Modified Theories of Relativistic Gravity: Theoretical Foundations, Phenomenology, and Applications in Physical Cosmology

by

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A thesis submitted to the School of Graduate Studies in partial fulfillment of the requirements for the degree of

Doctor of Philosophy

Department of Theoretical Physics (Interdisciplinary Program)
Faculty of Science

Date of graduation: October 2016

Memorial University of Newfoundland

March 2016

St. John's Newfoundland and Labrador

Abstract

This thesis studies the theories and phenomenology of modified gravity, along with their applications in cosmology, astrophysics, and effective dark energy. This thesis is organized as follows. Chapter 1 reviews the fundamentals of relativistic gravity and cosmology, and Chapter 2 provides the required Co-authorship Statement for Chapters 3 ∼ 6. Chapter 3 develops the $\mathscr{L} = f(R, R_c^2, R_m^2, \mathscr{L}_m)$ class of modified gravity that allows for nonminimal matter-curvature couplings ($R_c^2 := R_{\mu\nu}R^{\mu\nu}$, $R_m^2 := R_{\mu\alpha\nu\beta}R^{\mu\alpha\nu\beta}$), derives the "coherence condition" $f_{R^2} = f_{R_m^2} = -f_{R_c^2}/4$ for the smooth limit to $f(R, \mathcal{G}, \mathscr{L}_m)$ generalized Gauss-Bonnet gravity, and examines stress-energy-momentum conservation in more generic $f(R, \mathcal{R}_1, \ldots, \mathcal{R}_n, \mathscr{L}_m)$ gravity. Chapter 4 proposes a unified formulation to derive the Friedmann equations from (non)equilibrium thermodynamics for modified gravities $R_{\mu\nu} - Rg_{\mu\nu}/2 = 8\pi G_{\text{eff}} T_{\mu\nu}^{(\text{eff})}$, and applies this formulation to the Friedman-Robertson-Walker Universe governed by $f(R)$, generalized Brans-Dicke, scalar-tensor-chameleon, quadratic, $f(R, \mathcal{G})$ generalized Gauss-Bonnet and dynamical Chern-Simons gravities. Chapter 5 systematically restudies the thermodynamics of the Universe in ΛCDM and modified gravities by requiring its compatibility with the holographic-style gravitational equations, where possible solutions to the long-standing confusions regarding the temperature of the cosmological apparent horizon and the failure of the second law of thermodynamics are proposed. Chapter 6 proposes the Lovelock-Brans-Dicke theory of alternative gravity with $\mathscr{L}_{\text{LBD}} = \frac{1}{16\pi}\left[\phi\left(R + \frac{a}{\sqrt{-g}}{}^*RR + b\mathcal{G}\right) - \frac{\omega_{\text{L}}}{\phi}\nabla_\alpha\phi\nabla^\alpha\phi\right]$, where ${}^*RR$ and $\mathcal{G}$ respectively denote the topological Chern-Pontryagin and Gauss-Bonnet invariants; as a quick application, Chapter 7 looks into traversable wormholes and energy conditions in Lovelock-Brans-Dicke gravity, along with an extensive comparison to wormholes in Brans-Dicke gravity. Chapter 8, for a large class of scalar-tensor-like gravity $\mathcal{S} = \int d^4x\sqrt{-g}\left(\mathscr{L}_{\text{HE}} + \mathscr{L}_{\text{G}} + \mathscr{L}_{\text{NC}} + \mathscr{L}_\phi\right) + \mathcal{S}_m$ whose action contains nonminimal couplings between a scalar field $\phi(x^\alpha)$ and generic curvature invariants $\{\mathcal{R}\}$ beyond the Ricci scalar, proves the local energy-momentum conservation and introduces the "Weyl/conformal dark energy". Chapter 9 investigates the primordial nucleosynthesis in $\mathscr{L} = \varepsilon^{2-2\beta}R^\beta + 16\pi m_{Pl}^{-2}\mathscr{L}_m$ gravity from the the semianalytical approach for ^{4}He, and from the empirical approach for D, ^{4}He, and ^{7}Li; also, consistency with the gravitational baryogenesis is estimated. Within the same gravitational framework as in Chapter 9, Chapter 10 continues to study thermal relics as hot, warm, and cold dark matter, and revises the Lee-Weinberg bound for the mass of speculated heavy neutrinos.

Key Words cosmic acceleration, dark energy, modified gravity, physical cosmology, early Universe

Publications and Declaration

Here is the list of publications (including manuscripts under review) during my PhD studies, where the first item is the fruit of my MSc studies, and the others belong to my PhD projects.

[1] Ivan Booth, David Wenjie Tian. Some spacetimes containing nonrotating extremal isolated horizons. *Classical and Quantum Gravity* **30** (2013), 145008. [arXiv:1210.6889]

[2] David Wenjie Tian, Ivan Booth. Lessons from $f(R, R_c^2, R_m^2, \mathscr{L}_m)$ gravity: Smooth Gauss-Bonnet limit, energy-momentum conservation, and nonminimal coupling. *Physical Review D* **90** (2014), 024059. [arXiv:1404.7823]

[3] David Wenjie Tian, Ivan Booth. Friedmann equations from nonequilibrium thermodynamics of the Universe: A unified formulation for modified gravity. *Physical Review D* **90** (2014), 104042. [arXiv: 1409.4278]

[4] David Wenjie Tian, Ivan Booth. Apparent horizon and gravitational thermodynamics of the Universe: Solutions to the temperature and entropy confusions, and extensions to modified gravity. *Physical Review D* **92** (2015), 024001. [arXiv:1411.6547]

[5] David Wenjie Tian, Ivan Booth. Lovelock-Brans-Dicke gravity. *Classical and Quantum Gravity* **33** (2016), 045001. [arXiv:1502.05695]

[6] David Wenjie Tian. Local energy-momentum conservation in scalar-tensor-like gravity with generic curvature invariants. *General Relativity and Gravitation* **48** (2016): 110. [arXiv:1507.07448].

[7] David Wenjie Tian. Traversable wormholes and energy conditions in Lovelock-Brans-Dicke gravity. [arXiv:1508.02291].

[8] David Wenjie Tian. Big Bang nucleosynthesis in power-law $f(R)$ gravity: Corrected constraints from the semianalytical approach. [arXiv:1511.03258]

[9] David Wenjie Tian. Thermal relics as hot, warm and cold dark matter in power-law $f(R)$ gravity. [arXiv:1512.09117]

This thesis is written in the *manuscript style* following the university guidlines, and the papers [2]~[9] above have been adopted to produce Chapter 3 to Chapter 10, where [2]~[5] are coauthored with Dr. Ivan Booth. I hereby confirm that I am the main contributor to [2]~[5], and I have been granted the permission by Dr. Ivan Booth to use [2]~[5] in this thesis.

Acknowledgement

When looking back at my graduate studies, above all I am most grateful to Prof. Ivan Booth, who is the supervisor for both my MSc and PhD studies. I joined Dr. Booth's research group in September 2010, with a poor background in relativistic gravity and physical cosmology at that time. Dr. Booth patiently taught me general relativity (GR) and differential geometry, from the introductory to the advanced levels; when I was not good enough at GR, he patiently answered all my naive (sometimes even funny or stupid) questions during our weekly meetings, suggested helpful reading materials, and guided me to move ahead towards correct directions; he funded my MSc and PhD studies, so that I was able to focus on research and academics without worrying about milk and bread; every year he took me to GR conferences, so that I can give presentations, learn from other relativists, and make friends with them; when I run into trouble in my life, he always stood behind me and helped me. Pains and gains, I gradually grew up in GR after years of effort; Dr. Booth witnessed every step of my progress, and did his best to help me establish my physics career. Nearly six years have passed: how time flies! Nowadays I have become capable to do independent research, to design and accomplish projects on my own, while from last year on, I found Dr. Booth began to get gray hairs. In my heart, he is not just my supervisor, but also like an uncle to me.

Also, I would like to thank Prof. Hari Kunduri in our gravity group. Although he is not my supervisor, he helped a lot for the development of my physics career. Time and time again, he generously supported my scholarship applications and job applications. He is a very friendly person, and it is always very pleasant, peaceful and inspiring to discuss physics and talk with him.

In addition, I want to thank Prof. John K.C. Lewis (Physics Department of our university), Prof. Valerio Faraoni (Bishop's University), and Prof. Sanjeev Seahra (University of New Brunswick). They were very friendly to me, always encouraged me to bravely pursued my physics career, kindly had stimulating talks with me, and generously helped with my postdoctoral applications.

Last but not least, the works comprising this thesis were financially supported by the Natural Sciences and Engineering Research Council of Canada, under the grant 261429-2013 held by Prof. Ivan Booth. I was also funded by the scholarship from the School of Graduate Studies in our university.

Dedication

To all unsung heroes in Earth history ❀

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List of Symbols

G	Newton's gravitational constant
a	Cosmic scale factor
H	Hubble parameter
H_0	Hubble constant
z	Cosmological redshift
Λ	Cosmological constant or vacuum energy
w	Equation of state parameter
$\rho_{\rm cr}$	Critical energy density of the Universe
Ω_M	Fractional energy density of baryonic and dark matter
$\Omega_{\rm r}$	Fractional energy density of radiation
Ω_Λ	Fractional energy density of the cosmological constant
Ω_k	Fractional energy density due to spatial curvature
$\mathscr{L}$	Lagrangian density
$\mathscr{L}_M$	Lagrangian density of physical matter
$\mathcal{G}$	Gauss-Bonnet invariant
$^*RR$	Chern-Pontryagin density
$\mathcal{R}$	Generic curvature invariant beyond the Ricci scalar
$\cong$	Equality in variations by neglecting total-derivative terms
$\Box$	Covariant d'Alembertian
$T_{\mu\nu}^{\rm (MG)}$	Modified-gravity effects in stress-energy-momentum tensor
Υ	Astrophysical areal radius
$m_{\rm Pl}$	Planck mass
$\bar{m}_{\rm Pl}$	Reduced Planck mass
Q	Mass gap between neutrons and protons
g_*	Number of statistical degree of freedom for relativistic species
X_n	Fractional abundance of free neutrons
Y_p	Primordial mass fraction of ^{4}He
$y_{\rm D}$	Primordial abundance of deuteron
$y_{{\rm L}i}$	Primordial abundance of ^{7}Li
s	Entropy density of the Universe
$\sum m_\nu$	Summed mass for the three generations of neutrinos

Chapter 1

Introduction and overview: Physical cosmology and relativistic gravity

In this chapter, we will prepare for the whole thesis by reviewing the foundations of some necessary topics, including the standard model of cosmology within the gravitational framework of general relativity (GR), accelerated expansion of the Universe, dark energy, and modified theories of relativistic gravity beyond GR.

Throughout this chapter, for the spacetime geometry, we adopt the metric signature $(-,+++)$ along with the conventions $\Gamma^{\alpha}_{\beta\gamma} = \Gamma^{\alpha}{}_{\beta\gamma} = g^{\alpha\mu}\Gamma_{\mu\beta\gamma}$ for the Christoffel symbols (i.e. the first index being contravariant), $R^{\alpha}{}_{\beta\gamma\delta} = \partial_\gamma\Gamma^{\alpha}_{\delta\beta} - \partial_\delta\Gamma^{\alpha}_{\gamma\beta} + \Gamma^{\alpha}_{\gamma\lambda}\Gamma^{\lambda}_{\delta\beta} - \Gamma^{\alpha}_{\delta\lambda}\Gamma^{\lambda}_{\gamma\beta}$ for the Riemann curvature tensor, and $R_{\mu\nu} = R^{\alpha}{}_{\mu\alpha\nu}$ for the Ricci tensor. Moreover, for the physical quantities, we primarily use the natural unit system of high energy physics which sets $c = \hbar = k_B = 1$ and is related to le système international d'unités by 1 GeV $= 1.1604 \times 10^{13}$ kelvin $= 1.7827 \times 10^{-27}$ kg $= (1.9732 \times 10^{-16}$ meters$)^{-1} = (6.5820 \times 10^{-25}$ seconds$)^{-1}$.

1.1 Standard cosmology

"*My goal is simple. It is complete understanding of the universe: why it is as it is and why it exists at all.*"

Stephen Hawking

1.1.1 Einstein's equation

To look into modern cosmology, firstly let us quickly recall GR. Since gravity dominates at large scales, we need not concern ourselves with local complexity arising from the electromagnetic and nuclear interactions. GR, with the equivalence principle and the general principle of relativity as two cornerstones, is the first established and best accepted theory of relativistic gravity. From the perspective of the action principle, the field equation of GR can be derived by the stationary variation of the Hilbert-Einstein action

$$\mathcal{I}_{\text{HE}} = \int d^4x\,\sqrt{-g}\left(R + 16\pi G\mathscr{L}_m\right), \tag{1.1}$$

where G is Newton's constant, $\mathscr{L}_m$ denotes the matter Lagrangian density, and $16\pi G \int d^4x \sqrt{-g}\, \mathscr{L}_m =: \mathcal{I}_m$ constitutes the matter action. Extremizing $\mathcal{I}_{\rm HE}$ with respect to the inverse metric, i.e. $\delta\mathcal{I}_{\rm HE}/\delta g^{\mu\nu} = 0$ with the variational derivative given by

$$\frac{\delta\mathcal{I}_{\rm HE}}{\delta g^{\mu\nu}} := \sum(-1)^n \partial_{\alpha_1}\cdots\partial_{\alpha_n} \frac{\partial\mathcal{I}_{\rm HE}}{\partial\left(\partial_{\alpha_1}\cdots\partial_{\alpha_n} g^{\mu\nu}\right)} = \frac{\partial\mathcal{I}_{\rm HE}}{\partial g^{\mu\nu}} - \partial_\alpha \frac{\partial\mathcal{I}_{\rm HE}}{\partial(\partial_\alpha g^{\mu\nu})} + \partial_\alpha\partial_\beta \frac{\partial\mathcal{I}_{\rm HE}}{\partial(\partial_\alpha\partial_\beta g^{\mu\nu})}\,, \tag{1.2}$$

one obtains Einstein's equation [1]

$$R_{\mu\nu} - \frac{1}{2}R\, g_{\mu\nu} = 8\pi G T^{(m)}_{\mu\nu}\,, \tag{1.3}$$

where the stress-energy-momentum tensor $T^{(m)}_{\mu\nu}$ for the physical matter is defined via

$$\delta\mathcal{I}_m = -\frac{1}{2}\times 16\pi G \int d^4x \sqrt{-g}\, T^{(m)}_{\mu\nu}\delta g^{\mu\nu} \quad \text{with} \quad T^{(m)}_{\mu\nu} := \frac{-2}{\sqrt{-g}} \frac{\delta\left(\sqrt{-g}\,\mathscr{L}_m\right)}{\delta g^{\mu\nu}}\,. \tag{1.4}$$

Due to the minimal curvature-matter coupling in $\mathcal{I}_{\rm HE}$, $T^{(m)}_{\mu\nu}$ is covariant conserved (see Subsection 1.2.9 for more details),

$$\nabla^\mu T^{(m)}_{\mu\nu} = 0\,, \tag{1.5}$$

which is consistent with the contracted Bianchi identity $\nabla^\mu\left(R_{\mu\nu} - \frac{1}{2}R g_{\mu\nu}\right) = 0$ and supplements Einstein's equation.

Einstein's equation relates the geometry of the spacetime continuum with the physical energy-momentum distribution. Given $T^{(m)}_{\mu\nu}$, one can solve Einstein's equation for $g_{\mu\nu}$, such as the Schwarzschild solution for the vacuum exterior of a static spherically symmetric body, and the Kerr solution for the vacuum exterior of a stationary axially symmetric body. Inversely, one can "design" the spacetime metric with desired geometric properties, and then reconstruct the matter fields; for example, the Morris-Thorne metric for traversable Lorentzian wormholes was proposed this way, which requires $T^{(m)}_{\mu\nu}$ to violate the standard null energy condition within GR [2].

1.1.2 Friedmann and continuity equations

Modern observations strongly support the traditional cosmological principle: for example, the Sloan Digital Sky Survey found that the distribution of galaxies in the Universe appears homogeneous at scales $\gtrsim 100$ Mpc [3], while the Wilkinson Microwave Anisotropy Probe (WMAP) confirmed that the cosmic microwave background (CMB) radiation is highly isotropic in the full-sky temperature map [4]. Mathematically, the most general spacetime for a *spatially* homogeneous and isotropic universe is described by the Friedman-Robertson-Walker (FRW) metric. In the (t, r, θ, φ) comoving coordinates, its line element reads

$$g_{\mu\nu}dx^\mu dx^\nu = ds^2 = -dt^2 + \frac{a(t)^2}{1-kr^2}\,dr^2 + a(t)^2 r^2\left(d\theta^2 + \sin^2\theta\, d\varphi^2\right), \tag{1.6}$$

where the curvature index k is normalized to one of $\{+1\,, 0\,, -1\}$ which correspond to closed, flat and open universes, respectively. The metric function $a(t)$ refers to the cosmic scale factor, which is a function of the comoving time and needs to be determined by Einstein's equation.

At cosmological scale, the matter content of the Universe is usually portrayed by a perfect-fluid type stress-energy-momentum tensor, which in the metric-independent form reads

$$T^{\mu\,(m)}_{\ \nu} = \mathrm{diag}[\,-\rho_m, P_m, P_m, P_m\,]\,. \tag{1.7}$$

With this $T^{(m)}_{\mu\nu}$ and the FRW metric Eq.(1.6), the $t-t$ component of Einstein's equation leads to the first Friedmann equation

$$H^2 + \frac{k}{a^2} = \frac{8\pi G}{3}\rho_m\,, \tag{1.8}$$

while the spatial components yield the second Friedmann equation

$$\dot{H} - \frac{k}{a^2} = -4\pi G\,(\rho_m + P_m) \quad \text{or} \quad 2\dot{H} + 3H^2 + \frac{k}{a^2} = -8\pi G P_m\,, \tag{1.9}$$

where H refers to the Hubble parameter

$$H := \frac{\dot{a}}{a} = \frac{d\ln a}{dt}\,, \tag{1.10}$$

with $\ddot{a}/a = \dot{H}+H^2$ and the overdot denoting the derivative with respect to the comoving time t. Practically, H describes the fractional change of the distance between any pair of galaxies per unit time, and thus measures the expansion rate of the Universe.

Eqs.(1.8) and (1.9) jointly govern the the evolution of the generic FRW Unverse. The first and second Friedmann equations are just first and second order differential equations for the scale factor $a(t)$, respectively, as $a(t)$ is the only FRW metric function to be specified. Moreover, Eq.(1.5) for local energy-momentum conservation[1] gives rise to the continuity equation

$$\dot{\rho}_m + 3H(\rho_m + P_m) = 0\,. \tag{1.11}$$

It is actually consistent with the adiabatic cosmic expansion: for the energy $U = \rho_m V$ in the comoving volume $V = a^3$, the first law of thermodynamics $dU = TdS - P_m dV$ with $dQ = TdS = 0$ yields $[d(\rho_m a^3) + P_m da^3]/dt = 0$, which still expands into Eq.(1.11).

1.1.3 Multiple components in the Universe

The physical content of the observable Universe is quite diverse. Primarily, she contains nonrelativistic baryonic matter of the $\mathrm{SU}(3)_c\times\mathrm{SU}(2)_W\times\mathrm{U}(1)_Y$ minimal standard model, cold/nonrelativistic dark matter beyond the minimal standard model, photons like the cosmic microwave background (CMB), and neutrinos like the cosmic neutrino background. Accordingly, it is often useful to decompose the total energy density ρ_m and pressure P_m into different components, say $\rho_m = \sum \rho_m^{(i)} = \rho_b(\text{baryon}) + \rho_{\text{dm}}(\text{dark matter}) + \rho_\gamma(\text{photon}) +$

[1] As usual, we regard $\nabla^\mu T^{(m)}_{\mu\nu} = 0$ or $\partial^\mu\left(\sqrt{-g}\,T^{(m)}_{\mu\nu}\right) = 0$ as local conservation, and $\partial^\mu\left[\sqrt{-g}\,\left(T^{(m)}_{\mu\nu} + t_{\mu\nu}\right)\right] = 0$ as the speculated global conservation, where $t_{\mu\nu}$ denotes an energy-momentum pseudotensor for the gravitational field.

ρ_ν(neutrino) $+ \cdots$, and the same for $P_m = \sum P_m^{(i)}$.

Given a type of physical matter, its pressure $P_m^{(i)}$ is related to its energy density $\rho_m^{(i)}$ by some generic function $P_m^{(i)} = P_m^{(i)}\left(\rho_m^{(i)}\right)$ as the equation of state (EoS); usually, a simplest linear relation $P_m^{(i)} = w_m^{(i)} \cdot \rho_m^{(i)}$ is assumed, where the proportionality coefficient $w_m^{(i)}$ refers to the EoS parameter associated to each energy component. This way, the second Friedmann equation (1.9) can be rewritten into $\dot{H} - \frac{k}{a^2} = -4\pi G\,(1 + w_m)\,\rho_m$, where $w_m \coloneqq P_m/\rho_m$, and practically w_m can be regarded either as that of the absolutely dominant matter, or the weighted average for all relatively dominant components

$$w_m = \frac{\sum P_m^{(i)}}{\rho_m} = \frac{\sum w_m^{(i)} \rho_m^{(i)}}{\rho_m} = \sum \alpha_i\, w_m^{(i)}\,, \tag{1.12}$$

with the weight coefficient given by $\alpha_i = \rho_m^{(i)}/\rho_m$.

One should note that physically meaningful w_m cannot take an arbitrary value; instead, w_m for classical matter fields is constrained by the null, weak, strong, and dominant energy conditions, which are a cornerstone in many areas of GR, such as the classical black hole thermodynamics [5, 6]. As shown in Table 1.1, these energy conditions collectively require $-1/3 \le w_m \le 1$ or less stringently $-1 \le w_m \le 1$, along with the positivity of the energy density; only a small handful exceptions involving quantum effects are found to violate these energy conditions, such as the quantum Casimir effect and the semiclassical Hawking radiation.

Table 1.1: Standard energy conditions in GR for classical matter fields, which revise the Table 2.1 in Ref.[6], with ℓ^α being an arbitrary null vector, and v^α an arbitrary timelike vector.

energy condition	tensorial statement	perfect-fluid statement
null	$T^{(m)}_{\alpha\beta}\ell^\alpha\ell^\beta \ge 0$	$\rho_m\,(w_m + 1) \ge 0$
weak	$T^{(m)}_{\alpha\beta}v^\alpha v^\beta \ge 0$	$\rho_m \ge 0,\ \ w_m \ge -1$
strong	$\left(T^{(m)}_{\alpha\beta} - \frac{1}{2}T^{(m)}g_{\alpha\beta}\right)v^\alpha v^\beta \ge 0$	$\rho_m\left(w_m + \frac{1}{3}\right) \ge 0,\ \ \rho_m\,(w_m + 1) \ge 0$
dominant	$-T^{\alpha(m)}_{\ \ \beta}v^\beta$ future directed	$\rho_m \ge 0,\ \ -1 \le w_m \le 1$

Following Table 1.1, let us illustrate the EoS parameters for some typical matter fields.

- $w_m \simeq 1/3$ for radiation or relativistic matter, nowadays including photons, the three generations of massless or light neutrinos, and possibly other particles in the hot early Universe (see Chapters 9 and 10). This is because radiation has no intrinsic scale; as such, its stress-energy-momentum tensor must be conformally invariant with a vanishing trace, i.e. $g^{\mu\nu}T^{(m)}_{\mu\nu} = -\rho_{\rm rad} + 3P_{\rm rad} = 0$, which implies $w_m = 1/3$ for radiation.

- $w_m \simeq 0$ for nonrelativistic matter, which is dubbed as pressureless "dust" in cosmological literature.

- $w_m = -1$ for vacuum energy. As a supplement to Eq.(1.7), the complete expression of $T^{(m)}_{\mu\nu}$ for perfect fluid reads

$$T^{(m)}_{\mu\nu} = (\rho_m + P_m)\,u_\mu u_\nu + P_m\,g_{\mu\nu}\,, \tag{1.13}$$

where u_μ is the comoving four-velocity along the cosmic Hubble flow. For pure vacuum energy, $T^{(m)}_{\mu\nu}$ should be Lorentzian invariant and observer-independent, which requires $\rho_m + P_m \equiv 0$ in Eq.(1.13), and consequently $w_m = -1$.

- $w_m \simeq 1$ for stiff matter. A typical example is the canonical and homogeneous scalar field $\phi(t)$ in the FRW Universe, which is given by the Lagrangian density $\mathscr{L}_\phi = -\frac{1}{2}\nabla_\alpha\phi\nabla^\alpha\phi - V(\phi)$ and has the EoS parameter

$$w_\phi = \frac{P_\phi}{\rho_\phi} = \frac{\frac{1}{2}\dot{\phi}^2 - V}{\frac{1}{2}\dot{\phi}^2 + V}. \tag{1.14}$$

w_ϕ can fall into the domain $1/3 \lesssim w_\phi \leq 1$ when the scalar field is so fast-rolling that the kinetic-energy term $\frac{1}{2}\dot{\phi}^2$ dominates over the potential V. Specifically, one has $w_\phi \simeq 1^-$ when $\frac{1}{2}\dot{\phi}^2 \gg V$ or $V = 0$.

Once w_m is known, the spatially decaying rate of ρ_m with respect to the scale factor can be immediately determined, as the continuity equation (1.11) or equivalently "$d\ln\rho_m = -3(1+w_m)d\ln a$" integrates to yield

$$\rho_m = \rho_{m0}\left(\frac{a}{a_0}\right)^{-3(1+w_m)} \propto a^{-3(1+w_m)}. \tag{1.15}$$

Here the integration constants $\{\rho_{m0}, a_0\}$ respectively specify the present-day matter density and scale factor of the Universe. Hence, for the examples of matter fields listed above, we have

$$\rho_m \propto a^{-4}\ (\text{radiation}), \quad \rho_m \propto a^{-3}\ (\text{dust}), \quad \rho_m \propto a^{-6}\ (\text{stiff}), \quad \text{and} \quad \rho_m = \text{contant (vacuum)}. \tag{1.16}$$

Considering its sharp decreasing rate, ρ_m of stiff matter could only, if ever, play important roles in the early Universe. On the other hand, since ρ_m for vacuum energy remains constant despite the cosmic expansion, it will eventually become the dominant component in an always expanding Universe – provided that ρ_m of vacuum is nonzero. In addition, when w_m is time-dependent, Eq.(1.11) along with $w_m = w_m(t) = w_m(a)$ implies

$$\rho_m = \rho_{m0}\exp\left\{-3\int_{a_0}^{a}\left[1 + w_m(\hat{a})\right]\frac{d\hat{a}}{\hat{a}}\right\}, \tag{1.17}$$

or equivalently

$$\rho_m = \rho_{m0}\left(\frac{a}{a_0}\right)^{-3\left[1+\tilde{w}_m(a)\right]} \quad \text{with} \quad \tilde{w}_m(a) = \frac{1}{\ln(a/a_0)}\int_{a_0}^{a} w_m(\hat{a})\frac{d\hat{a}}{\hat{a}}. \tag{1.18}$$

1.1.4 Acceleration of the late-time Universe and dark energy

"*Observations always involve theory.*"
Edwin Powell Hubble

In terms of the scale factor itself rather than the Hubble parameter, the second Friedmann equation (1.9) can be rewritten into the acceleration equation

$$\frac{\ddot{a}}{a} = -\frac{4\pi G}{3}(\rho_m + 3P_m) = -\frac{4\pi G}{3}\sum\left(1 + 3w_m^{(i)}\right)\rho_m^{(i)}. \tag{1.19}$$

Hence, the Universe would be undergoing decelerated spatial expansion if it were dominated by ordinary matter with $-1/3 < w_m \leq 1$, as was commonly believed two decades ago. There is a minus sign inside the so-called "deceleration parameter" $q := -a\ddot{a}/\dot{a}^2$, which was introduced for the traditional belief of cosmic deceleration.

However, this old thought of cosmic expansion was revolutionized in the year 1998, when the Supernova Search Team Collaboration (Adam G. Riess *et al.*) [7] and the Supernova Cosmology Project Collaboration (S. Perlmutter *et al.*) [8] reported their measurements on high-redshift type-Ia supernovae that their peak luminosities appear dimmer than expected; among the different explanations like changes in the chemical composition of the progenitor stars, failure of type-Ia supernovae as standard candles, and absorptions by intergalactic dust, the most natural possibility is that lights from these supernovae have traveled greater distances than previously predicted, which implies the Universe undergoing *accelerated* spatial expansion! Shortly afterwards, speed-up of the Universe was solidified by other sources of observational data like the CMB anisotropy [4], Hubble constant [9], and galaxy (super)clusters [10, 11]. There is no doubt that the cosmic acceleration was of greatest importance and had far-reaching implications in contemporary physics.

According to Eq.(1.19), the spatial acceleration $\ddot{a} > 0$ happens for the FRW Universe when $\rho_m + 3P_m < 0$ (assuming the positivity of the energy density $\rho_m > 0$); that is to say, the cosmic perfect-fluid must be dominated by some exotic component with large negative pressure that satisfies $w_m^{(i)} < -1/3$ and thus violates the standard energy conditions. This component has been dubbed as *dark energy*.

One might think dark energy to be a bit counter-intuitive, whose large negative pressure produces repulsive gravitational effect to accelerate the Universe. Contrarily, in our daily experience, it feels that positive pressure is repulsive and would push particles away from each other, while negative pressure (i.e. tension) is attractive and would pull particles together. How to reconcile this conflict? The answer is simple: such "daily experience" is unreliable. In fact, it is the *gradient* of the positive pressure that pushes particles away, and the gradient of negative pressure/tension that pulls particles together; for example, air in the atmosphere can flow towards lower-pressure regions, while the gas inside a tank has no macroscopic kinetics as there is no lower-pressure region to expand into. However, the cosmic perfect fluid is homogeneous and isotropic, and the pressure $P_m = \sum P_m^{(i)}$ has no spatial gradient; instead, similar to the role of ρ_m, P_m also serves as a source of gravity that affects the expansion $\dot{a}$ and acceleration $\ddot{a}$ of the Universe, as shown by the Friedmann equations (1.8), (1.9) and (1.19).

1.1.5 Cosmological constant and ΛCDM cosmology

The cosmological constant, which is conventionally denoted by Λ, was originally introduced as a geometric term that slightly extends Einstein's equation (1.3) into the Einstein-Λ equation

$$R_{\mu\nu} - \frac{1}{2}R\, g_{\mu\nu} + \Lambda\, g_{\mu\nu} \;=\; 8\pi G T_{\mu\nu}^{(m)}\,. \tag{1.20}$$

It still satisfies the covariant invariance $\nabla^\mu \left(R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} + \Lambda g_{\mu\nu}\right) \equiv 0$ for consistency with the local conservation $\nabla^\mu T_{\mu\nu}^{(m)} = 0$, and from a variational approach, it arises from the Hilbert-Einstein-Λ action

$$\mathcal{I}_{\text{HE}\Lambda} \;=\; \int d^4x\,\sqrt{-g}\,\Big(R - 2\Lambda + 16\pi G \mathscr{L}_m\Big). \tag{1.21}$$

Historically, Einstein firstly employed Λ in an attempt to maintain a static universe [12], and abandoned it after Edwin Hubble's discovery of extragalactic recession and cosmic expansion.

However, relativists never really forgot Λ. After the establishment of cosmic acceleration, the cosmological constant immediately became the simplest model of dark energy, as Λ measures the ground-state energy density of the vacuum and has the EoS parameter $w_\Lambda = -1$. Note that nowadays Λ is generally treated as an energy component supplementing $T^{(m)}_{\mu\nu}$ rather than a geometric term supplementing the Einstein tensor $G_{\mu\nu} := R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu}$, and the terms "cosmological constant" and "vacuum energy" are used interchangeably in cosmology. In this sense, Eq.(1.20) can be rearranged into

$$R_{\mu\nu} - \frac{1}{2}R\,g_{\mu\nu} \;=\; 8\pi G\left(T^{(m)}_{\mu\nu} - \frac{\Lambda}{8\pi G}g_{\mu\nu}\right), \tag{1.22}$$

and thus the energy density and pressure of the vacuum are given by

$$\rho_\Lambda = -P_\Lambda = \frac{\Lambda}{8\pi G}\,. \tag{1.23}$$

In Eq.(1.22), $T^{(m)}_{\mu\nu}$ still collects the cosmic Hubble flow of ordinary and dark matters that are diluted along spatial expansion, while Λ plays the role of an unlimited vacuum energy reservoir; this way, Λ deserves to be highlighted as an individual term that is unabsorbed by $T^{(m)}_{\mu\nu}$.

Substituting the FRW metric into the Einstein-Λ equation (1.20) or (1.22), one obtains the expansion equation with multiple energy components,

$$H^2 = \frac{8\pi G}{3}\left(\rho_M + \rho_{\rm r}\right) + \frac{\Lambda}{3} - \frac{k}{a^2}\,, \tag{1.24}$$

where $\rho_M = \rho_b$(baryon)+$\rho_{\rm cdm}$(cold dark matter) for nonrelativistic matter, and $\rho_{\rm r} = \rho_{\rm r}$(radiation) $= \rho_\gamma$(photon) $+\rho_\nu$(neutrino). Recall that $\rho_m \propto a^{-3}$, $\rho_{\rm r} \propto a^{-4}$ and ρ_Λ = constant, so Eq.(1.24) can be converted into

$$H^2 = \frac{8\pi G}{3}\left[\rho_{M0}\left(\frac{a_0}{a}\right)^3 + \rho_{\rm r0}\left(\frac{a_0}{a}\right)^4\right] + \frac{\Lambda}{3} - \frac{k}{a_0^2}\left(\frac{a_0}{a}\right)^2\,, \tag{1.25}$$

where the "0" in the subscript means "the present-day value". Define the the fractional densities as

$$\Omega_{M0} = \frac{\rho_{M0}}{\rho_{\rm cr0}}\,,\quad \Omega_{\rm r0} = \frac{\rho_{\rm r0}}{\rho_{\rm cr0}}\,,\quad \Omega_{\Lambda0} = \frac{\rho_\Lambda}{\rho_{\rm cr0}} = \frac{\Lambda}{3H_0^2}\,,\quad \Omega_{k0} = -\frac{k}{a_0^2H_0^2}\,, \tag{1.26}$$

where $\rho_{\rm cr0}$ denotes the critical density of the current Universe,

$$\rho_{\rm cr0} := \frac{3H_0^2}{8\pi G}\,, \tag{1.27}$$

and Eq.(1.25) becomes

$$H^2 = H_0^2\left[\Omega_{M0}\left(\frac{a_0}{a}\right)^3 + \Omega_{r0}\left(\frac{a_0}{a}\right)^4 + \Omega_{\Lambda 0} + \Omega_{k0}\left(\frac{a_0}{a}\right)^2\right]. \tag{1.28}$$

Moreover, if we introduce the cosmological redshift parameter

$$\frac{a_0}{a} = 1 + z\,, \tag{1.29}$$

which reduces to $\frac{1}{a} = 1+z$ in the popular convention $a_0 = 1$, then Eq.(1.28) further leads to the parameterized Friedmann equation

$$H = H(z; H_0, \boldsymbol{p}) = H_0\sqrt{\Omega_{M0}(1+z)^3 + \Omega_{r0}(1+z)^4 + \Omega_{\Lambda 0} + \Omega_{k0}(1+z)^2}\,, \tag{1.30}$$

where $\boldsymbol{p} = (\Omega_{M0}, \Omega_{r0}, \Omega_{\Lambda 0})$ for the ΛCDM cosmology[2] under discussion. In fact, the phase-space vector $\boldsymbol{p}$ varies for different dark-energy or cosmological models, and typically, the phase space $\{\boldsymbol{p}\}$ is explored by the Markov-Chain Monte-Carlo engine CosmoMC [13].

Since $\Omega_{M0} + \Omega_{r0} + \Omega_{\Lambda 0} + \Omega_{k0} = 1$ in accordance with Eq.(1.28), one learns that $k = 0$ and the universe would be spatially flat if $\Omega_{M0} + \Omega_{r0} + \Omega_{\Lambda 0} = 1$; $k = -1$ and the universe would be spatially open if $\Omega_{M0} + \Omega_{r0} + \Omega_{\Lambda 0} < 1$; $k = +1$ and the universe would be spatially closed if $\Omega_{M0} + \Omega_{r0} + \Omega_{\Lambda 0} > 1$. This agrees with the intuitive expectation that over-dense physical energy wraps and closes the space.

On the other hand, following Eqs.(1.23), (1.26), (1.27) and (1.29), the Friedmann acceleration equation (1.19) can be parameterized into

$$\begin{aligned}\frac{\ddot{a}}{a} &= -\frac{4\pi G}{3}\sum\left(1 + 3w_m^{(i)}\right)\rho_m^{(i)} + \frac{\Lambda}{3}\\ &= -H_0^2\left[\frac{1}{2}\Omega_{M0}(1+z)^3 + \Omega_{r0}(1+z)^4 - \Omega_{\Lambda 0}\right],\end{aligned} \tag{1.31}$$

which does not contain an Ω_{k0} term as Eq.(1.19) for $\ddot{a}/a$ is independent of the spatial curvature. In cosmology and astrophysics, there are two principal types of constraints for the viability of Λ and more complicated dark-energy models (see Subsection 1.1.8 below): one is related to the cosmic structure growth, while the other is relevant with the expansion history of the Universe, for which Eq.(1.30) and its modified forms play a fundamental role. Eq.(1.31) is however not so important as Eq.(1.30) in testing dark energies, and is mainly used to check the deceleration-acceleration phase transition. In fact, instead of Eq.(1.31), it proves more convenient to use the dimensionless deceleration parameter $q := -a\ddot{a}/(\dot{a})^2 = -\ddot{a}/(aH^2)$; with H^2 parameterized by Eq.(1.30), it follows that q is related to the componential energy densities by

$$q = -\frac{\ddot{a}}{aH^2} = \frac{\frac{1}{2}\Omega_{M0}(1+z)^3 + \Omega_{r0}(1+z)^4 - \Omega_{\Lambda 0}}{\Omega_{M0}(1+z)^3 + \Omega_{r0}(1+z)^4 + \Omega_{\Lambda 0} + \Omega_{k0}(1+z)^2}\,. \tag{1.32}$$

[2]The full meaning of ΛCDM is the inflationary and Big Bang cosmology with the present-day Universe dominated by the cosmological constant and cold dark matter, while cosmic inflation will be partially discussed in Subsection 1.1.9.

1.1.6 Observational data

For the cosmic fluid, how is the total energy allocated to its multiple components? Also, how quickly does the Universe expand? To answer these questions, in Table 1.2 we collect nine global FRW parameters from the second Planck data release [14], where $\{\Omega_{b0}h^2, \Omega_{\text{cdm}0}h^2\}$ are *best-fit* values in the flat ΛCDM model, $\{h, \Omega_{\Lambda 0}, \Omega_{M0}, z_{\text{eq}}, t_0\}$ are *derived* values in flat ΛCDM, and $\{\Omega_k, w_m\}$ are *derived* values in nonflat extended ΛCDM. Here h denotes the normalized value of the Hubble constant H_0 in the unit of 100 km/s/Mpc, which is dimensionless and more convenient to use in numerical calculations.

Table 1.2: Nine global FRW parameters based on the 2015 Planck data in Ref.[14] , where $\{\Omega_{b0}h^2, \Omega_{\text{cdm}0}h^2, h, \Omega_{\Lambda 0}, \Omega_{M0}, t_0, z_{\text{eq}}\}$ come from the "TT,TE,EE+lowP+lensing+ext" column of its Table 4, and $\{\Omega_k, w_m\}$ from the "TT, TE, EE+lensing+ext" column of its Table 5.

symbol	meaning	value
$\Omega_{b0}h^2$	h^2-coupled fractional density of baryons	0.02230 ± 0.00014
$\Omega_{\text{cdm}0}h^2$	h^2-coupled fractional density of cold dark matter	0.1188 ± 0.0010
h	normalized Hubble constant, $H_0 = 100h$ km/s/Mpc	0.6774 ± 0.0046
$\Omega_{\Lambda 0}$	fractional density of Λ	0.6911 ± 0.0062
Ω_{M0}	fractional density of nonrelativistic matter	0.3089 ± 0.0062
z_{eq}	redshift of matter-radiation equality	3371 ± 23
t_0	age of the observable Universe	13.799 ± 0.021 Gyr
Ω_{k0}	fractional density of spatial curvature	$0.0008^{+0.0040}_{-0.0039}$
w_m	EoS parameter of dark energy	$-1.019^{+0.075}_{-0.080}$

An immediate implication of Table 1.2 is that the Universe is nearly flat: the base ΛCDM model with a flatness assumption matches well with the observed expansion history (and structure growth), and the nonflat extended ΛCDM turns out to carry a tiny fractional density $\Omega_{k0} = 0.0008^{+0.0040}_{-0.0039}$ for the spatial curvature. Besides Table 1.2, the WMAP nine-years data and other sources like the Baryon Acoustic Oscillations (BAO) yield $\Omega_{k0} = -0.0027^{+0.0039}_{-0.0038}$ [15], independently the time-delay measurements of two strong gravitational lensing systems along with the seven-years WMAP data find $\Omega_{k0} = 0.003^{+0.005}_{-0.006}$ [16], while recent analyses based on BAO data give $\Omega_{k0} = -0.003 \pm 0.003$ [17]. Recall that in Subsection 1.1.2 we started from the generic FRW metric Eq.(1.6) which allows for a nontrivial spatial curvature; this was mainly for theoretical generality, and also because the Universe may not be *absolutely* flat.

With $z_{\text{eq}} = 3371 \pm 23$ measured for the redshift of matter-radiation equality in the early Universe, we can find out the present-day fractional density $\Omega_{\text{r}0}$ for relativistic matter. The matter-radiation equality $\rho_M(t) = \rho_{\text{r}}(t)$ yields

$$\rho_{M0}\left(\frac{a_0}{a_{\text{eq}}}\right)^3 = \rho_{\text{r}0}\left(\frac{a_0}{a_{\text{eq}}}\right)^4 \quad \Rightarrow \quad \frac{\rho_{M0}}{\rho_{\text{r}0}} = \frac{\Omega_{M0}}{\Omega_{\text{r}0}} = \frac{a_0}{a_{\text{eq}}} = 1 + z_{\text{eq}}\,, \tag{1.33}$$

and it follows that

$$\Omega_{\text{r}0} = \frac{\Omega_{M0}}{1 + z_{\text{eq}}} = 9.1607 \times 10^{-5}\,. \tag{1.34}$$

Hence, it is generally an acceptable approximation to neglect Ω_{k0} and Ω_{r0} in the parameterized Friedmann equations (1.30) and (1.31).

With $\Omega_{k0} \simeq 0 \simeq \Omega_{r0}$ and $\Omega_{M0} + \Omega_{\Lambda 0} \simeq 1$ in Eq.(1.32), Table 1.2 gives rise to the present-day ($z = 0$) deceleration parameter

$$q_0 \simeq \frac{1}{2}\Omega_{M0} - \Omega_{\Lambda 0} = -0.5367\,, \tag{1.35}$$

which, as expected, corresponds to an accelerated phase. Moreover, numerically the present-day critical density is [18]

$$\rho_{\mathrm{cr}0} \coloneqq \frac{3H_0^2}{8\pi G} = 1.8785 h^2 \times 10^{-29}\ \mathrm{g/cm^3} = 1.0538 h^2 \times 10^{-5}\ \mathrm{GeV/cm^3}\,, \tag{1.36}$$

and with $h = 0.6774$, one obtains

$$\rho_{\mathrm{cr}0} = 0.8620 \times 10^{-29}\ \mathrm{g/cm^3} = 0.4835 \times 10^{-5}\ \mathrm{GeV/cm^3}\,, \tag{1.37}$$

from which the current vacuum energy density $\rho_\Lambda = \Omega_{\Lambda 0}\rho_{\mathrm{cr}0}$ and dust density $\rho_{M0} = \Omega_{M0}\rho_{\mathrm{cr}0}$ can be immediately determined. In addition, one might have noticed that the quantities $\{\Omega_{b0}h^2\,,\Omega_{\mathrm{cdm}0}h^2\,,h\}$ in Table 1.2 imply

$$\begin{aligned} \Omega_{b0} &= (0.02230 \pm 0.00014)\,h^{-2} = 0.04904 \pm 0.00111 \\ \Omega_{\mathrm{cdm}0} &= (0.1188 \pm 0.0010)\,h^{-2} = 0.2642 \pm 0.0072\,, \end{aligned} \tag{1.38}$$

and the recovered value $\Omega_{b0} + \Omega_{\mathrm{cdm}0} = (0.14110 \pm 0.00114)h^{-2} = 0.31324 \pm 0.00831$ slightly differs from $\Omega_{M0} = 0.3089 \pm 0.0062$. This is because $\{\Omega_{b0}h^2\,,\Omega_{\mathrm{cdm}0}h^2\}$ come directly from the best fitting (i.e. the maximal-likelihood fitting) of the observational data, while the value $\Omega_{M0} = 0.3089 \pm 0.0062$ is a simple subtraction $\Omega_{M0} = 1 - \Omega_{\Lambda 0}$ after $\Omega_{\Lambda 0} = 0.6911 \pm 0.0062$ being derived, and the latter approach carries extra systematic errors for neglecting $\{\Omega_{k0}\,,\Omega_{r0}\}$.

1.1.7 Some implications of ΛCDM

Having introduced the ΛCDM model, the parameterized Friedmann equations, and the observational data, we will proceed to investigate some interesting implications.

(1) *Dimming of type Ia supernovae*. In Subsection 1.1.4, we emphasized that detections of high-z type Ia supernovae shed first light on the cosmic acceleration. In fact, the difference between the apparent m_L and absolute M_L magnitudes of luminosity (i.e. the distance modulus $\mu_L \coloneqq m_L - M_L$) for this type of standard candle is positively related to the luminosity distance d_L by [19]

$$m_L - M_L = 5\log_{10}\left(\frac{d_L}{\mathrm{Mpc}}\right) + 25\,, \tag{1.39}$$

and with $\Omega_{k0} \simeq 0 \simeq \Omega_{r0}$ in Eq.(1.30), d_L is given by [20]

$$d_L = \frac{1+z}{H_0} \int_0^z \frac{d\hat{z}}{\sqrt{\Omega_{M0}(1+\hat{z})^3 + \Omega_{\Lambda 0}}}\,, \tag{1.40}$$

which integrates to yield

$$d_L = \begin{cases} \dfrac{2}{H_0}\Big(1+z-\sqrt{1+z}\Big) & \text{if} \quad \Omega_{M0}=1\,, \Omega_{\rm de0}=0\,, \\ \dfrac{1}{H_0} z(1+z) & \text{if} \quad \Omega_{M0}=0\,, \Omega_{\rm de0}=1\,. \end{cases} \tag{1.41}$$

Since $z(1+z) > 2\Big(1+z-\sqrt{1+z}\Big)$ for $z > 0$[3], thus a supernova would have a longer luminosity distance and appear dimmer/reddened in a Λ-dominated universe.

(2) *The cosmological constant problem.* In Subsection 1.1.5 we mentioned that the terms "cosmological constant" and "vacuum energy" can be used interchangeably in cosmology. However, from the perspective of quantum field theory or high energy physics, "vacuum energy" becomes a more serious terminology. Adding up all vacuum modes below the ultraviolet cutoff at the Planck scale, one obtains the quantum vacuum energy density (i.e. zero-point energy density) $\rho_\Lambda^{\rm QFT} \sim m_{\rm Pl}^4/(16\pi^2) = 3.7873 \times 10^{73}\,{\rm GeV}^{-4}$ where $m_{\rm Pl} := 1/\sqrt{G} = 1.2209 \times 10^{19}$ GeV denotes the Planck mass [21], while in light of Eq.(1.37), the cosmological ρ_Λ has the observed density

$$\rho_\Lambda = \Omega_{\Lambda 0}\rho_{\rm cr0} = 0.4835 \times 10^{-5}\ {\rm GeV/cm}^3 = 3.7151 \times 10^{-47}\ {\rm GeV}^4\,. \tag{1.42}$$

Thus, $\rho_\Lambda^{\rm QFT}/\rho_\Lambda = 1.0194 \times 10^{120}$, with a huge energy discrepancy of 120 orders of magnitude, and this discrepancy is often called the cosmological constant problem or the vacuum catastrophe.

(3) *Deceleration-acceleration transition before Λ-dominance.* With the approximations $\Omega_{k0} \simeq 0 \simeq \Omega_{r0}$, Eq.(1.32) becomes

$$q(z) \simeq \frac{\frac{1}{2}\Omega_{M0}(1+z)^3 - \Omega_{\Lambda 0}}{\Omega_{M0}(1+z)^3 + \Omega_{\Lambda 0}}\,. \tag{1.43}$$

Thus, the Universe transits from the decelerated state to the accelerated state at

$$z_1 \simeq \left(\frac{2\Omega_{\Lambda 0}}{\Omega_{M0}}\right)^{1/3} - 1 = 0.6478\,, \tag{1.44}$$

and at z_1, the fractional densities for nonrelativistic matter and Λ are respectively

$$\Omega_M = \Omega_{M0}(1+z_1)^3 = 0.6667\,, \quad \Omega_\Lambda = 1 - \Omega_M = 0.3333\,. \tag{1.45}$$

[3] According to the definition $a_0/a := 1+z$, one has $-1 < z < \infty$, where $z \to \infty$ traces back to the initial Big Bang with $a \to 0$, and $z \to -1$ corresponds to the distant future of eternal expansion with $a \gg a_0$. In astronomical observations, the domain of interest is $z > 0$, which means "looking into the past".

In addition, Ω_Λ begins to dominate over Ω_M at the time

$$\Omega_{M0}(1+z_2)^3 \simeq \Omega_{\Lambda 0} \quad \Rightarrow \quad z_2 \simeq \left(\frac{\Omega_{\Lambda 0}}{\Omega_{M0}}\right)^{1/3} - 1 = 0.3080\,. \tag{1.46}$$

Comparing z_1 with z_2, one can see that the Universe enters the accelerating phase considerably earlier than the cosmological constant becomes the dominant component.

1.1.8 *w*CDM and more complicated examples of dark energy

As reflected by Table 1.2, it is really shocking that ordinary matter only comprises $4\% \sim 5\%$ of the total energy of the Universe, and enormous efforts have been spent to understand dark matter and dark energy. As an alternative to the cosmological constant, quite a few theories of dark energy have been developed [22]. The simplest extension of ΛCDM is to consider dark energy with a constant EoS parameter $w_{\text{de}} < -1/3$; this way, ρ_{de} evolves by $\rho_{\text{de}} \propto a^{-3(1+w_{\text{de}})}$, and thus the parameterized Friedmann equations (1.30) and (1.32) are generalized into

$$H = H_0\sqrt{\Omega_{M0}(1+z)^3 + \Omega_{r0}(1+z)^4 + \Omega_{\text{de}0}(1+z)^{3(1+w_{\text{de}})} + \Omega_{k0}(1+z)^2}\,, \tag{1.47}$$

$$\text{and} \quad \frac{\ddot{a}}{a} = -H_0^2\left[\frac{1}{2}\Omega_{M0}(1+z)^3 + \Omega_{r0}(1+z)^4 - \Omega_{\text{de}0}(1+z)^{3(1+w_{\text{de}})}\right]. \tag{1.48}$$

This situation is usually called the *w*CDM model of the Universe, which recovers ΛCDM for $w_{\text{de}} = w_\Lambda = -1$, and to date, ΛCDM and *w*CDM are two best tested models in astrophysics and cosmology.

More generally, dark energy may have a time-dependent EoS parameter $w_{\text{de}} = w_{\text{de}}(z) < -1/3$, and the evolution of ρ_{de} respects Eq.(1.17). This way, the parameterized *w*CDM Friedmann equations (1.47) and (1.48) are further extended into

$$H = H_0\sqrt{\Omega_{M0}(1+z)^3 + \Omega_{r0}(1+z)^4 + \Omega_{\text{de}0}\exp\left\{3\int_0^z \frac{1+w_{\text{de}}(\hat{z})}{1+\hat{z}}d\hat{z}\right\} + \Omega_{k0}(1+z)^2}\,, \tag{1.49}$$

$$\text{and} \quad \frac{\ddot{a}}{a} = -H_0^2\left[\frac{1}{2}\Omega_{M0}(1+z)^3 + \Omega_{r0}(1+z)^4 - \Omega_{\text{de}0}\exp\left\{3\int_0^z \frac{1+w_{\text{de}}(\hat{z})}{1+\hat{z}}d\hat{z}\right\}\right]. \tag{1.50}$$

Some typical examples of dark energy with an evolving w_{de} are collected as follows.

(1) *Scalar fields and ϕCDM*. For a homogeneous scalar field $\phi(t)$ in the FRW Universe whose kinetics traces back to the standard Lagrangian density $\mathscr{L}_\phi = -\frac{1}{2}\nabla_\alpha\phi\nabla^\alpha\phi - V(\phi)$, its EoS parameter $w_\phi(t)$ is still given by Eq.(1.14). One might have noticed that, contrary to stiff matter, $w_\phi(t)$ behaves like $w_\phi(t) \simeq -1^+$ when $\phi(t)$ rolls slowly so that the potential $V(\phi)$ absolutely dominates over the kinetic-energy effect $\frac{1}{2}\dot{\phi}^2$. Also, $w_\phi(t)$ can fall into the domain $-1 < w_\phi(t) \lesssim -1/3$ when $\phi(t)$ is suitably strongly self-interacting with appropriate $V(\phi)$-dominance.

Hence, such a scalar field acts exactly like dark energy, and then leads to the ϕCDM extension of ΛCDM. Typical examples of this class include the canonical quintessence scalar field $\mathscr{L}_\phi = -\frac{1}{2}\nabla_\alpha\phi\nabla^\alpha\phi$ $-V(\phi)$ with $-1^+ < w_{\text{de}} < -1/3$ [23], and the noncanonical phantom scalar field $\mathscr{L}_\phi = \frac{1}{2}\nabla_\alpha\phi\nabla^\alpha\phi - V(\phi)$

with $w_{\rm de} < -1^-$ [24]. In addition, the double-scalar-field quintom model $\mathscr{L}_\phi = -\frac{1}{2}\nabla_\alpha\phi\nabla^\alpha\phi + \frac{1}{2}\nabla_\alpha\varphi\nabla^\alpha\varphi - U(\phi,\varphi)$ has the EoS parameter

$$w_{\rm de}^{\rm (quintom)} = \frac{\frac{1}{2}\dot{\phi}^2 - \frac{1}{2}\dot{\varphi}^2 - U}{\frac{1}{2}\dot{\phi}^2 - \frac{1}{2}\dot{\varphi}^2 + U}\,, \tag{1.51}$$

which allows to cross the so-called "phantom divide" $w_{\rm de} = -1$ when $\dot{\phi}^2 = \dot{\varphi}^2$ [25]. Moreover, by generalizing the Lagrangian density into $\mathscr{L} = -f(\frac{1}{2}\nabla_\alpha\phi\nabla^\alpha\phi) + V(\phi)$ and keeping $-1 < w_{\rm de} < -1/3$, i.e. replacing the kinetic term $\frac{1}{2}\nabla_\alpha\phi\nabla^\alpha\phi$ by some positively defined function $f(\frac{1}{2}\nabla_\alpha\phi\nabla^\alpha\phi)$, one obtains the "kinetic quintessence" or k-essence model [26].

(2) *Dark energy with nonlinear EoS rather than* $P_{\rm de} = w_{\rm de}\rho_{\rm de}$, such as the generalized Chaplygin gas whose pressure and energy density satisfies $P_{\rm de} = -A/\rho_{\rm de}^\alpha$ ($\{A,\alpha\}$ being positive constants), and this model has even been used to provide a unified description of dark matter and dark energy [27, 28].

(3) *Phenomenological modifications of the GR Friedmann equations (1.8), (1.9) and (1.19)*, such as the holographic dark energy with $\rho_{\rm de} = \dfrac{3\tilde{c}}{8\pi G}R_{\rm IR}^{-1}$ where $\tilde{c}$ is a constant and $R_{\rm IR}$ is the infrared cut-off scale [29], QCD ghost $\rho_{\rm de} = \alpha H^2$ [30], Ricci dark energy $\rho_{\rm de} \propto 2H^2 + \dot{H}$ [31], andc Pilgrim dark energy $\rho_{\rm de} = \alpha H^2 + \beta H^4$ models [32]. They can help produce the expected cosmic acceleration, but the physical motivations for these modifications of the standard Friedmann equations are unclear.

However, as we shall shortly see in Section 1.2, dark energy is not the only choice, and relativistic gravities beyond GR can also provide solutions to the cosmic acceleration problem.

1.1.9 Acceleration of the early Universe: Inflation

"Inflation hasn't won the race, but so far it's the only horse."
Andrei Linde

In Subsections 1.1.4~1.1.8, we have discussed the spatial acceleration of the late-time Universe. In fact, it is generally believed that acceleration also happens in the very early Universe, i.e. violent inflation right after the initial Big Bang and before the radiation-dominated era.

Unlike the problem of late-time acceleration which was inspired by astronomical observations, the motivations behind the cosmic inflation are mainly theoretical. Let's take anisotropies of the CMB background as an example. According to the 2015 Planck data [14], the last scattering which is the source of the CMB photons happens at the redshift $z_* = 1089.90 \pm 0.23$, or equivalently $a_* = 1/1090.90$. Moreover, with $\Omega_{M0} = 0.3089 \pm 0.0062$, $\Omega_{\Lambda 0} = 0.6911 \pm 0.0062$ and $\Omega_{r0} \simeq 0 \simeq \Omega_{k0}$ in the parameterized Friedmann equation (1.30), the particle horizon at z_* and the angular diameter distance to the last-scattering surface [20] are respectively

$$d_* = a_*\int_0^{a_*}\frac{da}{a^2H(a)} = \frac{1}{1+z_*}\int_{z_*}^{\infty}\frac{dz}{H(z)} \simeq \frac{8.7561\times 10^{-5}}{H_0}\,, \tag{1.52}$$

$$D_A^* = a_*\int_{a_*}^{1}\frac{da}{a^2H(a)} = \frac{1}{1+z_*}\int_0^{z_*}\frac{dz}{H(z)} \simeq \frac{2.6550\times 10^{-3}}{H_0}\,. \tag{1.53}$$

Accordingly, the angular size between causally connected patches on the full-sky CMB map is simply

$$\theta_* = \frac{d_*}{D_A^*} \simeq 3.2980 \times 10^{-2} \text{ rad} \simeq 1.8896^\circ\,, \tag{1.54}$$

so regions separated by $\theta > 1.8896^\circ$ should have little heat exchange. However, ever since the discovery of CMB, it has been long known that the CMB temperature is highly uniform and isotropic, and recent WMAP and Planck data have shown that the CMB unisotropy exists only at $\lesssim 10^{-5}$ level [14, 15]. This is completely unnatural in light of Eq.(1.54), so there must be some mechanism to synchronize the CMB temperature; as a result, an era of cosmic inflation has been proposed, which supplements the hot Big Bang theory to overcome its shortcomings [33].

In the simplest model, the inflation era is dominated by the inflaton scalar field $\phi(x^\alpha)$, whose kinetics is given by the action

$$\mathcal{I}_\phi = \int d^4x \sqrt{-g}\left(-\frac{1}{2}\nabla_\alpha\phi\nabla^\alpha\phi - V(\phi)\right). \tag{1.55}$$

The stress-energy-momentum tensor of $\mathcal{I}_\phi$ is

$$T^{(\phi)}_{\mu\nu} = -\frac{2}{\sqrt{-g}}\frac{\delta\left(\sqrt{-g}\mathscr{L}_\phi\right)}{\delta g^{\mu\nu}} = \nabla_\mu\phi\nabla_\nu\phi - \left(\frac{1}{2}\nabla_\alpha\phi\nabla^\alpha\phi + V\right)g_{\mu\nu}\,, \tag{1.56}$$

and under the flat FRW metric Eq.(1.6), the perfect inflaton fluid $T^{\mu(\phi)}_{\ \nu} = [-\rho_\phi, P_\phi, P_\phi, P_\phi]$ leads to

$$\rho_\phi = \frac{1}{2}\dot{\phi}^2 + V \quad \text{and} \quad P_\phi = \frac{1}{2}\dot{\phi}^2 - V\,. \tag{1.57}$$

Thus, according to Eqs.(1.8) and (1.19), in the inflation era the cosmic expansion satisfies the Friedmann equations

$$H^2 = \frac{8\pi G}{3}\left(\frac{1}{2}\dot{\phi}^2 + V\right) \quad \text{and} \quad \frac{\ddot{a}}{a} = -\frac{8\pi G}{3}\left(\dot{\phi}^2 - V\right), \tag{1.58}$$

which indicate that the Universe accelerates when the potential energy $V(\phi)$ dominates over the kinetic energy $\frac{1}{2}\dot{\phi}^2$. Clearly the slow-rolling inflaton field does not belong to the stiff matter in Eq.(1.14), which contrarily requires ϕ to be fast-rolling so that $\dot{\phi}^2 \gg V$; instead, inflaton behaves pretty like the quintessence described in the previous subsection, and this similarity had inspired the investigations to unify the early and the late-time accelerations into a common framework (eg. [34]).

In Chapter 9 we will calculate the "gravitational baryogenesis" that dynamically produces the required baryon-antibaryon asymmetry for an expanding Universe by violating the combined charge, parity and time reversal symmetry in thermal equilibrium. The net baryon abundance relies on the upper temperature bound T_d for the tensor-mode fluctuations at the inflationary scale, while the energy scale of inflation is related to the tensor-to-scalar ratio $\tilde{r}$ by [35]

$$T_d = \text{upper lim}\left(V^{1/4}\right) \simeq 1.06 \times 10^{16} \times \left(\frac{\tilde{r}}{0.01}\right)^{1/4} \text{ [GeV]}\,. \tag{1.59}$$

This result is extremely useful as the ratio $\tilde{r}$ can be measured in astrophysical observations (for example, the observed B-mode power spectrum in inflationary gravitational waves by the BICEP2 experiment gives $\tilde{r} = 0.20^{+0.07}_{-0.05}$ [36], and Planck has placed a 95% upper limit on $\tilde{r} < 0.113$ by the combinations of Planck power spectra, Planck lensing and external data [14]). However, one should note that Eq.(1.59) is built upon the standard paradigm of single-field slow-rolling inflation as above, and in the situation of *nonstandard* cosmic expansion that modifies Eq.(1.58), the inflation scenario and thus Eq.(1.59) should also be updated when one looks for T_d.

1.2 Modified gravity

> "*No one will be able to read the great book of the universe if he does not understand its language which is that of mathematics.*"
> *Galileo Galilei*

1.2.1 Lovelock theorem and modifications of GR

As an alternative to the various models of dark energy with large negative pressure that violates the standard energy conditions, the accelerated expansion of the Universe has inspired the reconsideration of relativistic gravity and modifications of GR, which can explain the cosmic acceleration and reconstruct the entire expansion history without dark energy. To date, quite a few alternative or modified theories of gravity have been developed, and a good way to organize and understand these theories is through the classic Lovelock's theorem, as they actually encode the possible ways to go beyond Lovelock's theorem and its necessary conditions [37] which limit the second-order field equation in four dimensions to $R_{\mu\nu} - Rg_{\mu\nu}/2 + \Lambda g_{\mu\nu} = 8\pi G T^{(m)}_{\mu\nu}$, i.e. Einstein's equation carrying the cosmological constant Λ. Note that for brevity, we will use the terminology "modified gravity" to denote both modified and alternative theories of relativistic gravity without discrimination whenever appropriate.

As shown in Subsection 1.1.1, it is somewhat amazing that although the Ricci scalar $R = g^{\alpha\beta}R_{\alpha\beta} = g^{\alpha\beta}g^{\mu\nu}R_{\alpha\mu\beta\nu}$ contains up to second-order derivative of $g_{\mu\nu}$, the Euler-Lagrange-type derivative $\delta\mathcal{I}_{\text{HE}}/\delta g^{\mu\nu}$ in Eq.(1.2) leads to a second-order rather than fourth-order field equation. This is because the higher-order curvature terms turn out to be total derivatives, the integration of which becomes a negligible surface integral over the boundary (i.e. the well-known Gibbons-Hawking-York boundary term [5]) in light of the Stokes theorem. In fact, there exist infinitely many *algebraic* Riemannian invariants $\widetilde{\mathcal{R}} = \widetilde{\mathcal{R}}(g_{\rho\sigma}, R_{\alpha\mu\beta\nu})$ as a function of the products/contractions of the metric tensor $g_{\rho\sigma}$ and the Riemann tensor $R_{\alpha\mu\beta\nu}$. In general, the action $\int d^4x\sqrt{-g}\,\widetilde{\mathcal{R}}$ leads to fourth-order gravitational field equations by the variational derivative

$$\frac{\delta\left(\sqrt{-g}\widetilde{\mathcal{R}}\right)}{\delta g^{\mu\nu}} = \frac{\partial\left(\sqrt{-g}\widetilde{\mathcal{R}}\right)}{\partial g^{\mu\nu}} - \partial_\alpha \frac{\partial\left(\sqrt{-g}\widetilde{\mathcal{R}}\right)}{\partial(\partial_\alpha g^{\mu\nu})} + \partial_\alpha\partial_\beta \frac{\partial\left(\sqrt{-g}\widetilde{\mathcal{R}}\right)}{\partial(\partial_\alpha\partial_\beta g^{\mu\nu})}. \tag{1.60}$$

However, remarkably it has been proved that in *four* dimensions, the following Lanczos-Lovelock action is the most general one which could yield a second-order gravitational field equation [37]

$$\mathcal{I}_{\text{LL}} = \int d^4x\sqrt{-g}\cdot\left(a\cdot R - 2\Lambda + b\cdot\delta_{\alpha\beta\gamma\eta}R^{\mu\nu\alpha\beta}R_{\mu\nu}{}^{\gamma\eta} + c\cdot\mathcal{G} + 16\pi G\mathscr{L}_m\right), \tag{1.61}$$

where $\{a = 1\,, \Lambda\,, b\,, c\}$ are all constants and we have set $a = 1$ in $\mathscr{L}_{\rm LL}$ without any loss of generality, while $\mathcal{G}$ refers to the Gauss-Bonnet invariant:

$$\mathcal{G} \;:=\; R^2 - 4R_{\alpha\beta}R^{\alpha\beta} + R_{\alpha\mu\beta\nu}R^{\alpha\mu\beta\nu}\,. \tag{1.62}$$

The first two terms in $\mathcal{I}_{\rm LL}$ are just the Hilbert-Einstein-Λ action as in Eq.(1.21). For the third term, $\sqrt{-g}\,\delta_{\alpha\beta\gamma\eta}R^{\mu\nu\alpha\beta}R_{\mu\nu}{}^{\gamma\eta} \equiv \epsilon_{\alpha\beta\gamma\eta}R^{\mu\nu\alpha\beta}R_{\mu\nu}{}^{\gamma\eta}$ actually refers to the Chern-Pontryagin density, where $\epsilon_{\alpha\beta\mu\nu} = \sqrt{-g}\delta_{\alpha\beta\mu\nu}$ refers to the totally antisymmetric Levi-Civita pseudotensor with $\epsilon_{0123} = \sqrt{-g}$, $\epsilon^{0123} = \frac{1}{\sqrt{-g}}$, and $\{\epsilon_{\alpha\beta\mu\nu},\ \epsilon^{\alpha\beta\mu\nu}\}$ can be obtained from each other by raising or lowering the indices with the metric tensor. $\epsilon_{\alpha\beta\gamma\eta}R^{\mu\nu\alpha\beta}R_{\mu\nu}{}^{\gamma\eta}$ is proportional to the divergence of the topological Chern-Simons four-current K^μ [38]:

$$\epsilon_{\alpha\beta\mu\nu}R^{\mu\nu}{}_{\gamma\delta}R^{\alpha\beta\gamma\delta} = -8\,\partial_\mu K^\mu \quad \text{with} \quad K^\mu = \epsilon^{\mu\alpha\beta\gamma}\left(\frac{1}{2}\Gamma^\xi_{\alpha\tau}\partial_\beta\Gamma^\tau_{\gamma\xi} + \frac{1}{3}\Gamma^\xi_{\alpha\tau}\Gamma^\tau_{\beta\eta}\Gamma^\eta_{\gamma\xi}\right), \tag{1.63}$$

and $b\int d^4x\,\sqrt{-g}\,\delta_{\alpha\beta\gamma\eta}R^{\mu\nu\alpha\beta}R_{\mu\nu}{}^{\gamma\eta} \equiv b\int d^4x\,\epsilon_{\alpha\beta\gamma\eta}R^{\mu\nu\alpha\beta}R_{\mu\nu}{}^{\gamma\eta}$ is equivalent to a surface integral in *all* dimensions [39] with no contribution to the field equation. Similarly for the fourth term, the covariant density $\sqrt{-g}\,\mathcal{G}$ has the topological current [40]

$$\sqrt{-g}\,\mathcal{G} = -\partial_\mu J^\mu \quad \text{with} \quad J^\mu = \sqrt{-g}\,\epsilon^{\mu\alpha\beta\gamma}\epsilon_{\rho\sigma}{}^{\xi\zeta}\Gamma^\rho_{\xi\alpha}\left(\frac{1}{2}R^\sigma{}_{\zeta\beta\gamma} - \frac{1}{3}\Gamma^\sigma_{\lambda\beta}\Gamma^\lambda_{\zeta\gamma}\right), \tag{1.64}$$

and $c\int d^4x\,\sqrt{-g}\,\mathcal{G}$ reduces to a surface integral in *four* (and lower-than-four) dimensions[4] and therefore makes no difference to the field equation, either; equivalently, the Bach-Lanczos tensor which vanishes identically in four and lower-than-four dimensions arises from the variational derivative $\delta(\sqrt{-g}\,\mathcal{G})/\delta g^{\mu\nu} = 0$,

$$\frac{\delta(\sqrt{-g}\,\mathcal{G})}{\delta g^{\mu\nu}} = -\frac{1}{2}\mathcal{G}\,g_{\mu\nu} + 2R\,R_{\mu\nu} - 4R_\mu{}^\alpha R_{\alpha\nu} - 4R_{\alpha\mu\beta\nu}R^{\alpha\beta} + 2R_{\mu\alpha\beta\gamma}R_\nu{}^{\alpha\beta\gamma} \equiv 0\,. \tag{1.66}$$

Thus, the Lanczos-Lovelock action Eq.(1.61) finally yields the same field equation as the Hilbert-Einstein-Λ action Eq.(1.21)). That is to say [37]:

Lovelock theorem: In four dimensions, the Einstein-Λ equation $R_{\mu\nu} - Rg_{\mu\nu}/2 + \Lambda g_{\mu\nu} = 8\pi G T^{(m)}_{\mu\nu}$ is the only second-order gravitational field equation in pure metric gravities.

Here by metric gravity we mean its mathematical scope is pseudoRiemannian geometry that is equipped with a metric tensor, a metric-compatible covariant derivative, and a torsion-free Levi-Civita connection. Hence, according to the Lovelock theorem, we can take the following approaches to develop relativistic theories of gravity as modifications or alternatives of GR.

[4]On the other hand, the Euler-Poincaré topological density for a four-dimensional Lorentzian manifold is (with $\chi(S^{2n})$ normalized to 2)

$$\mathcal{E}^{(4)} = \frac{1}{128\pi^2}\epsilon^{\mu\nu\rho\sigma}\epsilon^{\alpha\beta\zeta\eta}R_{\mu\nu\alpha\beta}R_{\rho\sigma\zeta\eta} = \frac{1}{32\pi^2}\Big(R^2 - 4R_{\alpha\beta}R^{\alpha\beta} + R_{\alpha\mu\beta\nu}R^{\alpha\mu\beta\nu}\Big) = \frac{\mathcal{G}}{32\pi^2}\,. \tag{1.65}$$

Hence, $\int d^4x\,\sqrt{-g}\,\mathcal{G}$ just gives rise to the Euler number χ which is a constant characterizing the topology of the spacetime. Hence, once again we have $\delta\int d^4x\,\sqrt{-g}\,\mathcal{G} \equiv 0$.

(1) Consider fourth- and even higher-order theories of gravity, such as the $\mathscr{L} = f(R) + 16\pi G\mathscr{L}_m$ [41], $\mathscr{L} = R + f(\mathcal{G}) + 16\pi G\mathscr{L}_m$ [42] and $\mathscr{L} = f(R, \mathcal{G}) + 16\pi G\mathscr{L}_m$ [43] models in existing literature[5]. Fourth-order gravity focuses on the nine parity-even (thus respect time-reversal and space-reflection symmetries) invariants out of the 14 *independent* algebraic Riemannian invariant which are introduced based on the Petrov and the Segre classifications of a spacetime [44], while higher-than-fourth-order theories will take differential Riemannian invariants into account. However, since fundamental physical laws are all expressed as second-order differential equations (like the Maxwell, Schrödinger and Einstein equations), higher-than-fourth-order theories are generally regarded with skepticism and not favored. However, fortunately fourth-order gravity is partially acceptable, because most of the results can be translated into second-order ones in the more general Einstein-Palatini formulation and can be helpful in quantizing gravity.

(2) Go to higher dimensions. For example, reconsider the Lanczos-Lovelock action Eq.(1.61) (with $a = 1$) in *five* dimensions, collect all terms nontrivially contributing to the field equation, and one obtains the action of the well-known Einstein-Gauss-Bonnet gravity:

$$\mathcal{I}_{\text{EGB}} = \int d^{(5)}x \sqrt{-g} \cdot \Big(R - 2\Lambda + c \cdot \mathcal{G} + 16\pi G\mathscr{L}_m \Big). \tag{1.67}$$

This time, $\delta(\sqrt{-g}\,\mathcal{G})/\delta g^{\mu\nu}$ will add a *nonzero* Bach-Lanczos tensor $-\frac{1}{2}\mathcal{G}\, g_{\mu\nu} + 2R\, R_{\mu\nu} - 4R_\mu{}^\alpha R_{\alpha\nu} - 4R_{\alpha\mu\beta\nu}R^{\alpha\beta} + 2R_{\mu\alpha\beta\gamma}R_\nu{}^{\alpha\beta\gamma}$ to the second-order field equation. More generally, Lovelock gravity arises as the topological generalizations of the Hilbert-Einstein action to generic N dimensions that still preserves second-order field equations [45].

(3) Go beyond pure Riemann geometry and metric gravity, and consider more *geometric* degrees of freedom (like torsion and independent affine connections) as field quantities, such as the teleparallel equivalence of GR in the pure-torsion Weitzenböck spacetime, modified teleparallel gravity $\mathcal{I} = \int dx^4 \sqrt{-g}\, [f(\mathcal{T}) + 16\pi G\mathscr{L}_m]$ with $\mathcal{T}$ being the torsion scalar [46], Einstein-Cartan gravity [47], and metric-affine gravity [47]. The diagram below quickly illustrates the relations between Riemannian spacetime and some other geometric spacetimes.

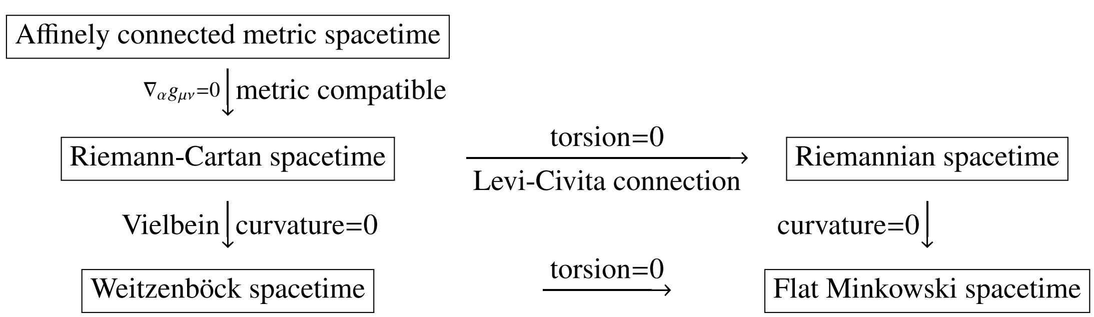

Figure 1.1: Relativistic gravities and torsion

(4) Consider extra *physical* degrees of freedom, most typically an extra scalar field. From the viewpoint of classical field theory, the field quantity for gravity is the metric $g_{\mu\nu}$ (rank-2 tensor), and that for

[5]We will deal with total Lagrangian density instead of the full action whenever appropriate for the sake of simplicity.

electromagnetic interaction is the covector potential A_μ (rank-1 tensor). Thus, it is natural to assume the existence of a scalar field (rank-0 tensor) or multi-scalar fields mediating a long-range interaction. Chern-Simons gravity [38], Brans-Dicke theory [48], generic scalar-tensor theories [49], Gauss-Bonnet effective dark energy [50], Horndeski [51] and Galileon [52] gravities are all fruits of this type.

(5) Einstein's equation implies the minimal coupling between the curvature invariants used in $\mathcal{I}_{\text{LL}}$ and the matter Lagrangian density $\mathscr{L}_m$. Thus, allowing for possibly nonminimal curvature-matter coupling[6] [54] opens a new window for modified gravity, and has brought theories like $\mathscr{L} = f(R) + 16\pi G\mathscr{L}_m + \tilde{f}(R)\mathscr{L}_m$ [55], generic $\mathscr{L} = f(R, \mathscr{L}_m)$ [56], and $\mathscr{L} = f(R, g^{\mu\nu}T^{(m)}_{\mu\nu}) + 16\pi G\mathscr{L}_m$ [57].

1.2.2 $f(R)$ gravity and construction of effective dark energy

From this subsection on, we will look into the theoretical structures of some specific modified gravities. We will begin with the minimally coupled $f(R)$ gravity, which is the simplest class of fourth-order gravity. As a straightforward generalization of the Hilbert-Einstein action $\mathcal{I}_{\text{HE}}$, $f(R)$ gravity is given by [41]

$$\mathcal{I} = \int d^4x\sqrt{-g}\left[f(R) + 16\pi G\mathscr{L}_m\right], \tag{1.68}$$

which replaces the Ricci scalar R in $\mathcal{I}_{\text{HE}} = \int \sqrt{-g}\, d^4x\,(R + 16\pi G\mathscr{L}_m)$ by an arbitrary function $f(R)$.

To find out the covariant field equation, one needs to vary the $f(R)$ action with respect to the inverse metric, which leads to

$$\begin{aligned}\delta\mathcal{I} &= \int d^4x\left[\sqrt{-g}\cdot\delta f(R) + f(R)\cdot\delta\sqrt{-g} + 16\pi G\cdot\delta\left(\sqrt{-g}\mathscr{L}_m\right)\right]\\ &= \int d^4x\,\sqrt{-g}\left(\frac{f_R\cdot\delta R}{\delta g^{\mu\nu}} - \frac{1}{2}g_{\mu\nu}f - 8\pi G T^{(m)}_{\mu\nu}\right)\delta g^{\mu\nu}\,,\end{aligned} \tag{1.69}$$

where $f_R = f_R(R) \coloneqq df(R)/dR$, and the definition of $T^{(m)}_{\mu\nu}$ in Eq.(1.4) has been used. Here one should note that total derivatives in the isolated variation δR are not necessarily pure divergences anymore, because the nontrivial coefficient f_R will be absorbed into the nonlinear and higher-order-derivative terms produced by δR. Based on the Palatini identity $\delta R^\alpha{}_{\mu\beta\nu} = \nabla_\beta\delta\Gamma^\alpha_{\mu\nu} - \nabla_\nu\delta\Gamma^\alpha_{\mu\beta}$ [5], contraction of the indices $\{\alpha, \beta\}$ yields

$$\delta R_{\mu\nu} \;=\; \nabla_\lambda\delta\Gamma^\lambda_{\mu\nu} - \nabla_\nu\delta\Gamma^\lambda_{\lambda\mu}\,. \tag{1.70}$$

Thus, $f_R\cdot\delta R = f_R\cdot\delta(g^{\mu\nu}R_{\mu\nu}) = f_R\cdot\left(R_{\mu\nu}\delta g^{\mu\nu} + g^{\mu\nu}\delta R_{\mu\nu}\right) = f_R\cdot\left[R_{\mu\nu}\delta g^{\mu\nu} + g^{\mu\nu}(\nabla_\lambda\delta\Gamma^\lambda_{\mu\nu} - \nabla_\nu\delta\Gamma^\lambda_{\lambda\mu})\right]$. Recall that variation of the Christoffel symbol satisfies [5]

$$\delta\Gamma^\lambda_{\mu\nu} = \frac{1}{2}g^{\lambda\alpha}\delta\Gamma_{\alpha\mu\nu} = \frac{1}{2}g^{\lambda\alpha}\left(\nabla_\mu\delta g_{\alpha\nu} + \nabla_\nu\delta g_{\alpha\mu} - \nabla_\alpha\delta g_{\mu\nu}\right), \tag{1.71}$$

[6]The terms *geometry-matter* coupling and *curvature-matter* coupling are both used in this thesis. They are not identical: the former can be either nonminimal or minimal, while the latter by its name is always nonminimal since a curvature invariant contains at least second-order derivative of the metric tensor. Here nonminimal coupling happens between algebraic or differential Riemannian scalar invariants and $\mathscr{L}_m$, so we will mainly use curvature-matter coupling.

and the the indices of $\delta g_{\alpha\beta}$ can be raised by $\delta g_{\alpha\beta} = -g_{\alpha\rho}g_{\beta\sigma}\delta g^{\rho\sigma}$, so

$$
\begin{aligned}
& f_R \cdot g^{\mu\nu} \left(\nabla_\lambda \delta\Gamma^\lambda_{\mu\nu} - \nabla_\nu \delta\Gamma^\lambda_{\lambda\mu}\right) \\
&= f_R \cdot g^{\mu\nu} \left\{ \frac{1}{2} g^{\lambda\alpha}\, \nabla_\lambda \Big(\nabla_\mu \delta g_{\alpha\nu} + \nabla_\nu \delta g_{\alpha\mu} - \nabla_\alpha \delta g_{\mu\nu} \Big) - \frac{1}{2} g^{\lambda\alpha}\, \nabla_\nu \Big(\nabla_\mu \delta g_{\alpha\lambda} + \nabla_\lambda \delta g_{\alpha\mu} - \nabla_\alpha \delta g_{\lambda\mu} \Big) \right\} \\
&= f_R \cdot \frac{1}{2} g^{\mu\nu} g^{\lambda\alpha} \left\{ \Big(\nabla_\lambda \nabla_\mu \delta g_{\alpha\nu} + \nabla_\lambda \nabla_\nu \delta g_{\alpha\mu} - \nabla_\lambda \nabla_\alpha \delta g_{\mu\nu} \Big) - \Big(\nabla_\nu \nabla_\mu \delta g_{\alpha\lambda} + \nabla_\nu \nabla_\lambda \delta g_{\alpha\mu} - \nabla_\nu \nabla_\alpha \delta g_{\lambda\mu} \Big) \right\} \\
&= f_R \cdot \Big(\nabla_\mu \nabla_\nu \delta g^{\mu\nu} - g^{\mu\nu} \Box \delta g_{\mu\nu} \Big) \cong \Big(- \nabla_\mu \nabla_\nu f_R + g_{\mu\nu} \Box f_R \Big)\, \delta g^{\mu\nu} \,.
\end{aligned}
\tag{1.72}
$$

where $\Box$ denotes the covariant d'Alembertian $\Box := g^{\alpha\beta}\nabla_\alpha\nabla_\beta$. Integrating Eq.(1.72) by parts and neglecting the total-derivative terms, one obtains

$$
f_R \cdot \delta R = \Big(f_R R_{\mu\nu} + g_{\mu\nu} \Box f_R - \nabla_\mu \nabla_\nu f_R \Big) \cdot \delta g^{\mu\nu} \,, \tag{1.73}
$$

Thus, the extremization $\delta\mathcal{I}/\delta g^{\mu\nu} = 0$ finally gives rise to the field equation

$$
f_R R_{\mu\nu} - \frac{1}{2} f g_{\mu\nu} + \Big(g_{\mu\nu} \Box - \nabla_\mu \nabla_\nu \Big) f_R = 8\pi G T^{(m)}_{\mu\nu} \,. \tag{1.74}
$$

However, in cosmology it is not so convenient to utilize Eq.(1.74) directly. Instead, it proves much more enlightening and helpful to rewrite the $f(R)$ field equation into a GR form, which people feel more familiar to deal with. This way, Eq.(1.74) can be rearranged into

$$
R_{\mu\nu} - \frac{1}{2} R g_{\mu\nu} \;=\; 8\pi G f_R^{-1} T^{(m)}_{\mu\nu} + f_R^{-1} \cdot \left[\frac{1}{2} (f - f_R R) g_{\mu\nu} + (\nabla_\mu \nabla_\nu - g_{\mu\nu} \Box) f_R \right], \tag{1.75}
$$

and it can be compactified into the GR form $R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} = 8\pi G_{\text{eff}} T^{(\text{eff})}_{\mu\nu}$, where G_{eff} denotes the effective gravitational coupling strength, and $T^{(\text{eff})}_{\mu\nu}$ represents the effective stress-energy-momentum tensor. From Eq.(1.75) one can observe that

$$
\begin{aligned}
8\pi G_{\text{eff}} T^{(\text{eff})}_{\mu\nu} &= 8\pi G f_R^{-1} \left\{ T^{(m)}_{\mu\nu} + (8\pi G)^{-1} \left[\frac{1}{2} (f - f_R R) g_{\mu\nu} + (\nabla_\mu \nabla_\nu - g_{\mu\nu} \Box) f_R \right] \right\} \\
&= 8\pi G f_R^{-1} \Big[T^{(m)}_{\mu\nu} + T^{(\text{MG})}_{\mu\nu} \Big],
\end{aligned}
\tag{1.76}
$$

so we have $G_{\text{eff}} = G f_R^{-1}$ and $T^{(\text{eff})}_{\mu\nu} = T^{(m)}_{\mu\nu} + (8\pi G)^{-1} \left[\frac{1}{2} (f - f_R R)\, g_{\mu\nu} + \Big(\nabla_\mu \nabla_\nu - g_{\mu\nu} \Box \Big) f_R \right]$. Thus, $T^{(\text{eff})}_{\mu\nu}$ contains two parts: $T^{(m)}_{\mu\nu}$ for the physical matter content, and the remaining part $T^{(\text{MG})}_{\mu\nu} = (8\pi G)^{-1} \Big[\frac{1}{2} (f - f_R R) g_{\mu\nu} + (\nabla_\mu \nabla_\nu - g_{\mu\nu} \Box) f_R \Big]$ to collect all nonlinear and higher-order terms of modified gravity [hence the superscript (MG)] so that $T^{(\text{eff})}_{\mu\nu} = T^{(m)}_{\mu\nu} + T^{(\text{MG})}_{\mu\nu}$. Eq.(1.75) takes a similar form with the Einstein−Λ equation (1.22) of ΛCDM cosmology, with $T^{(\text{MG})}_{\mu\nu}$ plays the role of the cosmological constant Λ or other candidates of dark energy. In this spirit, we regard Eq.(1.75) as the form of $f(R)$ field equation that constructs the effective dark energy.

Generally an effective dark-energy fluid of modified gravity $T^{\mu\;(\text{MG})}_{\;\nu} = \text{diag}\Big[-\rho_{(\text{MG})}, P_{(\text{MG})}, P_{(\text{MG})}, P_{(\text{MG})} \Big]$

is assumed, along with a total effective fluid $T^{\mu\,(\text{eff})}_{\nu} = \text{diag}\Big[-\rho_{\text{eff}}, P_{\text{eff}}, P_{\text{eff}}, P_{\text{eff}}\Big]$. Then substitute the FRW metric Eq.(1.6) into the $T^{(\text{MG})}_{\mu\nu}$ of $f(R)$ gravity, and we obtain the modified Friedmann equations

$$H^2 + \frac{k}{a^2} = \frac{8\pi}{3}\frac{G}{f_R}\rho_m + \frac{1}{3f_R}\left(\frac{1}{2}f_R R - \frac{1}{2}f - 3H\dot{f}_R\right), \tag{1.77}$$

$$\dot{H} - \frac{k}{a^2} = -4\pi\frac{G}{f_R}\left(\rho_m + P_m\right) - \frac{1}{2f_R}\left(\ddot{f}_R - H\dot{f}_R\right), \tag{1.78}$$

while the density and pressure of the effective dark-energy fluid are respectively

$$\rho_{(\text{MG})} = \frac{1}{8\pi G}\left(\frac{1}{2}f_R R - \frac{1}{2}f - 3H\dot{f}_R\right) \quad \text{and} \quad P_{(\text{MG})} = \frac{1}{8\pi G}\left(\frac{1}{2}f - \frac{1}{2}f_R R + \ddot{f}_R + 2H\dot{f}_R\right). \tag{1.79}$$

Note that compact notations have been used in Eqs.(1.77) and (1.78), as f_R itself is treated as a function of the comoving time t. Otherwise, one can further write $\dot{f}_R$ into $f_{RR}\dot{R}$ and $\ddot{f}_R$ into $f_{RR}\ddot{R} + f_{RRR}\dot{R}^2$, and the Ricci scalar for the FRW spacetime is already known to be $R = R(t) = 6\Big(\dot{H} + 2H^2 + \frac{k}{a^2}\Big)$. This in turn indicates that second-order and third-order derivative $\{\ddot{H}, \dddot{H}\}$ (or equivalently third-order and fourth-order derivative $\{\dddot{a}, \ddddot{a}\}$) get involved in Eqs.(1.77) and (1.78), and these terms are gone once we return to GR with $f_R = 1$.

$f(R)$ gravity plays an important role in this thesis. For example, Chapter 4 involves the derivation of Eqs.(1.77) and (1.78) from the unified first law of gravitational thermodynamics on the apparent horizon of the FRW Universe. Chapter 9 will investigate the primordial nucleosynthesis in power-law $f(R)$ gravity from the the semianalytical approach for ^{4}He, and from the empirical approach for {D, ^{4}He, ^{7}Li}; also, consistency with the gravitational baryogenesis will be estimated. Still in power-law $f(R)$ gravity, Chapter 10 will study thermal relics as hot, warm, and cold dark matter, and revises the Lee-Weinberg bound for the mass of speculated heavy neutrinos.

1.2.3 Quadratic gravity

Having seen $f(R)$ gravity, we will continue with modified gravities that depend on curvature invariants beyond the Ricci scalar, and a simplest example is the quadratic modification of GR. The Lagrangian density of quadratic gravity is constructed by the linear superposition of GR with some typical quadratic (as opposed to cubic and quartic) algebraic curvature invariants, such as R^2, $R_{\mu\nu}R^{\mu\nu}$, $S_{\mu\nu}S^{\mu\nu}$ (with $S_{\mu\nu} := R_{\mu\nu} - \frac{1}{4}R\,g_{\mu\nu}$ being the traceless part of the Ricci tensor), $R_{\mu\alpha\nu\beta}R^{\mu\alpha\nu\beta}$, $C_{\mu\alpha\nu\beta}C^{\mu\alpha\nu\beta}$ [with $C_{\alpha\beta\gamma\delta} = R_{\alpha\beta\gamma\delta} + \frac{1}{2}\Big(g_{\alpha\delta}R_{\beta\gamma} - g_{\alpha\gamma}R_{\beta\delta} + g_{\beta\gamma}R_{\alpha\delta} - g_{\beta\delta}R_{\alpha\gamma}\Big) + \frac{1}{6}\left(g_{\alpha\gamma}g_{\beta\delta} - g_{\alpha\delta}g_{\beta\gamma}\right)R$ being the conformal Weyl tensor, which is the totally traceless part in the Ricci decomposition of Riemann tensor]. This way, generally quadratic gravity can be given by

$$\mathscr{L} = R + aR^2 + bR_{\mu\nu}R^{\mu\nu} + cS_{\mu\nu}S^{\mu\nu} + dR_{\mu\alpha\nu\beta}R^{\mu\alpha\nu\beta} + eC_{\mu\alpha\nu\beta}C^{\mu\alpha\nu\beta} + 16\pi G\mathscr{L}_m\,, \tag{1.80}$$

where the coefficients $\{a, b, c, d, e\}$ are all constants. However, these quadratic invariants are not completely independent with each other, as

$$S_{\mu\nu}S^{\mu\nu} = R_{\mu\nu}R^{\mu\nu} - \frac{1}{4}R^2 \quad , \quad C_{\mu\alpha\nu\beta}C^{\mu\alpha\nu\beta} = R_{\mu\alpha\nu\beta}R^{\mu\alpha\nu\beta} - 2R_{\mu\nu}R^{\mu\nu} + \frac{1}{3}R^2\,, \tag{1.81}$$

while $R_{\mu\alpha\nu\beta}R^{\mu\alpha\nu\beta}$ can be absorbed into the Gauss-Bonnet invariant by $R_{\mu\alpha\nu\beta}R^{\mu\alpha\nu\beta} = \mathcal{G} - R^2 + 4R_{\mu\nu}R^{\mu\nu}$ with $\mathcal{G}$ making no contribution to the field equation. Hence, it is sufficient to consider the following form of quadratic gravity [58]

$$\mathcal{I} = \int d^4x\sqrt{-g}\left(R + a\cdot R^2 + b\cdot R_{\alpha\beta}R^{\alpha\beta} + 16\pi G\mathscr{L}_m\right). \tag{1.82}$$

Variation of this action with respect to the inverse metric yields

$$\delta\mathcal{I} = \int d^4x\,\sqrt{-g}\left[\frac{\delta R}{\delta g^{\mu\nu}} + a\cdot\frac{2R\delta R}{\delta g^{\mu\nu}} + b\cdot\frac{\delta R_{\alpha\beta}R^{\alpha\beta}}{\delta g^{\mu\nu}} - \frac{1}{2}g_{\mu\nu}\Big(R + aR^2 + bR_{\alpha\beta}R^{\alpha\beta}\Big) - 8\pi GT^{(m)}_{\mu\nu}\right]\delta g^{\mu\nu}, \tag{1.83}$$

where

$$\delta R^2/\delta g^{\mu\nu} \;=\; 2R\,R_{\mu\nu} + 2\left(g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu\right)R\,, \tag{1.84}$$

and $\delta R_{\mu\nu}R^{\mu\nu}$ can be reduced into the variation of the Riemann tensor [59],

$$\begin{aligned}\delta R_{\alpha\beta}R^{\alpha\beta} \;&=\; \delta\Big[R_{\alpha\beta}\cdot(g^{\alpha\rho}g^{\beta\sigma}R_{\rho\sigma})\Big] \;=\; 2R_\mu{}^\alpha R_{\alpha\nu}\cdot\delta g^{\mu\nu} + 2R^{\mu\nu}\cdot\delta R^\alpha{}_{\mu\alpha\nu}\\ &=\; \Big(2R_\mu{}^\alpha R_{\alpha\nu} - \nabla_\alpha\nabla_\nu R_\mu{}^\alpha - \nabla_\alpha\nabla_\mu R_\nu{}^\alpha + \Box R_{\mu\nu} + g_{\mu\nu}\cdot\nabla_\alpha\nabla_\beta R^{\alpha\beta}\Big)\delta g^{\mu\nu}\,.\end{aligned} \tag{1.85}$$

Thus, the field equation is

$$\begin{aligned}&-\frac{1}{2}(R + a\cdot R^2 + b\cdot R_{\alpha\beta}R^{\alpha\beta})\,g_{\mu\nu} + (1+2aR)\,R_{\mu\nu} + 2a\,(g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu)\,R\\ &+ b\cdot\Big(2R_\mu{}^\alpha R_{\alpha\nu} - \nabla_\alpha\nabla_\nu R_\mu{}^\alpha - \nabla_\alpha\nabla_\mu R_\nu{}^\alpha + \Box R_{\mu\nu} + g_{\mu\nu}\nabla_\alpha\nabla_\beta R^{\alpha\beta}\Big) = 8\pi GT^{(m)}_{\mu\nu}\,.\end{aligned} \tag{1.86}$$

Considering that the second Bianchi identity $\nabla_\gamma R_{\alpha\mu\beta\nu} + \nabla_\nu R_{\alpha\mu\gamma\beta} + \nabla_\beta R_{\alpha\mu\nu\gamma} = 0$ implies

$$\nabla^\beta\nabla^\alpha R_{\alpha\beta} \;=\; \frac{1}{2}\,\Box R \quad \text{and} \tag{1.87}$$

$$\nabla^\alpha\nabla_\mu R_{\alpha\nu} + \nabla^\alpha\nabla_\nu R_{\alpha\mu} \;=\; \nabla_\mu\nabla_\nu R - 2R_{\alpha\mu\beta\nu}R^{\alpha\beta} + 2R_\mu{}^\alpha R_{\alpha\nu}\,, \tag{1.88}$$

Eq.(1.86) can be recast into

$$\begin{aligned}&-\frac{1}{2}(R + a\cdot R^2 + b\cdot R_{\alpha\beta}R^{\alpha\beta})\,g_{\mu\nu} + (1+2aR)\,R_{\mu\nu} + 2a\,(g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu)\,R\\ &\quad + b\cdot\Big[2R_{\alpha\mu\beta\nu}R^{\alpha\beta} + (\frac{1}{2}\,g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu)\,R + \Box R_{\mu\nu}\Big] = 8\pi GT^{(m)}_{\mu\nu}\,.\end{aligned} \tag{1.89}$$

In the spirit of constructing the effective dark energy via $R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} = 8\pi G_{\text{eff}}\left(T^{(m)}_{\mu\nu} + T^{(\text{MG})}_{\mu\nu}\right)$, one can rewrite the field equation (1.89) into

$$R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} = \frac{8\pi G}{1+2aR}\bigg\{T^{(m)}_{\mu\nu} + (8\pi G)^{-1}\Big[\frac{1}{2}\Big(bR_{\alpha\beta}R^{\alpha\beta} - aR^2\Big)g_{\mu\nu} + (2a+b)\nabla_\mu\nabla_\nu R - (2a+\frac{b}{2})\, g_{\mu\nu}\Box R - 2b\left(2R_{\mu\alpha\nu\beta}R^{\alpha\beta} + \Box R_{\mu\nu}\right)\Big]\bigg\}. \tag{1.90}$$

From the coefficient of $T^{(m)}_{\mu\nu}$ we learn that the effective gravitational coupling strength for quadratic gravity is $G_{\text{eff}} = G/(1+2aR)$, while the modified-gravity effects contribute to the effective total fluid by $T^{(\text{MG})}_{\mu\nu} = (8\pi G)^{-1}\Big[\frac{1}{2}\Big(bR_c^2 - aR^2\Big)g_{\mu\nu} + (2a+b)\nabla_\mu\nabla_\nu R - (2a+\frac{b}{2})g_{\mu\nu}\Box R - 2b\Big(2R_{\mu\alpha\nu\beta}R^{\alpha\beta} + \Box R_{\mu\nu}\Big)\Big]$. Substitute the FRW metric into Eq.(1.113), we obtain the modified Friedmann equations

$$H^2 + \frac{k}{a^2} = \frac{8\pi G}{3(1+2aR)}\left\{\rho_m + \frac{1}{8\pi G}\Big[\frac{a}{2}R^2 - \frac{b}{2}R_{\alpha\beta}R^{\alpha\beta} + \frac{b}{2}\ddot{R} - (4a+b)H\dot{R} + 4bR^t{}_{\alpha t\beta} + 2b\Box R_t{}^t\Big]\right\}, \tag{1.91}$$

$$\dot{H} - \frac{k}{a^2} = \frac{-8\pi G}{2(1+2aR)}\left\{\rho_m + P_m + \frac{1}{8\pi G}\Big[(2a+b)\ddot{R} - \frac{b}{2}H\dot{R} + 4b(R^t{}_{\alpha t\beta} - R^r{}_{\alpha r\beta})R^{\alpha\beta} + 2b\Box(R_t{}^t - R_r{}^r)\Big]\right\}, \tag{1.92}$$

while the density and pressure of the effective dark-energy fluid are respectively

$$\rho_{(\text{MG})} = \frac{1}{8\pi G}\left(\frac{a}{2}R^2 - \frac{b}{2}R_{\alpha\beta}R^{\alpha\beta} + \frac{b}{2}\ddot{R} - (4a+b)H\dot{R} + 4bR^t{}_{\alpha t\beta} + 2b\Box R_t{}^t\right), \tag{1.93}$$

$$P_{(\text{MG})} = \frac{1}{8\pi G}\left(\frac{b}{2}R_{\alpha\beta}R^{\alpha\beta} - \frac{a}{2}R^2 + (2a+\frac{b}{2})\ddot{R} + (4a+\frac{b}{2})H\dot{R} - 4b\,R^r{}_{\alpha r\beta}R^{\alpha\beta} - 2b\,\Box R_r{}^r\right). \tag{1.94}$$

Just like the treatment of $f(R)$ gravity in Subsection 1.2.2, to keep the expressions of $\rho_{(\text{MG})}$, $P_{(\text{MG})}$ and the Friedmann equations (1.91) and (1.92) clear and readable, we continue using compact notations for R, $R_{\alpha\beta}R^{\alpha\beta}$, $\dot{R}$, $\ddot{R}$, $R^t{}_{\alpha t\beta}R^{\alpha\beta}$, $R^r{}_{\alpha r\beta}R^{\alpha\beta}$, $\Box R_t{}^t$ and $\Box R_r{}^r$, and one should keep in mind that for the FRW metric Eq.(1.6), these geometric quantities are already known and can be fully expanded into higher-derivative and nonlinear terms of H or a.

Quadratic gravity is one of the earliest modified gravities; it dates back to late 1970s and was employed to help quantize gravity [58]. In this thesis, quadratic gravity will be involved in Chapter 3 as a special example of $f(R, R_{\alpha\beta}R^{\alpha\beta}, R_{\alpha\mu\beta\nu}R^{\alpha\mu\beta\nu}, \mathscr{L}_m)$ gravity. Moreover, Chapters 3 and 4 will involve the gravitational thermodynamics of the FRW Universe governed by quadratic gravity, including the derivation of Eqs.(1.91) and (1.92) on the cosmological apparent horizon, and proofs of the standard and generalized second laws of thermodynamics for the Universe enclosed by different horizons.

1.2.4 $f(R,\mathcal{G})$ gravity

When discussing Lovelock's theorem in Subsection 1.2.1, we showed that an isolated Gauss-Bonnet invariant $\int d^4x\sqrt{-g}\,\mathcal{G}$ does not affect the field equation. However, things become different for generalized

$\mathcal{G}-$dependence. As an example, consider the generalized Gauss-Bonnet gravity given by the action [43]

$$\mathcal{I} = \int d^4x\sqrt{-g}\Big[f(R,\mathcal{G}) + 16\pi G\mathscr{L}_m\Big], \tag{1.95}$$

where $f(R,\mathcal{G})$ is a generic function of the Ricci scalar R and the Gauss-Bonnet invariant $\mathcal{G}$. Variation of the $f(R,\mathcal{G})$ action leads to

$$\begin{aligned}\delta\mathcal{I} &= \int d^4x\Big[\sqrt{-g}\cdot\delta f(R,\mathcal{G}) + f(R,\mathcal{G})\cdot\delta\sqrt{-g} + 16\pi G\cdot\delta\Big(\sqrt{-g}\mathscr{L}_m\Big)\Big]\\ &= \int d^4x\,\sqrt{-g}\Big[\frac{f_R\cdot\delta R}{\delta g^{\mu\nu}} + \frac{f_{\mathcal{G}}\cdot\delta\mathcal{G}}{\delta g^{\mu\nu}} - \frac{1}{2}g_{\mu\nu}f - 8\pi G T^{(m)}_{\mu\nu}\Big]\delta g^{\mu\nu}\,,\end{aligned} \tag{1.96}$$

where $f_R = f_R(R,\mathcal{G}) \coloneqq df(R,\mathcal{G})/dR$, and $f_{\mathcal{G}} = f_{\mathcal{G}}(R,\mathcal{G}) \coloneqq df(R,\mathcal{G})/dR$.

Following the standard procedures of variational derivative as before, we have $\delta\Big(\sqrt{-g}f_RR\Big)/\delta g^{\mu\nu} \cong f_RR_{\mu\nu} + (g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu)f_R$. Moreover, $f_{\mathcal{G}}\cdot\delta\mathcal{G} = f_{\mathcal{G}}\cdot\Big(\delta R^2 - 4\delta R_{\alpha\beta}R^{\alpha\beta} + \delta R_{\alpha\mu\beta\nu}R^{\alpha\mu\beta\nu}\Big)$, with

$$f_{\mathcal{G}}\cdot\frac{\delta R^2}{\delta g^{\mu\nu}} \cong 2f_{\mathcal{G}}RR_{\mu\nu} + 2\Big(g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu\Big)\left(f_{\mathcal{G}}R\right)\,, \tag{1.97}$$

$$f_{\mathcal{G}}\cdot\frac{\delta R_{\alpha\beta}R^{\alpha\beta}}{\delta g^{\mu\nu}} \cong 2f_{\mathcal{G}}R_\mu{}^\alpha R_{\alpha\nu} + \Box\Big(f_{\mathcal{G}}R_{\mu\nu}\Big) - \nabla_\alpha\nabla_\nu\Big(f_{\mathcal{G}}R_\mu{}^\alpha\Big) - \nabla_\alpha\nabla_\mu\left(f_{\mathcal{G}}R_\nu{}^\alpha\right) + g_{\mu\nu}\nabla_\alpha\nabla_\beta\Big(f_{\mathcal{G}}R^{\alpha\beta}\Big)\,, \tag{1.98}$$

$$f_{\mathcal{G}}\cdot\frac{\delta R_{\alpha\mu\beta\nu}R^{\alpha\mu\beta\nu}}{\delta g^{\mu\nu}} \cong 2f_{\mathcal{G}}R_{\mu\alpha\beta\gamma}R_\nu{}^{\alpha\beta\gamma} + 4\nabla^\beta\nabla^\alpha\Big(f_{\mathcal{G}}R_{\alpha\mu\beta\nu}\Big)\,, \tag{1.99}$$

where total-derivative terms have been removed. Recall that besides Eqs.(1.87) and (1.88), the second Bianchi identity also has the following implications which transform the derivative of a high-rank curvature tensor into those of lower-rank tensors plus nonlinear algebraic terms:

$$\nabla^\alpha R_{\alpha\mu\beta\nu} = \nabla_\beta R_{\mu\nu} - \nabla_\nu R_{\mu\beta} \tag{1.100}$$

$$\nabla^\alpha R_{\alpha\beta} = \frac{1}{2}\nabla_\beta R \tag{1.101}$$

$$\nabla^\beta\nabla^\alpha R_{\alpha\mu\beta\nu} = \Box R_{\mu\nu} - \frac{1}{2}\nabla_\mu\nabla_\nu R + R_{\alpha\mu\beta\nu}R^{\alpha\beta} - R_\mu{}^\alpha R_{\alpha\nu}\,. \tag{1.102}$$

Using Eqs.(1.87), (1.88) and (1.100)-(1.102) to expand the second-order covariant derivatives in Eqs.(1.97)-(1.99), and after some algebra, we finally obtain

$$\begin{aligned}f_{\mathcal{G}}\cdot\frac{\delta\mathcal{G}}{\delta g^{\mu\nu}} \coloneqq \mathcal{H}^{(\mathrm{GB})}_{\mu\nu} &= f_{\mathcal{G}}\Big(2RR_{\mu\nu} - 4R_\mu{}^\alpha R_{\alpha\nu} - 4R_{\alpha\mu\beta\nu}R^{\alpha\beta} + 2R_{\mu\alpha\beta\gamma}R_\nu{}^{\alpha\beta\gamma}\Big) + 2R\Big(g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu\Big)f_{\mathcal{G}}\\ &\quad -4R_{\mu\nu}\Box f_{\mathcal{G}} + 4R_\mu{}^\alpha\nabla_\alpha\nabla_\nu f_{\mathcal{G}} + 4R_\nu{}^\alpha\nabla_\alpha\nabla_\mu f_{\mathcal{G}} - 4g_{\mu\nu}R^{\alpha\beta}\nabla_\alpha\nabla_\beta f_{\mathcal{G}} + 4R_{\alpha\mu\beta\nu}\nabla^\beta\nabla^\alpha f_{\mathcal{G}}\,,\end{aligned} \tag{1.103}$$

where unlike Eqs.(1.97)-(1.99), the second-order derivatives $\{\Box, \nabla_\alpha\nabla_\nu, \mathrm{etc}\}$ now only act on $f_{\mathcal{G}}$. Recall that the Bach-Lanczos tensor vanishes identically in four dimensions, as in Eq.(1.66), so $2RR_{\mu\nu} - 4R_\mu{}^\alpha R_{\alpha\nu} -$

$4R_{\alpha\mu\beta\nu}R^{\alpha\beta} + 2R_{\mu\alpha\beta\gamma}R_{\nu}{}^{\alpha\beta\gamma} = \frac{1}{2}\mathcal{G}g_{\mu\nu}$, which simplifies Eq.(1.103) into

$$\begin{aligned}\mathcal{H}_{\mu\nu}^{(\mathrm{GB})} = \frac{1}{2}f_{\mathcal{G}}\mathcal{G}g_{\mu\nu} + 2R\left(g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu\right)f_{\mathcal{G}} - 4R_{\mu\nu}\Box f_{\mathcal{G}} + 4R_{\mu}{}^{\alpha}\nabla_\alpha\nabla_\nu f_{\mathcal{G}} \\ +4R_{\nu}{}^{\alpha}\nabla_\alpha\nabla_\mu f_{\mathcal{G}} - 4g_{\mu\nu}R^{\alpha\beta}\nabla_\alpha\nabla_\beta f_{\mathcal{G}} + 4R_{\alpha\mu\beta\nu}\nabla^\beta\nabla^\alpha f_{\mathcal{G}}\,,\end{aligned} \tag{1.104}$$

whose trace is

$$g^{\mu\nu}H_{\mu\nu}^{(\mathrm{GB})} = f_{\mathcal{G}}\mathcal{G} + 2R\Box f_{\mathcal{G}} - 4R^{\alpha\beta}\nabla_\alpha\nabla_\beta f_{\mathcal{G}}\,. \tag{1.105}$$

Thus, the field equation of $f(R,\mathcal{G})$ gravity reads

$$f_R\,R_{\mu\nu} - \frac{1}{2}f\,g_{\mu\nu} + (g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu)\,f_R + \mathcal{H}_{\mu\nu}^{(\mathrm{GB})} \;=\; 8\pi G\,T_{\mu\nu}^{(m)}\,, \tag{1.106}$$

where $\{f, f_R, f_{\mathcal{G}}\}$ are all functions of $(R,\mathcal{G})$.

In the extant literature, the effects of the generalized and thus nontrivial Gauss-Bonnet dependence for the field equations are generally depicted in the form analogous to Eq.(1.103), such as the string-inspired Gauss-Bonnet effective dark energy [50] with $\mathscr{L} = \frac{1}{16\pi G}R - \frac{\gamma}{2}\nabla_\mu\varphi\nabla^\mu\varphi - V(\varphi) + f(\varphi)\mathcal{G}$, as well as the $\mathscr{L} = R + f(\mathcal{G}) + 16\pi G$ [42], $\mathscr{L} = f(R,\mathcal{G}) + 16\pi\mathscr{L}_m$ [43] and $f(R,\mathcal{G},\mathscr{L}_m)$ [60] generalized Gauss-Bonnet gravities. Here we emphasize that the Gauss-Bonnet effects therein could all be simplified into similar forms of Eq.(1.104) via our method.

The generalized $\mathcal{G}$ dependence is very important to this thesis. For example, in Chapter 3, $\mathscr{L} = f(R,\mathcal{G})+16\pi\mathscr{L}_m$ gravity will be extended into $\mathscr{L} = f(R,\mathcal{G},\mathscr{L}_m)$ gravity that allows for nonminimal curvature couplings (see also Subsection 1.2.10), and the smooth transition from $\mathscr{L} = f(R, R_{\alpha\beta}R^{\alpha\beta}, R_{\alpha\mu\beta\nu}R^{\alpha\mu\beta\nu}, \mathscr{L}_m)$ gravity to $\mathscr{L} = f(R,\mathcal{G},\mathscr{L}_m)$ gravity will be derived. In Chapters 4 and 5, gravitational thermodynamics of the Universe governed by $\mathscr{L} = f(R,\mathcal{G}) + 16\pi\mathscr{L}_m$ gravity will be involved. Moreover, in Chapters 6 and 7, Lovelock-Brans-Dicke gravity will be developed and the applications to traversable wormholes will be extensively discussed, where the nonminimal coupling between a scalar field and $\mathcal{G}$ will play a key role.

1.2.5 Generalized Brans-Dicke gravity with self-interaction potential

So far, we have looked into $f(R)$, quadratic, and $f(R,\mathcal{G})$ gravities, which are all fourth-order theories. In this subsection, we will consider the modification of GR by a scalar field which serves as an extra physical degree of freedom. Perhaps the best known theory of this type is Brans-Dicke gravity with action [48]

$$\mathcal{I} \;=\; \int d^4x\sqrt{-g}\left(\phi R - \frac{\omega_{\mathrm{BD}}}{\phi}\,\nabla_\alpha\phi\nabla^\alpha\phi + 16\pi\mathscr{L}_m\right), \tag{1.107}$$

where the constant ω_{BD} refers to the Brans-Dicke parameter. However, we choose to move a step further and consider the following generalized Brans-Dicke gravity,

$$\mathcal{I} \;=\; \int d^4x\sqrt{-g}\left(\phi R - \frac{\omega(\phi)}{\phi}\,\nabla_\alpha\phi\nabla^\alpha\phi - V(\phi) + 16\pi G\mathscr{L}_m\right), \tag{1.108}$$

which has a Brans-Dicke field $\omega(\phi)$ in place of $\omega_{\rm BD}$ and a self-interaction potential $V(\phi)$. Here Eq.(1.108) has adopted the convention $16\pi G\mathscr{L}_m$ with a Newtonian constant G, as opposed to $16\pi\mathscr{L}_m$ in Eq.(1.107) which encodes G into ϕ^{-1}, so as to facilitate the comparison with $f(R)$ gravity in next subsection. Varying Eq.(1.108) with respect to the inverse metric, one obtains

$$\delta\mathcal{I} = \int d^4x\sqrt{-g}\left[\phi\frac{\delta R}{\delta g^{\mu\nu}} - \frac{\omega}{\phi}\nabla_\alpha\phi\nabla_\beta\phi\frac{\delta g^{\alpha\beta}}{\delta g^{\mu\nu}} - \frac{1}{2}\Big(\phi R - \frac{\omega}{\phi}\nabla_\alpha\phi\nabla^\alpha\phi - V\Big)g_{\mu\nu} - 8\pi G T^{(m)}_{\mu\nu}\right]\delta g^{\mu\nu}\,. \tag{1.109}$$

Thus, the gravitational field equation is

$$\phi\Big(R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu}\Big) - \frac{\omega}{\phi}\Big(\nabla_\mu\phi\nabla_\nu\phi - \frac{1}{2}g_{\mu\nu}\nabla_\alpha\phi\nabla^\alpha\phi\Big) + \Big(g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu\Big)\phi + \frac{1}{2}Vg_{\mu\nu} = 8\pi T^{(m)}_{\mu\nu}\,. \tag{1.110}$$

In addition to the metric tensor, the scalar field ϕ in Eq.(1.108) serves as a second physical field. Variation of Eq.(1.108) with respect to ϕ yields the *kinematical* wave equation

$$\frac{2\omega}{\phi}\Box\phi \;=\; -R - \frac{\phi\omega_\phi - \omega}{\phi^2}\cdot\nabla_\alpha\phi\nabla^\alpha\phi + V_\phi\,, \tag{1.111}$$

with $\Box\phi = g^{\alpha\beta}\nabla_\alpha\nabla_\beta\phi = \frac{1}{\sqrt{-g}}\partial_\alpha\Big(\sqrt{-g}\,g^{\alpha\beta}\partial_\beta\phi\Big)$, $\omega_\phi = \omega_\phi(\phi) := d\omega(\phi)/d\phi$, and $V_\phi = V_\phi(\phi) := dV(\phi)/d\phi$. By the trace of the field equation (1.110), $-R = \dfrac{1}{\phi}\Big(8\pi T^{(m)} - \dfrac{\omega}{\phi}\nabla_\alpha\phi\nabla^\alpha\phi - 3\Box\phi - 2V\Big)$, Eq.(1.111) can be recast into the following *dynamical* wave equation or Klein-Gordon equation

$$(2\omega+3)\Box\phi = 8\pi T^{(m)} - \omega_\phi\cdot\nabla_\alpha\phi\nabla^\alpha\phi - 2V + \phi V_\phi\,, \tag{1.112}$$

which explicitly relates the propagation of $\phi(x^\alpha)$ to the trace $T^{(m)}$ of the matter tensor for the stress-energy-momentum distribution.

In the spirit of constructing the effective dark energy via $R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} = 8\pi G_{\rm eff}\Big(T^{(m)}_{\mu\nu} + T^{(\rm MG)}_{\mu\nu}\Big)$, the field equation (1.110) can be rewritten as

$$R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} = 8\pi\frac{G}{\phi}T^{(m)}_{\mu\nu} + \frac{1}{\phi}\Big(\nabla_\mu\nabla_\nu - g_{\mu\nu}\Box\Big)\phi + \frac{\omega}{\phi^2}\Big(\nabla_\mu\phi\nabla_\nu\phi - \frac{1}{2}g_{\mu\nu}\nabla_\alpha\phi\nabla^\alpha\phi\Big) - \frac{1}{2\phi}Vg_{\mu\nu}\,, \tag{1.113}$$

so $G_{\rm eff} = G/\phi$ in accordance with the coefficient of $T^{(m)}_{\mu\nu}$, and $T^{(\rm MG)}_{\mu\nu} = (8\pi G)^{-1}\Big[\Big(\nabla_\mu\nabla_\nu - g_{\mu\nu}\Box\Big)\phi + \frac{\omega}{\phi}\Big(\nabla_\mu\phi\nabla_\nu\phi - \frac{1}{2\phi}g_{\mu\nu}\nabla_\alpha\phi\nabla^\alpha\phi\Big) - \frac{1}{2}Vg_{\mu\nu}\Big]$. Substituting the FRW metric into Eq.(1.113), one obtains the modified Friedmann equations

$$H^2 + \frac{k}{a^2} \;=\; \frac{8\pi}{3}\frac{G}{\phi}\rho_m + \frac{1}{3\phi}\Big(-3H\dot\phi + \frac{\omega}{2}\dot\phi^2 + \frac{1}{2}V\Big), \tag{1.114}$$

$$\dot H - \frac{k}{a^2} \;=\; -4\pi\frac{G}{\phi}\Big(\rho_m + P_m\Big) - \frac{1}{2\phi}\Big(\ddot\phi + 5H\dot\phi + \omega\dot\phi^2 - V\Big), \tag{1.115}$$

while the density and pressure of the generalized Brans-Dicke effective dark-energy fluid are respectively

$$\rho_{(\mathrm{MG})} = \frac{1}{8\pi G}\left(\frac{\omega}{2\phi}\dot{\phi}^2 - 3H\dot{\phi} + \frac{1}{2}V\right) \quad \text{with} \quad P_{(\mathrm{MG})} = \frac{1}{8\pi G}\left(-\frac{\omega}{2\phi}\dot{\phi}^2 + \ddot{\phi} + 2H\dot{\phi} - \frac{1}{2}V\right). \tag{1.116}$$

Moreover, the scalar field's dynamical wave equation (1.112) under the FRW metric becomes

$$(2\omega+3)\Big(\ddot{\phi} + 3H\dot{\phi}\Big) = 8\pi(\rho_m - 3P_m) - \dot{\phi}^2\omega_\phi - \phi V_\phi + 2V\,. \tag{1.117}$$

Here note that Eq.(1.117) does not mean that ϕ propagates the same way in vacuum ($\rho_m = 0 = P_m$) and in radiation ($\rho_m = 3P_m$). H differs for these two situations according to the first Friedmann equation (1.114).

1.2.6 Equivalence between $f(R)$ and nondynamical Brans-Dicke gravity

One might have a feeling of familiarity when going through the generalized Brans-Dicke gravity – yes, its behaviours are pretty similar to $\mathscr{L} = f(R) + 16\pi G\mathscr{L}_m$ gravity as discussed in Subsection 1.2.2. In fact, removing the kinetic term of ϕ in Eq.(1.108) so that $\mathcal{I} = \int d^4x\sqrt{-g}\,[\phi R - V(\phi) + 16\pi G\mathscr{L}_m]$, and comparing its field equation with that of $f(R)$ gravity, one has

$$\begin{aligned}\phi R_{\mu\nu} - \frac{1}{2}\Big(\phi R - V(\phi)\Big)g_{\mu\nu} + \Big(g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu\Big)\phi &= 8\pi G T^{(m)}_{\mu\nu},\\ f_R\, R_{\mu\nu} - \frac{1}{2}f(R)\, g_{\mu\nu} + \Big(g_{\mu\nu}\,\Box - \nabla_\mu\nabla_\nu\Big)f_R &= 8\pi G\, T^{(m)}_{\mu\nu}\,.\end{aligned} \tag{1.118}$$

Clearly, these two equations become identical for the following relations:

$$f_R = \phi \quad \text{and} \quad f(R) = \phi R - V(\phi) \quad \text{or} \quad f_R\,R - f(R) = V(\phi)\,. \tag{1.119}$$

More rigourously, introduce an auxiliary field $\chi = \chi(x^\alpha)$ and consider the following dynamically equivalent action of $f(R)$ gravity,

$$\mathcal{I} = \int d^4x\,\sqrt{-g}\Big[f(\chi) + f_\chi\cdot(R-\chi) + 16\pi G\mathscr{L}_m\Big], \tag{1.120}$$

whose variational derivative with respect to χ yields the constraint

$$f_{\chi\chi}(R-\chi) = 0\,, \tag{1.121}$$

with $f_\chi = f_\chi(\chi) \coloneqq df(\chi)/d\chi$ and $f_{\chi\chi} = f_{\chi\chi}(\chi) \coloneqq d^2f(\chi)/d\chi^2$. If $f_{\chi\chi}$ does not vanish identically, Eq.(1.121) leads to $\chi = R$. Redefining the χ field into the scalar field $\phi = f_\chi$ and introducing the potential $V(\phi) = \phi\cdot R(\phi) - f\Big(R(\phi)\Big)$, then $\mathscr{L} = f(R) + 16\pi G\mathscr{L}_m$ gravity becomes equivalent to $\mathscr{L} = \phi R - V(\phi) + 16\pi G\mathscr{L}_m$ gravity.

That is to say, the $f(R)$ fourth-order modified gravity in Subsection 1.2.2 and the generalized Brans-Dicke alternative gravity in Subsection 1.2.5 are not totally independent. Instead, the former can be regarded as a subclass of the latter with a vanishing Brans-Dicke function $\omega(\phi) \equiv 0$ for the kinetic term $\nabla_\alpha\phi\nabla^\alpha\phi$, and the equivalence is realized by Eq.(1.119). For example, applying the replacements $f_R \mapsto \phi$ and $f_R R - f(R) \mapsto V(\phi)$ to Subsection 1.2.2, one obtains the modified Friedmann equations

$$H^2 + \frac{k}{a^2} = \frac{8\pi}{3}\frac{G}{\phi}\rho_m + \frac{1}{3\phi}\left(-3H\dot{\phi} + \frac{1}{2}V\right) \quad \text{and} \quad \dot{H} - \frac{k}{a^2} = -4\pi\frac{G}{\phi}\left(\rho_m + P_m\right) - \frac{1}{2\phi}\left(\ddot{\phi} + 5H\dot{\phi} - V\right), \tag{1.122}$$

along with

$$\rho_{(\text{MG})} = \frac{1}{8\pi G}\left(-3H\dot{\phi} + \frac{1}{2}V\right) \quad \text{and} \quad P_{(\text{MG})} = \frac{1}{8\pi G}\left(\ddot{\phi} + 2H\dot{\phi} - \frac{1}{2}V\right), \tag{1.123}$$

which match Eqs.(1.114)~(1.116) with $\omega(\phi) \equiv 0$.

1.2.7 Scalar-tensor-chameleon gravity

The generalized Brans-Dicke gravity can be further extended into the scalar-tensor-chameleon gravity, which is given by the action (e.g. [61], and the usage of "chameleon" will be clarified soon)

$$\mathcal{I} = \int d^4x\sqrt{-g}\Big[F(\phi)R - Z(\phi)\cdot\nabla_\alpha\phi\nabla^\alpha\phi - 2U(\phi) + 16\pi G E(\phi)\mathscr{L}_m\Big], \tag{1.124}$$

where $\{F(\phi), Z(\phi), U(\phi), E(\phi)\}$ (and $\{F, Z, U, E\}$ for brevity) are arbitrary functions of the scalar ϕ, and $E(\phi)$ is the "chameleon" function nonminimally coupled to the matter Lagrangian density $\mathscr{L}_m$. Vary the action with respect to the inverse metric,

$$\begin{aligned}\delta\mathcal{I} = \int d^4x\sqrt{-g}\Bigg\{&F(\phi)\frac{\delta R}{\delta g^{\mu\nu}} - \frac{1}{2}\Big[F(\phi)R - Z(\phi)\cdot\nabla_\alpha\phi\nabla^\alpha\phi - 2U(\phi)\Big]g_{\mu\nu}\\ &-Z(\phi)\nabla_\alpha\phi\nabla_\beta\phi\frac{\delta g^{\alpha\beta}}{\delta g^{\mu\nu}} + \frac{16\pi G E(\phi)}{\sqrt{-g}}\frac{\delta\left(\sqrt{-g}\mathscr{L}_m\right)}{\delta g^{\mu\nu}}\Bigg\}\delta g^{\mu\nu},\end{aligned} \tag{1.125}$$

and it is easy to find the gravitational field equation:

$$F\Big(R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu}\Big) + (g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu)F - Z\left(\nabla_\mu\phi\nabla_\nu\phi - \frac{1}{2}g_{\mu\nu}\partial_\alpha\phi\,\partial^\alpha\phi\right) + Ug_{\mu\nu} = 8\pi G E T^{(m)}_{\mu\nu}\,. \tag{1.126}$$

On the other hand, the wave equation $\delta\mathcal{I}/\delta\phi = 0$ reads

$$2Z\Box\phi = 2U_\phi - F_\phi R - Z_\phi\cdot\nabla_\alpha\phi\nabla^\alpha\phi - E_\phi\mathscr{L}_m\,, \tag{1.127}$$

where $U_\phi = U_\phi(\phi) = dU(\phi)/d\phi$, and similarly for $\{F_\phi, Z_\phi, E_\phi\}$. Eqs.(1.126)~(1.127) indicate that due to the presence of $E(\phi)$, the net gravitational effects of $T^{(m)}_{\mu\nu}$ becomes reliant on the distribution of the scalar field, while the wave equation explicitly depends on the physical matter $\mathscr{L}_m$ (or $T^{(m)} = g^{\mu\nu}T^{(m)}_{\mu\nu}$ if one substitutes the trace of Eq.(1.126) into Eq.(1.127) to replace R). That is to say, both the field and the wave equations become *environment-dependent*: they vary among different cosmic epoches as the dominant matter changes and ϕ evolves, and they alters in different regions of the Universe. This is why the theory under consideration is dubbed scalar-tensor-chameleon gravity.

To construct the effective dark energy, we rearrange Eq.(1.126) into the form of $R_{\mu\nu}-\frac{1}{2}Rg_{\mu\nu} = 8\pi G_{\rm eff}\Big(T^{(m)}_{\mu\nu} + T^{\rm (MG)}_{\mu\nu}\Big)$ as

$$R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} = 8\pi G\frac{E}{F}T^{(m)}_{\mu\nu} + \frac{1}{F}\Big(\nabla_\mu\nabla_\nu - g_{\mu\nu}\Box\Big)F + \frac{Z}{F}\Big(\nabla_\mu\phi\nabla_\nu\phi - \frac{1}{2}g_{\mu\nu}\nabla_\alpha\phi\nabla^\alpha\Big) - \frac{U}{F}g_{\mu\nu}\,, \tag{1.128}$$

so one can observe that $G_{\rm eff} = \frac{E}{F}G$ and $T^{\rm (MG)}_{\mu\nu} = \frac{1}{8\pi GE}\Big[\Big(\nabla_\mu\nabla_\nu - g_{\mu\nu}\Box\Big)F + Z\Big(\nabla_\mu\phi\nabla_\nu\phi - \frac{1}{2}g_{\mu\nu}\nabla_\alpha\phi\nabla^\alpha\phi\Big) - Ug_{\mu\nu}\Big]$. Substitution of the FRW metric into Eq.(1.128) leads to the modified Friedmann equations

$$H^2 + \frac{k}{a^2} = \frac{8\pi}{3}\frac{GE}{F}\rho_m + \frac{1}{3F}\Big(-3HF_\phi\,\dot\phi + \frac{1}{2}Z\,\dot\phi^2 + U\Big), \tag{1.129}$$

$$\dot H - \frac{k}{a^2} = -4\pi\frac{GE}{F}\Big(\rho_m + P_m\Big) - \frac{1}{2F}\Big(F_\phi\,\ddot\phi + F_{\phi\phi}\,\dot\phi^2 + 5HF_\phi\,\dot\phi - Z\,\dot\phi^2 - 2U\Big), \tag{1.130}$$

where we have used $\dot F = F_\phi\dot\phi$ and $\ddot F = F_\phi\ddot\phi + F_{\phi\phi}\,\dot\phi^2$, while the energy density and pressure for $T^{\mu\,\rm (MG)}_{\ \nu} = {\rm diag}[-\rho_{\rm (MG)}, P_{\rm (MG)}, P_{\rm (MG)}, P_{\rm (MG)}]$ are

$$\begin{aligned} \rho_{\rm (MG)} &= \frac{1}{8\pi G\,E}\Big(-3HF_\phi\dot\phi + \frac{1}{2}Z\,\dot\phi^2 + U\Big) \\ P_{\rm (MG)} &= \frac{1}{8\pi G\,E}\Big(F_\phi\ddot\phi + F_{\phi\phi}\,\dot\phi^2 + 2HF_\phi\dot\phi - \frac{1}{2}Z\,\dot\phi^2 - U\Big). \end{aligned} \tag{1.131}$$

In the absence of the chameleon function, $E(\phi) \equiv 1$, $E_\phi = 0$, and with $F(\phi) \mapsto \phi$, $F_\phi \mapsto 1$, $F_{\phi\phi} \mapsto 0$, $Z(\phi) \mapsto \frac{\omega(\phi)}{\phi}$, $U(\phi) \mapsto \frac{1}{2}V(\phi)$, we recover the situation of generalized Brans-Dicke gravity in Subsection 1.2.5.

Note that to date it is still not clear whether cosmic acceleration arises from new physical fields or new laws of gravity, and scalar-tensor theories have the advantage of taking both possibilities into account. To move one step further, Horndeski [51] or Galileon [52] gravity is the most general scalar-tensor theory that contains at most second-order derivatives of the scalar field. For cosmological interest, the covariant Galileon gravity has the action [53]

$$\mathcal{I} = \int d^4x\sqrt{-g}\Big(R - \frac{c_1}{2}V(\phi) - \frac{c_2}{2}\nabla_\alpha\phi\nabla^\alpha\phi - \frac{1}{2}\sum_{i=3}^{5}c_i\mathscr{L}_i + 16\pi G\mathscr{L}_m\Big), \tag{1.132}$$

where $\{c_i\}$ are constant coefficients, and

$$\mathscr{L}_3 = 2\Box\phi\nabla_\alpha\phi\nabla^\alpha\phi/M^3\,, \tag{1.133}$$

$$\mathscr{L}_4 = \nabla_\alpha\phi\nabla^\alpha\phi\Big[2(\Box\phi)^2 - 2(\nabla_\alpha\nabla_\beta\phi)(\nabla^\alpha\nabla^\beta\phi) - \frac{1}{2}R\nabla_\alpha\phi\nabla^\alpha\phi\Big]/M^6\,, \tag{1.134}$$

$$\mathscr{L}_5 = \nabla_\alpha\phi\nabla^\alpha\phi\Big[(\Box\phi)^3 - 3(\Box\phi)(\nabla_\alpha\nabla_\beta\phi)(\nabla^\alpha\nabla^\beta\phi) + 2(\nabla_\alpha\nabla^\beta\phi)(\nabla_\beta\nabla^\gamma\phi)(\nabla_\gamma\nabla^\alpha\phi) - 6(\nabla_\alpha\phi)(\nabla^\alpha\nabla^\beta\phi)(\nabla^\gamma\phi)G_{\beta\gamma}\Big]/M^9, \tag{1.135}$$

with $M^3 = m_{\rm Pl}H_0^2$ to balance the dimensions. The full Galileon gravity is however too complicated to deal with, so in applications like best-fitting or prediction of cosmological parameters, one usually drops $\{\mathscr{L}_4, \mathscr{L}_5\}$ by setting $c_4 = c_5 = 0$, and preserves the $\{c_1, c_2, c_3\}$ terms to constitute the cubic Galileon theory.

1.2.8 A unified form of modified gravity

1.2.8.1 Field equations and modified Friedmann equations

We have looked into $f(R)$, quadratic, $f(R,\mathcal{G})$, generalized Brans-Dicke, scalar-tensor-chameleon gravities, and derived their field equations. One may have noticed that in the construction of effective dark energy for the modified Friedmann equations, they follow a similar pattern. More generally, consider modified gravities with the Lagrangian density

$$\mathscr{L} = \mathscr{L}_G(R, R_{\alpha\beta}R^{\alpha\beta}, \mathcal{R}_i\,, \vartheta\,, \nabla_\mu\vartheta\nabla^\mu\vartheta\,, \cdots) + 16\pi G\mathscr{L}_m\,, \tag{1.136}$$

where $\mathcal{R}_i = \mathcal{R}_i\,(g_{\alpha\beta}\,, R_{\mu\alpha\nu\beta}\,, \nabla_\gamma R_{\mu\alpha\nu\beta}\,, \ldots)$ refers to a generic Riemannian invariant beyond the Ricci scalar and ϑ denotes a scalarial extra degree of freedom unabsorbed by $\mathscr{L}_m$. Its field equation takes the form

$$\mathcal{H}_{\mu\nu} = 8\pi G T_{\mu\nu}^{(m)} \quad \text{with} \quad \mathcal{H}_{\mu\nu} := \frac{1}{\sqrt{-g}}\frac{\delta\left(\sqrt{-g}\,\mathscr{L}_G\right)}{\delta g^{\mu\nu}}\,, \tag{1.137}$$

where total-derivative/boundary terms should be removed in the derivation of $\mathcal{H}_{\mu\nu}$. In the spirit of constructing the effective dark energy from modified-gravity effects, Eq.(1.137) can be *intrinsically* recast into a compact GR form by isolating the $R_{\mu\nu}$ in $\mathcal{H}_{\mu\nu}$:

$$G_{\mu\nu} \equiv R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} = 8\pi G_{\rm eff}T_{\mu\nu}^{(\rm eff)} \quad \text{with} \quad \mathcal{H}_{\mu\nu} = \frac{G}{G_{\rm eff}}G_{\mu\nu} - 8\pi G T_{\mu\nu}^{(\rm MG)}\,, \tag{1.138}$$

where $T_{\mu\nu}^{(\rm eff)} = T_{\mu\nu}^{(m)} + T_{\mu\nu}^{(\rm MG)}$, and all terms beyond GR have been packed into $T_{\mu\nu}^{(\rm MG)}$ and $G_{\rm eff}$. Here $T_{\mu\nu}^{(\rm MG)}$ collects the modified-gravity nonlinear and higher-order effects, while $G_{\rm eff}$ denotes the effective gravitational coupling strength which can be directly recognized from the coefficient of the matter tensor $T_{\mu\nu}^{(m)}$ – for example, as previously shown, we have $G_{\rm eff} = G/f_R(R)$ for $f(R)$, $G_{\rm eff} = G/(1+2aR)$ for quadratic, $G_{\rm eff} = G/f_R(R,\mathcal{G})$ for $f(R,\mathcal{G})$ generalized Gauss-Bonnet, $G_{\rm eff} = G/\phi$ for (generalized) Brans-Dicke, and $G_{\rm eff} = GE(\phi)/F(\phi)$ for scalar-tensor-chameleon gravities. Moreover, $T_{\mu\nu}^{(\rm eff)}$ is assumed to be an effective perfect-fluid content,

$$T^{\mu}{}_{\nu}^{(\rm eff)} = {\rm diag}\left[-\rho_{\rm eff}, P_{\rm eff}, P_{\rm eff}, P_{\rm eff}\right] \quad \text{with} \quad P_{\rm eff}/\rho_{\rm eff} =: w_{\rm eff}, \tag{1.139}$$

along with $\rho_{\rm eff} = \rho_m + \rho_{(\rm MG)}$ and $P_{\rm eff} = P_m + P_{(\rm MG)}$.

Substituting the FRW metric Eq.(1.6) and the effective cosmic fluid Eq.(1.139) into the field equation

(1.138), one could obtain the modified Friedmann equations

$$\begin{aligned} H^2+\frac{k}{a^2} &= \frac{8\pi G_{\text{eff}}}{3}\Big[\rho_m+\rho_{(\text{MG})}\Big] \quad \text{and} \\ \dot{H}-\frac{k}{a^2} = -4\pi G_{\text{eff}}\Big[\rho_m+P_m+\rho_{(\text{MG})}+P_{(\text{MG})}\Big] &\quad \text{or} \quad 2\dot{H}+3H^2+\frac{k}{a^2} = -8\pi G_{\text{eff}}\Big[\rho_m+\rho_{(\text{MG})}\Big]\,. \end{aligned} \tag{1.140}$$

Obviously, by setting $G_{(\text{eff})} = G$ and $\rho_{(\text{MG})} = 0 = P_{(\text{MG})}$, we immediately recover the standard Friedmann equations in GR. Here one should note that the FRW metric depicts the observed Universe, so it is independent of and *a priori* applies to all theories of metric gravity. That is to say, we needn't worry about whether or not the FRW metric is a solution to the modified field equations when studying the cosmology in modified gravity; it must be a solution, and if not, it is the gravity theory that fails.

1.2.8.2 Generalized energy conditions

Having derived the modified Friedmann equations, let us go back to the generic field equation (1.138). Recall that $T_{\mu\nu}^{(m)}$ has to respect a set of standard energy conditions to be physically meaningful in GR, so we cannot help but ask that are there similar restrictions to $T_{\mu\nu}^{(\text{eff})}$? The answer is yes, and $T_{\mu\nu}^{(\text{eff})}$ has to obey a set of generalized energy conditions.

In a region of a spacetime, for the expansion rate $\theta_{(\ell)}$ of a null congruence along its null tangent vector field ℓ^μ, and the expansion rate $\theta_{(u)}$ of a timelike congruence along its timelike tangent u^μ, $\theta_{(\ell)}$ and $\theta_{(u)}$ respectively satisfy the Raychaudhuri equations [6]

$$\ell^\mu\nabla_\mu\theta_{(\ell)} = \frac{d\theta_{(\ell)}}{d\lambda} = \kappa_{(\ell)}\theta_{(\ell)} - \frac{1}{2}\,\theta_{(\ell)}^2 - \sigma_{\mu\nu}^{(\ell)}\sigma_{(\ell)}^{\mu\nu} + \omega_{\mu\nu}^{(\ell)}\omega_{(\ell)}^{\mu\nu} - R_{\mu\nu}\ell^\mu\ell^\nu\,, \tag{1.141}$$

$$u^\mu\nabla_\mu\theta_{(u)} = \frac{d\theta_{(u)}}{d\tau} = \kappa_{(u)}\theta_{(u)} - \frac{1}{3}\,\theta_{(u)}^2 - \sigma_{\mu\nu}^{(u)}\sigma_{(u)}^{\mu\nu} + \omega_{\mu\nu}^{(u)}\omega_{(u)}^{\mu\nu} - R_{\mu\nu}u^\mu u^\nu\,. \tag{1.142}$$

The inaffinity coefficients are zero $\kappa_{(\ell)} = 0 = \kappa_{(u)}$ under affine parameterizations, the twist vanishes $\omega_{\mu\nu}\omega^{\mu\nu} = 0$ for hypersurface-orthogonal foliations, and being spatial tensors $\left(\sigma_{\mu\nu}^{(\ell)}\ell^\mu = 0 = \sigma_{\mu\nu}^{(u)}u^\mu\right)$ the shears always satisfy $\sigma_{\mu\nu}\sigma^{\mu\nu} \geq 0$. Thus, to guarantee $d\theta_{(\ell)}/d\lambda \leq 0$ and $d\theta_{(u)}/d\tau \leq 0$ under all circumstances – even in the occasions $\theta_{(\ell)} = 0 = \theta_{(u)}$, so that the congruences focus and gravity is always an attractive force, the following geometric nonnegativity conditions are expected to hold:

$$R_{\mu\nu}\ell^\mu\ell^\nu \geq 0 \qquad , \qquad R_{\mu\nu}u^\mu u^\nu \geq 0\,. \tag{1.143}$$

Note that although this is the most popular approach to derive Eq.(1.143) for its straightforwardness and simplicity, it is not perfect. In general $\theta_{(\ell)}$ and $\theta_{(u)}$ are nonzero and one could only obtain $\frac{1}{2}\theta_{(\ell)}^2 + R_{\mu\nu}\ell^\mu\ell^\nu \geq 0$ and $\frac{1}{3}\theta_{(u)}^2 + R_{\mu\nu}u^\mu u^\nu \geq 0$. Thus, it is only safe to say that Eq.(1.143) provides the sufficient rather than necessary conditions to ensure $d\theta_{(\ell)}/d\lambda \leq 0$ and $d\theta_{(u)}/d\tau \leq 0$. Fortunately, this imperfectness is not a disaster and does not negate the conditions in Eq.(1.143); for example, one can refer to Ref. [62] for a rigorous derivation of the first inequality in Eq.(1.143) from the Virasoro constraint in the worldsheet string theory.

Following Eq.(1.138) along with its trace equation $R = -8\pi G_{\text{eff}}T^{(\text{eff})}$ and the equivalent form $R_{\mu\nu} = 8\pi G_{\text{eff}}\left(T_{\mu\nu}^{(\text{eff})} - \frac{1}{2}g_{\mu\nu}T^{(\text{eff})}\right)$, the geometric nonnegativity conditions in Eq.(1.143) can be translated into the generalized null and strong energy conditions (GNEC and GSEC for short)

$$G_{\text{eff}} T^{(\text{eff})}_{\mu\nu}\, \ell^\mu \ell^\nu \geq 0 \quad (\text{GNEC}) \quad , \quad G_{\text{eff}} \left(T^{(\text{eff})}_{\mu\nu} u^\mu u^\nu + \frac{1}{2} T^{(\text{eff})} \right) \geq 0 \quad (\text{GSEC}), \tag{1.144}$$

where $\ell^\mu \ell_\mu = 0$ for the GNEC, and $u_\mu u^\mu = -1$ in the GSEC for compatibility with the metric signature $(-,+++)$. We further supplement Eq.(1.144) by the generalized weak energy condition

$$G_{\text{eff}} T^{(\text{eff})}_{\mu\nu} u^\mu u^\nu \geq 0 \quad (\text{GWEC}), \tag{1.145}$$

and the generalized dominant energy condition (GDEC) that $G_{\text{eff}} T^{(\text{eff})}_{\mu\nu} u^\mu u^\nu \geq 0$ with $G_{\text{eff}} T^{(\text{eff})}_{\mu\nu} u^\mu$ being a causal vector.

Note that for the common pattern of field equations in modified gravities, we have chosen to adopt Eq.(1.138) rather than $R_{\mu\nu} - \frac{1}{2} R g_{\mu\nu} = 8\pi G \widehat{T}^{(\text{eff})}_{\mu\nu}$, where G is Newton's constant. That is to say, we do not absorb G_{eff} into $T^{(\text{eff})}_{\mu\nu}$ so that $G_{\text{eff}} T^{(\text{eff})}_{\mu\nu} = G \widehat{T}^{(\text{eff})}_{\mu\nu}$; as a consequence, G_{eff} shows up in the generalized energy conditions as well. This is because the effective matter-gravity coupling strength G_{eff} plays important roles in many physics problems, such as the Wald entropy of black-hole horizons [63], although the meanings and applications of G_{eff} have not been fully understood (say the relations between G_{eff} and the weak, Einstein, and strong equivalence principles).

For the FRW Universe, a unified formulation to derive the Friedmann equations from (non)equilibrium thermodynamics on the apparent horizon will be developed in Chapter 4, while in Chapter 5, after systematic restudies of the FRW cosmological thermodynamics by requiring its compatibility with the holographic-style gravitational equations, possible solutions will be proposed for the confusions regarding the temperature of the apparent horizon and the failure of the second law of thermodynamics. Both chapters are based on $R_{\mu\nu} - \frac{1}{2} R g_{\mu\nu} = 8\pi G_{\text{eff}} T^{(\text{eff})}_{\mu\nu}$, and these unified formulations will be applied to $f(R)$, quadratic, $f(R, \mathcal{G})$ generalized Gauss-Bonnet, generalized Brans-Dicke, scalar-tensor-chameleon, and dynamical Chern-Simons gravities.

1.2.9 More insights into $T^{(m)}_{\mu\nu}$ and energy-momentum conservation

In the theoretical structures of modified gravity, a remaining problem of concern is convariance of the field equations and validity of the local conservation equation $\nabla^\mu T^{(m)}_{\mu\nu} = 0$ for physical matter. We will look into this problem in this subsection.

1.2.9.1 Some comments on $T^{(m)}_{\mu\nu}$

Before tackling the conservation problem, we would like to make some quick comments on $T^{(m)}_{\mu\nu}$. In fact, the matter Lagrangian density $\mathscr{L}_m$ in the Hilbert-Einstein action $\mathcal{I}_{\text{HE}}$ and consequently $T^{(m)}_{\mu\nu}$ can be rescaled into

$$\mathcal{I} = \int d^4x \sqrt{-g} \left(R + 8\lambda\pi G\, \mathscr{L}_m \right), \tag{1.146}$$

and

$$T^{(m)}_{\mu\nu} := -\frac{\lambda}{\sqrt{-g}} \frac{\delta(\sqrt{-g}\mathscr{L}_m)}{\delta g^{\mu\nu}}, \tag{1.147}$$

where $\lambda > 0$ is a constant, and one still recovers Einstein's equation $R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} = 8\pi G T^{(m)}_{\mu\nu}$. It is simply a convention to set $\lambda = 2$ in Eqs.(1.1), (1.4), and (1.21).

Also, in general $\mathscr{L}_m$ does not explicitly depend on the derivatives of the metric tensor [1], i.e. $\mathscr{L}_m = \mathscr{L}_m\left(g_{\mu\nu}, \psi_m, \partial_\mu\psi_m\right) \neq \mathscr{L}_m\left(g_{\mu\nu}, \partial_\alpha g_{\mu\nu}, \partial_{\alpha\cdots} g_{\mu\nu}, \psi_m, \partial_\mu\psi_m\right)$ where ψ_m collects the matter fields. For example, $\mathscr{L}_m = \mathscr{L}_m(g_{\mu\nu}, A_\alpha, \nabla_\beta A_\alpha) = -\frac{1}{16\pi}F_{\alpha\beta}F^{\alpha\beta}$ with $F_{\alpha\beta} \coloneqq \nabla_\alpha A_\beta - \nabla_\beta A_\alpha$ for source-free electromagnetic field, and $\mathscr{L}_m = \mathscr{L}_m(g_{\mu\nu}, \phi, \nabla_\alpha\phi) = -\frac{1}{2}g^{\alpha\beta}\nabla_\alpha\phi\nabla_\beta\phi - V(\phi)$ for a massive scalar field. With $\delta\sqrt{-g} = -\frac{1}{2}\sqrt{-g}\,g_{\mu\nu}\delta g^{\mu\nu}$, $T^{(m)}_{\mu\nu}$ defined in Eq.(1.4) can be expanded and then recast into

$$T^{(m)}_{\mu\nu} = g_{\mu\nu}\mathscr{L}_m - 2\frac{\delta\mathscr{L}_m}{\delta g^{\mu\nu}}\,. \tag{1.148}$$

Instead of Eq.(1.4) or (1.148), it had been suggested that $T^{(m)}_{\mu\nu}$ could be derived solely from the equations of motion $\frac{\partial\mathscr{L}_m}{\partial\psi_m} - \nabla_\mu\frac{\partial\mathscr{L}_m}{\partial(\partial_\mu\psi_m)} = 0$ for the ψ_m field in $\mathscr{L}_m\left(g_{\mu\nu}, \psi_m, \partial_\mu\psi_m\right)$ [65]; however, further analyses have shown that this method does not hold a general validity, and Eqs.(1.4) and (1.148) remain as the most reliable approach to $T^{(m)}_{\mu\nu}$ [66].

1.2.9.2 $\nabla^\mu T^{(m)}_{\mu\nu} = 0$ and generalized contracted Bianchi identity

During the brief review of GR in Subsection 1.1.1, we have seen that in the contravariant derivative of Einstein's equation, Bianchi's identity $\nabla^\mu\left(R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu}\right) \equiv 0$ immediately guarantees $\nabla^\mu T^{(m)}_{\mu\nu} = 0$. Similarly for $f(R)$ gravity, taking the contravariant derivative of the field equation (1.74), we find

$$\begin{aligned}
\nabla^\mu T^{(m)}_{\mu\nu} &= \nabla^\mu\Big[f_R R_{\mu\nu} - \frac{1}{2}f g_{\mu\nu} + \left(g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu\right)f_R\Big] \\
&= R_{\mu\nu}\nabla^\mu f_R + f_R\nabla^\mu R_{\mu\nu} - \frac{1}{2}f_R g_{\mu\nu}\nabla^\mu R + (\nabla_\nu\Box - \Box\nabla_\nu)f_R \\
&= R_{\mu\nu}\nabla^\mu f_R + f_R\nabla^\mu\Big(R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu}\Big) - R_{\mu\nu}\nabla^\mu f_R \;\equiv\; 0\,,
\end{aligned} \tag{1.149}$$

where we have applied $\nabla^\mu(R_{\mu\nu} - Rg_{\mu\nu}/2) = 0$ and the third-order-derivative commutation relation $(\nabla_\nu\Box - \Box\nabla_\nu)f_R = -R_{\mu\nu}\nabla^\nu f_R$. Hence, $\nabla^\mu T^{(m)}_{\mu\nu} = 0$ holds in $\mathscr{L} = f(R) + 16\pi G\mathscr{L}_m$ gravity.

For quadratic and $f(R, \mathcal{G})$ gravities in Subsections 1.2.3 and 1.2.4, direct proofs by the contravariant derivatives of their field equations (as in GR and $f(R)$) are hard to establish. Instead, we will move ahead to the bigger scenario of $\mathcal{I} = \int d^4x\sqrt{-g}\left[f(R, \cdots, \mathcal{R}) + 16\pi G\mathscr{L}_m\right]$ gravity with extended dependence on generic algebraic or differential Riemannian invariants $\mathcal{R} = \mathcal{R}(g_{\alpha\beta}, R_{\mu\alpha\nu\beta}, \nabla_\gamma R_{\mu\alpha\nu\beta}, \ldots)$. Formally we write down the variation as $\delta\mathcal{I} \cong \int d^4x\sqrt{-g}\left[\mathcal{H}^{(G)}_{\mu\nu} - 8\pi T^{(m)}_{\mu\nu}\right]\delta g^{\mu\nu}$, where $\mathcal{H}^{(G)}_{\mu\nu}$ resembles and generalizes the Einstein tensor by

$$\mathcal{H}^{(G)}_{\mu\nu} \;\cong\; \frac{1}{\sqrt{-g}}\,\frac{\delta\left[\sqrt{-g}\,f(R, \cdots, \mathcal{R})\right]}{\delta g^{\mu\nu}}\,. \tag{1.150}$$

Due to the coordinate invariance of the gravitational part $\mathcal{I}_G = \int d^4x\sqrt{-g}\,f(R, \cdots, \mathcal{R})$, $\mathcal{H}^{(G)}_{\mu\nu}$ satisfies the *generalized contracted Bianchi identity* [67, 68]

$$\nabla^\mu \left(\frac{1}{\sqrt{-g}} \frac{\delta \left[\sqrt{-g}\, f(R, \cdots, \mathcal{R}) \right]}{\delta g^{\mu\nu}} \right) = 0\,, \tag{1.151}$$

or just $\nabla^\mu \mathcal{H}^{(\mathrm{G})}_{\mu\nu} = 0$ by the definition of $\mathcal{H}^{(\mathrm{G})}_{\mu\nu}$. Similar to the relation $G_{\mu\nu} = R_{\mu\nu} - \frac{1}{2} R g_{\mu\nu}$, one can further expand $\mathcal{H}^{(\mathrm{G})}_{\mu\nu}$ to rewrite Eq.(1.151) into

$$\nabla^\mu \left(f_R R_{\mu\nu} + \sum f_{\mathcal{R}} \mathcal{R}_{\mu\nu} - \frac{1}{2} f(R, \cdots, \mathcal{R})\, g_{\mu\nu} \right) = 0\,, \tag{1.152}$$

where $f_R = f_R(R, \cdots, \mathcal{R}) := \partial f(R, \cdots, \mathcal{R}) / \partial R$, $f_{\mathcal{R}} = f_{\mathcal{R}}(R, \cdots, \mathcal{R}) := \partial f(R, \cdots, \mathcal{R}) / \partial \mathcal{R}$, and $\mathcal{R}_{\mu\nu} \cong \left(f_{\mathcal{R}} \delta \mathcal{R} \right) / \delta g^{\mu\nu}$ – note that in the calculation of $\mathcal{R}_{\mu\nu}$, $f_{\mathcal{R}}$ will serve as a nontrivial coefficient if $f_{\mathcal{R}} \neq$ constant and should be absorbed into the variation $\delta\mathcal{R}$ when integrated by parts. Specifically, when $f\,(R, \cdots, \mathcal{R}) = R + a \cdot R^2 + b \cdot R_{\alpha\beta} R^{\alpha\beta}$ or $f\,(R, \cdots, \mathcal{R}) = f(R, \mathcal{G})$, Eq.(1.151) becomes the generalized contracted Bianchi identities for quadratic and generalized Gauss-Bonnet gravities, respectively, which implies $\nabla^\mu T^{(m)}_{\mu\nu} = 0$.

1.2.9.3 $\nabla^\mu T^{(m)}_{\mu\nu} = 0$ in Brans-Dicke and scalar-tensor-like gravity

In modified gravities that contain nonminimal couplings between scalar fields and the curvature invariants, the generalized contracted Bianchi identity Eq.(1.151) for $\mathcal{I} = \int d^4 x \sqrt{-g} \left[f\,(R, \cdots, \mathcal{R}) + 16\pi G \mathscr{L}_m \right]$ gravity is no longer valid, and the conservation problem becomes more complicated than for pure tensorial gravity.

For generalized Brans-Dicke gravity in Subsection 1.2.5, let us take contravariant derivative of its field equation (1.110). With the Bianchi identity $\nabla^\mu \left(R_{\mu\nu} - \frac{1}{2} R g_{\mu\nu} \right) = 0$ and the third-order-derivative commutator $\left(\nabla_\nu \Box - \Box \nabla_\nu \right) \phi = -R_{\mu\nu} \nabla^\mu \phi$, it follows that

$$\nabla^\mu \left[\phi \left(R_{\mu\nu} - \frac{1}{2} R g_{\mu\nu} \right) + \left(g_{\mu\nu} \Box - \nabla_\mu \nabla_\nu \right) \phi + \frac{1}{2} V g_{\mu\nu} \right] = \frac{1}{2} \nabla_\nu \phi \cdot \left(-R + V_\phi \right); \tag{1.153}$$

moreover,

$$\nabla^\mu \left[-\frac{\omega}{\phi} \left(\nabla_\mu \phi \nabla_\nu \phi - \frac{1}{2} g_{\mu\nu} \nabla_\alpha \phi \nabla^\alpha \phi \right) \right] = \frac{1}{2} \nabla_\nu \phi \cdot \left(\frac{\omega - \omega_\phi}{\phi^2} \nabla_\alpha \phi \nabla^\alpha \phi - \frac{2\omega}{\phi} \Box \phi + V_\phi \right) = \frac{1}{2} \nabla_\nu \phi \cdot \left(R - V_\phi \right), \tag{1.154}$$

where the kinematical wave equation (1.111) has been employed for the replacement $\frac{\omega - \omega_\phi}{\phi^2} \nabla_\alpha \phi \nabla^\alpha \phi - \frac{2\omega}{\phi} \Box \phi = R - V_\phi$. Adding up Eqs.(1.153) and (1.154), one could see that the generalized Brans-Dicke field equation (1.110) is covariant invariant and $\nabla^\mu T^{(m)}_{\mu\nu} = 0$.

More generic scalar-tensor gravities can involve the nonminimal couplings between scalar fields and more complicated curvature invariants, which needs more effort to confirm the stress-energy-momentum conservation. For example, in the construction of Lovelock-Brans-Dicke gravity in Chapter 6, we will discuss the nonminimal $\phi-$couplings to Chern-Pontryagin density and Gauss-bonnet invariant, and prove

$\nabla^\mu T^{(m)}_{\mu\nu} = 0$. Moreover, for a large class of scalar-tensor-like gravity

$$\mathcal{I} = \int d^4x\sqrt{-g}\Big[R + f(R,\cdots,\mathcal{R}) + h(\phi)\cdot\widehat{f}(R,\cdots,\mathcal{R}) - \lambda(\phi)\cdot\nabla_\alpha\phi\nabla^\alpha\phi - V(\phi) + 16\pi G\mathscr{L}_m\Big], \quad (1.155)$$

where $h(\phi)$ is an arbitrary function of the scalar field $\phi = \phi(x^\alpha)$, and $\widehat{f}(R,\cdots,\mathcal{R})$ has generic dependence on curvature invariants $\mathcal{R}$; the covariant invariance of its field equation and $\nabla^\mu T^{(m)}_{\mu\nu} = 0$ will be proved in Chapter 8.

1.2.9.4 $\nabla^\mu T^{(m)}_{\mu\nu} = 0$ and minimal geometry-matter coupling

So far we have been establishing the stress-energy-momentum conservation by the covariant invariance of the field equations, and alternatively, one can look at $\nabla^\mu T^{(m)}_{\mu\nu} = 0$ from the perspective of minimal geometry-matter coupling. For GR, $f(R)$, quadratic, $f(R,\mathcal{G})$ and generalized Brans-Dicke gravities, the matter fields are always minimally coupled to the spacetime geometry, with an isolated matter density $\mathscr{L}_m$ in the total lagrangian density $\mathscr{L}_{\text{total}} = \mathscr{L}_{\text{gravity}} + 16\pi G\mathscr{L}_m$, and thus there are no curvature-matter coupling terms like $R\cdot\mathscr{L}_m$; in other words, the gravity/geometry part and the matter part in the total action are fully separable, $\mathcal{I}_{\text{total}} = \mathcal{I}_{\text{gravity}} + \mathcal{I}_m$.

Consider an arbitrary infinitesimal coordinate transformation $x^\mu \mapsto x^\mu + \delta x^\mu$, where $\delta x^\mu = k^\mu$ is an infinitesimal vector field that vanishes on the boundary, i.e. $k^\mu = 0\,|_{\partial\mathcal{M}}$, so that the spacetime manifold $\mathcal{M}$ is mapped onto itself. Since $\mathscr{L}_m = \mathscr{L}_m\left(g_{\mu\nu}, \psi_m, \partial_\mu\psi_m\right)$ is a scalar invariant that respects the diffeomorphism invariance under the active transformation $x^\mu \mapsto x^\mu + k^\mu$, Noether's conservation law directly yields

$$\nabla^\mu\left(\frac{1}{\sqrt{-g}}\frac{\delta\left(\sqrt{-g}\,\mathscr{L}_m\right)}{\delta g^{\mu\nu}}\right) = 0\,. \quad (1.156)$$

Comparison with Eq.(1.4) yields that Eq.(1.156) can be rewritten into $-\frac{1}{2}\nabla^\mu T^{(m)}_{\mu\nu} = 0$. That is to say, under minimal geometry-matter coupling with an isolated $\mathscr{L}_m$ in the total Lagrangian density, the matter tensor $T^{(m)}_{\mu\nu}$ in Eq.(1.4) has been defined in a *practical* way so that $T^{(m)}_{\mu\nu}$ is automatically symmetric, Noether compatible, and covariant invariant, which naturally guarantees the stress-energy-momentum conservation $\nabla^\mu T^{(m)}_{\mu\nu} = 0$. In this sense, and borrowing $\mathcal{H}_{\mu\nu} = 8\pi G T^{(m)}_{\mu\nu}$ in Eq.(1.137) as the generic field equation, one can regard the vanishing divergence $\nabla^\mu\mathcal{H}_{\mu\nu} = 0$ to either *imply* or *confirm* the conservation $\nabla^\mu T^{(m)}_{\mu\nu} = 0$.

1.2.10 Nonminimal curvature-matter couplings: $f(R,\mathscr{L}_m)$ gravity

In this subsection, we will consider an unusual modification of GR: allowing for nonminimal curvature-matter couplings like $R\cdot\mathscr{L}_m$. We will take generic $I = \int d^4x\sqrt{-g}\,f(R,\mathscr{L}_m)$ gravity as an example, which was proposed in Ref.[56] and is the maximal extension of GR and $\mathcal{I}_{\text{HE}}$ within the dependence of $\{R,\mathscr{L}_m\}$. Variation of the action $I = \int d^4x\sqrt{-g}\,f(R,\mathscr{L}_m)$ yields

$$\delta\mathcal{I} = \int d^4x\sqrt{-g}\left(f_R\cdot\frac{\delta R}{\delta g^{\mu\nu}} + f_{\mathscr{L}_m}\cdot\frac{\delta\mathscr{L}_m}{\delta g^{\mu\nu}} - \frac{1}{2}g_{\mu\nu}f\right)\delta g^{\mu\nu}\,, \quad (1.157)$$

where $f_R = f_R(R, \mathscr{L}_m) := df(R, \mathscr{L}_m)/dR$, $f_{\mathscr{L}_m} = f_{\mathscr{L}_m}(R, \mathscr{L}_m) := df(R, \mathscr{L}_m)/d\mathscr{L}_m$, according to Eq.(1.148), one has

$$f_{\mathscr{L}_m} \cdot \frac{\delta \mathscr{L}_m}{\delta g^{\mu\nu}} = \frac{1}{2} f_{\mathscr{L}_m} \cdot \left(g_{\mu\nu} \mathscr{L}_m - T^{(m)}_{\mu\nu} \right). \tag{1.158}$$

With $f_R \delta R / \delta g^{\mu\nu}$ already calculated in Eq.(1.73) [though now it becomes $f_R = f_R(R, \mathscr{L}_m)$ as opposed to $f_R = f_R(R)$], $\delta \mathcal{I} / \delta g^{\mu\nu} = 0$ leads to the field equation

$$f_R R_{\mu\nu} - \frac{1}{2} f g_{\mu\nu} + \left(g_{\mu\nu} \Box - \nabla_\mu \nabla_\nu \right) f_R = \frac{1}{2} f_{\mathscr{L}_m} \left(T^{(m)}_{\mu\nu} - g_{\mu\nu} \mathscr{L}_m \right), \tag{1.159}$$

whose trace is $f_R R - 2f(R, \mathscr{L}_m) + 3\Box f_R = \frac{1}{2} f_{\mathscr{L}_m} \left(T^{(m)} - 4\mathscr{L}_m \right)$. Moreover, taking the contravariant derivative of Eq.(1.159), one can see that $\nabla^\mu T^{(m)}_{\mu\nu} = 0$ no longer holds. Instead, $\nabla^\mu T^{(m)}_{\mu\nu}$ satisfies the divergence equation

$$\nabla^\mu T^{(m)}_{\mu\nu} = \left(\mathscr{L}_m \, g_{\mu\nu} - T_{\mu\nu} \right) \nabla^\mu \ln f_{\mathscr{L}_m} . \tag{1.160}$$

This generalized conservation equation indicates that there would be direct energy exchange between spacetime geometry and the energy-matter content under nonminimal curvature-matter couplings; for example, Eq.(1.160) has been interpreted as a matter creation process with an irreversible energy flow from the gravitational field to the created matter in accordance with the second law of thermodynamics [69, 70].

Specifically, when the matter content is minimally coupled to the spacetime metric, the coupling coefficient $f_{\mathscr{L}_m}$ reduces to become a constant. In accordance with the gravitational coupling strength in GR, this constant is necessarily equal to $16\pi G$. That is,

$$f_{\mathscr{L}_m} = \text{constant} = 16\pi G \quad \text{and} \quad f(R\,, \mathscr{L}_m) = \tilde{f}(R) + 16\pi G \mathscr{L}_m \,. \tag{1.161}$$

while the field equation (1.159) becomes (with the tilde on $\tilde{f}$ omitted)

$$-\frac{1}{2} f \, g_{\mu\nu} + f_R \, R_{\mu\nu} + \left(g_{\mu\nu} \Box - \nabla_\mu \nabla_\nu \right) f_R = 8\pi G T^{(m)}_{\mu\nu} \,, \tag{1.162}$$

which recovers the situation of minimally coupled $f(R)$ gravity in Subsection 1.2.2. Moreover, as an extension of $f(R, \mathscr{L}_m)$ gravity, in Chapter 3 we will extensively investigate $f(R, R_{\alpha\beta} R^{\alpha\beta}, R_{\alpha\mu\beta\nu} R^{\alpha\mu\beta\nu}, \mathscr{L}_m)$ and $f(R, \mathcal{G}, \mathscr{L}_m)$ gravities, including the equations of nongeodesic motion in different matter fields and the generalized energy-momentum conservation.

1.3 Summary

In this chapter, we have reviewed the fundamentals of GR, physical cosmology, dark energy, and relativistic gravity. All necessary preparations have been made, and after the Statement of Co-authorship in Chapter 2, we will begin to investigate the applications of modified gravities from Chapter 3 until Chapter 10.

1.4 Addendum

1.4.1 Sign conventions

Throughout this thesis, we adopt the geometric conventions $R^{\alpha}{}_{\beta\gamma\delta} = \partial_\gamma \Gamma^{\alpha}_{\delta\beta} - \partial_\delta \Gamma^{\alpha}_{\gamma\beta} \cdots$ and $R_{\mu\nu} = R^{\alpha}{}_{\mu\alpha\nu}$ along with the metric signature $(-,+++)$. In the literature of relativistic gravity and cosmology, there exists another set of conventions that uses $R^{\alpha}{}_{\beta\gamma\delta} = \partial_\delta \Gamma^{\alpha}_{\gamma\beta} - \partial_\gamma \Gamma^{\alpha}_{\delta\beta} \cdots$ and the metric signature $(+,---)$, while the definitions of Christoffel symbols and the contraction $R_{\mu\nu} = R^{\alpha}{}_{\mu\alpha\nu}$ remain the same [1].

The table below shows the changes of signs from the $(-,+++)$ system into the $(+,---)$ system, and one should bear in mind that the definition of the Riemann tensor differs by an overall minus sign between the two sets of conventions.

Metric tensor and its inverse	$g_{\alpha\beta}\,,\ g^{\alpha\beta}$	Changing sign
Christoffel symbols of first kind	$\Gamma_{\alpha\beta\gamma} = \frac{1}{2}\left(\partial_\gamma g_{\alpha\beta} + \partial_\beta g_{\alpha\gamma} - \partial_\alpha g_{\beta\gamma}\right)$	Changing sign
Christoffel symbols of second kind	$\Gamma^{\alpha}{}_{\beta\gamma} = \frac{1}{2}\, g^{\alpha\delta}\left(\partial_\gamma g_{db} + \partial_\beta g_{\delta\gamma} - \partial_\delta g_{\beta\gamma}\right)$	No change
Riemann tensor (redefined)	$R^{\alpha}{}_{\beta\gamma\delta} = \partial_\gamma \Gamma^{\alpha}{}_{\beta\delta} - \partial_\delta \Gamma^{\alpha}{}_{\beta\gamma} + \Gamma^{\epsilon}{}_{\beta\delta}\Gamma^{\alpha}{}_{\epsilon\gamma} - \Gamma^{\epsilon}{}_{\beta\gamma}\Gamma^{\alpha}{}_{\epsilon\delta}$	Changing sign
Ricci tensor	$R_{\alpha\beta} = R^{\gamma}{}_{\alpha\gamma\beta}$	Changing sign
Scalar curvature	$R = g^{\alpha\beta} R_{\alpha\beta}$	No change
Einstein tensor	$G_{\alpha\beta} = R_{\alpha\beta} - \frac{1}{2} g_{\alpha\beta} R$	Changing sign
Stress-energy-momentum tensor	$T^{(m)}_{\alpha\beta}$	Changing sign
Cosmological constant	$R_{\alpha\beta} - \frac{1}{2} g_{\alpha\beta} R + g_{\alpha\beta}\Lambda = T_{\alpha\beta}$	No change

1.4.2 Fundamentals of error analysis

Besides the theories and phenomenology, this thesis also investigates the cosmological applications of modified gravity. Especially, in Chapters 9 and 10 we will deal with observational data, so let us quickly review the fundamentals of error analyses.

Given a set of discrete measurements $\{x_i\}$ for the observable x, the best estimated value is the average or mean value

$$\bar{x} = \frac{1}{n} \sum_{1}^{n} x_i\,, \tag{1.163}$$

and the standard deviation of x is given by

$$\sigma = \sqrt{\frac{\sum_1^n (x_i - \bar{x})^2}{n-1}}\,. \tag{1.164}$$

while the standard deviation (or standard error) of the mean value $\bar{x}$ is

$$\sigma_m = \frac{\sigma}{\sqrt{n}} = \sqrt{\frac{\sum_1^n (x_i - \bar{x})^2}{n(n-1)}}\,. \tag{1.165}$$

Then the measured value of x can be written as $x = \bar{x} + \Delta x = \bar{x} + \sigma_m$.

For the algebraic combination of multiple and uncorrelated measurements, the propagation of independent errors satisfy the following rules.

(1) If two mutually independent quantities are being added or subtracted, i.e. $y = x_i \pm x_j$, then

$$\Delta y = \sqrt{(\Delta x_i)^2 + \left(\Delta x_j\right)^2}\,; \tag{1.166}$$

(2) If two mutually independent quantities are being multiplied or divided, i.e. $y = x_i x_j$ or $y = x_i/x_j (i \neq j)$, then

$$\frac{\Delta y}{y} = \sqrt{\left(\frac{\Delta x_i}{x_i}\right)^2 + \left(\frac{\Delta x_j}{x_j}\right)^2}\,. \tag{1.167}$$

Particularly, if one takes the power of a quantity, i.e. $y = x^n$, Eq.(1.167) implies $\Delta y = \sqrt{n} x^{n-1} \Delta x$.

Note that these rules were already used in Eq.(1.38) to derive $\{\Omega_{b0}, \Omega_{\rm cdm0}\}$ from $\{\Omega_{b0} h^2, \Omega_{\rm cdm0} h^2, h\}$.

Chapter 2

Statement of Co-authorship

Chapters 3~6 are based on the following publications by David Wenjie Tian and Dr. Ivan Booth:

- David Wenjie Tian, Ivan Booth. Lessons from $f(R, R_c^2, R_m^2, \mathscr{L}_m)$ gravity: Smooth Gauss-Bonnet limit, energy-momentum conservation, and nonminimal coupling. *Physical Review D* **90** (2014), 024059. [arXiv:1404.7823]
- David Wenjie Tian, Ivan Booth. Friedmann equations from nonequilibrium thermodynamics of the Universe: A unified formulation for modified gravity. *Physical Review D* **90** (2014), 104042. [arXiv: 1409.4278]
- David Wenjie Tian, Ivan Booth. Apparent horizon and gravitational thermodynamics of the Universe: Solutions to the temperature and entropy confusions, and extensions to modified gravity. *Physical Review D* **92** (2015), 024001. [arXiv:1411.6547]
- David Wenjie Tian, Ivan Booth. Lovelock-Brans-Dicke gravity. *Classical and Quantum Gravity* **33** (2016), 045001. [arXiv:1502.05695]

We hereby confirm that for each paper, David Wenjie Tian was the main contributor in the primary four steps: (1) Design and identification of the research proposal; (2) Practical aspects of the research; (3) Data analysis; (4) Manuscript preparation.

Chapter 3. Lessons from $f(R, R_c^2, R_m^2, \mathscr{L}_m)$ gravity: Smooth Gauss-Bonnet limit, energy-momentum conservation and nonminimal coupling

[*Phys. Rev. D* **90** (2014), 024059]

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Abstract

This paper studies a generic fourth-order theory of gravity with Lagrangian density $f(R, R_c^2, R_m^2, \mathscr{L}_m)$, where R_c^2 and R_m^2 respectively denote the square of the Ricci and Riemann tensors. By considering explicit R^2 dependence and imposing the "coherence condition" $f_{R^2} = f_{R_m^2} = -f_{R_c^2}/4$, the field equations of $f(R, R^2, R_c^2, R_m^2, \mathscr{L}_m)$ gravity can be smoothly reduced to that of $f(R, \mathcal{G}, \mathscr{L}_m)$ generalized Gauss-Bonnet gravity with $\mathcal{G}$ denoting the Gauss-Bonnet invariant. We use Noether's conservation law to study the $f(\mathcal{R}_1, \mathcal{R}_2 \ldots, \mathcal{R}_n, \mathscr{L}_m)$ model with nonminimal coupling between $\mathscr{L}_m$ and Riemannian invariants $\mathcal{R}_i$, and conjecture that the gradient of nonminimal gravitational coupling strength $\nabla^\mu f_{\mathscr{L}_m}$ is the only source for energy-momentum nonconservation. This conjecture is applied to the $f(R, R_c^2, R_m^2, \mathscr{L}_m)$ model, and the equations of continuity and nongeodesic motion of different matter contents are investigated. Finally, the field equation for Lagrangians including the traceless-Ricci square and traceless-Riemann (Weyl) square invariants is derived, the $f(R, R_c^2, R_m^2, \mathscr{L}_m)$ model is compared with the $f(R, R_c^2, R_m^2, T) + 2\kappa\mathscr{L}_m$ model, and consequences of nonminimal coupling for black hole and wormhole physics are considered.

PACS numbers: 04.20.Cv , 04.20.Fy , 04.50.Kd

3.1 Introduction

There are two main proposals to explain the accelerated expansion of the Universe [1]. The first assumes the existence of negative-pressure dark energy as a dominant component of the cosmos [2, 3]. The second approach seeks viable modifications of both general relativity (GR) and its alternatives [4, 5].

Focusing on modifications of GR, the original Lagrangian density can be modified in two ways: (1) extending its dependence on the curvature invariants, and (2) considering nonminimal curvature-matter coupling. The simplest curvature-invariant modification is $f(R) + 2\kappa\mathscr{L}_m$ gravity [5, 6] ($\kappa = 8\pi G/c^4 \equiv 8\pi G$ and $c = 1$ hereafter), where the isolated Ricci scalar R in the Hilbert-Einstein action is replaced by a generic function of R. In this case standard energy-momentum conservation $\nabla^\mu T_{\mu\nu} = 0$ continues to hold. Further extensions have introduced dependence on such things as the Gauss-Bonnet invariant $\mathcal{G}$ [4, 7] and squares of Ricci and Riemann tensors $\{R_c^2, R_m^2\}$ [8], leading to models with Lagrangian densities like $R + f(\mathcal{G}) + 2\kappa\mathscr{L}_m$, $f(R, \mathcal{G}) + 2\kappa\mathscr{L}_m$

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and $R + f(R, R_c^2, R_m^2) + 2\kappa\mathscr{L}_m$. In all these models, the spacetime geometry remains minimally coupled to the matter Lagrangian density $\mathscr{L}_m$.

On the other hand, following the spirit of nonminimal $f(R)\mathscr{L}_d$ coupling in scalar-field dark-energy models [9], for modified theories of gravity an extra term $\lambda\tilde{f}(R)\mathscr{L}_m$ was respectively added to the standard actions of GR and $f(R)+2\kappa\mathscr{L}_m$ gravity in [10] and [11], which represents nonminimal curvature-matter coupling between R and $\mathscr{L}_m$. These ideas soon attracted a lot of attention in other modifications of GR after the work in [11], and nonminimal coupling was introduced to other gravity models such as generalized Gauss-Bonnet gravity [6, 12] with terms like $\lambda f(\mathcal{G})\mathscr{L}_m$. From these initial models, some general consequences of nonminimal coupling were revealed. Most significantly, $\mathscr{L}_m$ enters the gravitational field equation directly, nonminimal coupling violates the equivalence principle, and in general, energy-momentum conservation is violated with nontrivial energy-momentum-curvature transformation. In [13], $f(R, \mathscr{L}_m)$ theory as the most generic extension of GR within the dependence of $\{R, \mathscr{L}_m\}$ was developed, while another type of nonminimal coupling, the $f(R,T)+2\kappa\mathscr{L}_m$ model, was considered in [14].

In this paper, we consider modifications to GR from both invariant-dependence and nonminimal-coupling aspects, and introduce a new model of generic fourth-order gravity with Lagrangian density $f(R, R_c^2, R_m^2, \mathscr{L}_m)$. This can be regarded as a generalization of the $f(R, \mathscr{L}_m)$ model [13] by adding R_c^2 and R_m^2dependence, and an extension of the $f(R, R_c^2, R_m^2)+2\kappa\mathscr{L}_m$ model [8] by allowing nonminimal curvature-matter coupling. Among the fourteen independent algebraic invariants which can be constructed from the Riemann tensor and metric tensor [15, 16], besides R we focus on Ricci square R_c^2 and Riemann square (Kretschmann scalar) R_m^2, not only because they are the two simplest square invariants (as opposed to cubic and quartic invariants [16]), but also because they provide a bridge to generalized Gauss-Bonnet theories of gravity [6] and quadratic gravity [17, 18]. By studying this model, we hope to get further insights into the effects of nonminimal coupling and dependence on extra curvature invariants.

This paper is organized as follows. First of all, the field equations for $\mathscr{L} = f(R, R_c^2, R_m^2, \mathscr{L}_m)$ gravity are derived and nonminimal couplings with $\mathscr{L}_m$ and T are compared in Sec. 3.2. In Sec. 3.3, we consider an explicit dependence on R^2, and introduce the condition $f_{R^2} = f_{R_m^2} = -f_{R_c^2}/4$ to smoothly transform $f(R, R^2, R_c^2, R_m^2, \mathscr{L}_m)$ gravity to the generalized Gauss-Bonnet gravity $\mathscr{L} = f(R, \mathcal{G}, \mathscr{L}_m)$; employing $\mathcal{G}$, quadratic gravity is revisited and traceless models like $\mathscr{L} = f(R, R_S^2, C^2, \mathscr{L}_m)$ are discussed. In Sec. 3.4, we commit ourselves to understanding the energy-momentum divergence problem associated with $f(R, R_c^2, R_m^2, \mathscr{L}_m)$ gravity and most generic $\mathscr{L} = f(\mathcal{R}_1, \mathcal{R}_2 \ldots, \mathcal{R}_n, \mathscr{L}_m)$ gravity with nonminimal coupling, as an application of which, the equations of continuity and nongeodesic motion are derived in Sec. 3.5. Finally, in Sec. 3.6, two implications of nonminimal coupling for black hole physics and wormholes are discussed. In the Appendix generalized energy conditions of $f(R, \mathcal{R}_1, \mathcal{R}_2 \ldots, \mathcal{R}_n, \mathscr{L}_m)$ and $f(R, R_c^2, R_m^2, \mathscr{L}_m)$ gravity are considered. Throughout this paper, we adopt the sign convention $R^\alpha{}_{\beta\gamma\delta} = \partial_\gamma\Gamma^\alpha_{\delta\beta} - \partial_\delta\Gamma^\alpha_{\gamma\beta} \cdots$ with the metric signature $(-, +++)$, and follow the straightforward metric approach rather than first-order Einstein-Palatini.

3.2 Field equation and its properties

3.2.1 Action and field equations

The action we propose for a generic fourth-order theory of gravity with possibly nonminimal curvature-matter coupling is

$$\mathcal{S} = \int d^4x\sqrt{-g}\, f(R\,, R_c^2\,, R_m^2\,, \mathscr{L}_m)\,, \tag{3.1}$$

where R_c^2 and R_m^2 denote the square of Ricci and Riemann curvature tensor, respectively,

$$R_c^2 := R_{\alpha\beta}R^{\alpha\beta} \quad , \quad R_m^2 := R_{\alpha\mu\beta\nu}R^{\alpha\mu\beta\nu}\,. \tag{3.2}$$

Varying the action Eq.(3.1) with respect to the inverse metric $g^{\mu\nu}$, we get[1]

$$\delta\mathcal{S} = \int d^4x\sqrt{-g}\left\{-\frac{1}{2}f\, g_{\mu\nu}\cdot\delta g^{\mu\nu} + f_R\cdot\delta R + f_{R_c^2}\cdot\delta R_c^2 + f_{R_m^2}\cdot\delta R_m^2 + f_{\mathscr{L}_m}\cdot\delta\mathscr{L}_m\right\}, \tag{3.3}$$

where $f_R := \partial f/\partial R$, $f_{R_c^2} := \partial f/\partial R_c^2$, $f_{R_m^2} := \partial f/\partial R_m^2$, and $f_{\mathscr{L}_m} := \partial f/\partial\mathscr{L}_m$. δR_c^2 and δR_m^2 can be reduced into variations of Riemann tensor,

$$\delta R_c^2 = \delta\Big[R_{\alpha\beta}\cdot(g^{\alpha\rho}g^{\beta\sigma}R_{\rho\sigma})\Big] = 2R_\mu{}^\alpha R_{\alpha\nu}\cdot\delta g^{\mu\nu} + 2R^{\mu\nu}\cdot\delta R^\alpha{}_{\mu\alpha\nu}\,, \tag{3.4}$$

$$\delta R_m^2 = \delta\Big[R_{\alpha\beta\gamma\epsilon}\cdot(g^{\alpha\rho}g^{\beta\sigma}g^{\gamma\zeta}g^{\epsilon\eta}R_{\rho\sigma\zeta\eta})\Big] = 4R_{\mu\alpha\beta\gamma}R_\nu{}^{\alpha\beta\gamma}\cdot\delta g^{\mu\nu} + 2R^{\alpha\beta\gamma\epsilon}\cdot\left(R^\rho{}_{\beta\gamma\epsilon}\,\delta g_{\alpha\rho} + g_{\alpha\rho}\,\delta R^\rho{}_{\beta\gamma\epsilon}\right), \tag{3.5}$$

while $\delta R^\lambda{}_{\alpha\beta\gamma}$ traces back to $\delta\Gamma^\lambda_{\alpha\beta}$ through the Palatini identity

$$\delta R^\lambda{}_{\alpha\beta\gamma} = \nabla_\beta(\delta\Gamma^\lambda_{\gamma\alpha}) - \nabla_\gamma(\delta\Gamma^\lambda_{\beta\alpha})\,. \tag{3.6}$$

Also, as is well known, $\delta\Gamma^\lambda_{\alpha\beta} = \frac{1}{2}\,g^{\lambda\sigma}\left(\nabla_\alpha\delta g_{\sigma\beta} + \nabla_\beta\delta g_{\sigma\alpha} - \nabla_\sigma\delta g_{\alpha\beta}\right)$ [19, 20], and we keep in mind that when raising the indices on $\delta g_{\alpha\beta}$ a minus sign appears: $\delta g_{\alpha\beta} = -g_{\alpha\mu}\,g_{\beta\nu}\,\delta g^{\mu\nu}$. Then, Eqs.(3.4-3.6) yield

$$f_R\cdot\delta R \cong \Big[f_R\,R_{\mu\nu} + (g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu)\,f_R\Big]\cdot\delta g^{\mu\nu} =: H^{(fR)}_{\mu\nu}\cdot\delta g^{\mu\nu}\,, \tag{3.7}$$

$$f_{R_c^2}\cdot\delta R_c^2 \cong \Big[2f_{R_c^2}\,R_\mu{}^\alpha R_{\alpha\nu} - \nabla_\alpha\nabla_\nu(R_\mu{}^\alpha f_{R_c^2}) - \nabla_\alpha\nabla_\mu(R_\nu{}^\alpha f_{R_c^2}) + \Box(R_{\mu\nu}f_{R_c^2}) + g_{\mu\nu}\nabla_\alpha\nabla_\beta(R^{\alpha\beta}f_{R_c^2})\Big]\cdot\delta g^{\mu\nu} =: H^{(fR_c^2)}_{\mu\nu}\cdot\delta g^{\mu\nu}, \tag{3.8}$$

$$\text{and}\quad f_{R_m^2}\cdot\delta R_m^2 \cong \Big[2\,f_{R_m^2}\cdot R_{\mu\alpha\beta\gamma}R_\nu{}^{\alpha\beta\gamma} + 4\,\nabla^\beta\nabla^\alpha(R_{\alpha\mu\beta\nu}f_{R_m^2})\Big]\cdot\delta g^{\mu\nu} =: H^{(fR_m^2)}_{\mu\nu}\cdot\delta g^{\mu\nu}\,. \tag{3.9}$$

Here, $\Box \equiv \nabla^\alpha\nabla_\alpha$ represents the covariant d'Alembertian, and the symbol $\cong$ denotes an effective equivalence by neglecting a surface integral after integration by parts twice to extract $\{H^{(fR)}_{\mu\nu}, H^{(fR_c^2)}_{\mu\nu}, H^{(fR_m^2)}_{\mu\nu}\}$. Especially, Eq.(3.9) has utilized the combination $2\nabla^\beta\nabla^\alpha(R_{\alpha\mu\beta\nu}f_{R_m^2}) + 2\nabla^\beta\nabla^\alpha(R_{\alpha\nu\beta\mu}f_{R_m^2}) = 4\nabla^\beta\nabla^\alpha(R_{\alpha\mu\beta\nu}f_{R_m^2})$, where the symmetry of $\nabla^\beta\nabla^\alpha(R_{\alpha\mu\beta\nu}f_{R_m^2})$ under the index switch $\mu \leftrightarrow \nu$ is guaranteed by $\nabla^\beta\nabla^\alpha R_{\alpha\mu\beta\nu} = \nabla^\beta\nabla^\alpha R_{\alpha\mu\beta\nu}$,

[1] The terms *geometry-matter* coupling and *curvature-matter* coupling are both used in this paper. They are not identical: the former can be either nonminimal or minimal, while the latter by its name is always nonminimal since a curvature invariant contains at least second-order derivative of the metric tensor. Here nonminimal coupling happens between algebraic or differential Riemannian scalar invariants and $\mathscr{L}_m$, so we will mainly use curvature-matter coupling.

$\nabla^\alpha\nabla^\beta f_{R^2_m} = \nabla^\beta\nabla^\alpha f_{R^2_m}$ as well as the $\mu \leftrightarrow \nu$ symmetry of its remaining expanded terms. Note that in these equations, total derivatives in individual variations $\{\delta R\,, \delta R^2_c\,, \delta R^2_m\}$ are not necessarily pure divergences anymore, because the nontrivial coefficients $\{f_R\,, f_{R^2_c}\,, f_{R^2_m}\}$ will be absorbed by the variations into the nonlinear and higher-order-derivative terms in $\{H^{(fR)}_{\mu\nu}, H^{(fR^2_c)}_{\mu\nu}, H^{(fR^2_m)}_{\mu\nu}\}$.

In the $f_{\mathscr{L}_m}\cdot\delta\mathscr{L}_m$ term in Eq.(3.3), we make use of the standard definition of stress-energy-momentum (SEM) density tensor used in GR (e.g. [10]- [14]), which is introduced in accordance with minimal geometry-matter coupling and automatic energy-momentum conservation (for further discussion see Sec. 3.4.1),

$$T_{\mu\nu} := \frac{-2}{\sqrt{-g}}\frac{\delta(\sqrt{-g}\,\mathscr{L}_m)}{\delta g^{\mu\nu}} \tag{3.10}$$

$$= \mathscr{L}_m\, g_{\mu\nu} - 2\frac{\delta\mathscr{L}_m}{\delta g^{\mu\nu}}\,. \tag{3.11}$$

The equivalence from Eq.(3.10) to Eq.(3.11) is built upon the common assumption that $\mathscr{L}_m$ does not explicitly depend on derivatives of the metric, $\mathscr{L}_m = \mathscr{L}_m(g_{\mu\nu}, \psi_m) \neq \mathscr{L}_m(g_{\mu\nu}, \partial_\alpha g_{\mu\nu}, \psi_m)$ with ψ_m collectively denoting all relevant matter fields.

After some work, Eqs.(3.3), (3.7), (3.8), (3.9) and (3.11) eventually give rise to the field equation for $f(R, R^2_c, R^2_m, \mathscr{L}_m)$ gravity:

$$-\frac{1}{2}f\, g_{\mu\nu} + f_R\, R_{\mu\nu} + (g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu)\, f_R + H^{(fR^2_c)}_{\mu\nu} + H^{(fR^2_m)}_{\mu\nu} \;=\; \frac{1}{2}\, f_{\mathscr{L}_m}\,(T_{\mu\nu} - \mathscr{L}_m\, g_{\mu\nu})\,, \tag{3.12}$$

where $H^{(fR^2_c)}_{\mu\nu}$ and $H^{(fR^2_m)}_{\mu\nu}$ were introduced in Eqs.(3.8) and (3.9) to collect all terms arising from R^2_c- and R^2_m-dependence in f,

$$\begin{aligned} H^{(fR^2_c)}_{\mu\nu} + H^{(fR^2_m)}_{\mu\nu} \;&= 2\, f_{R^2_c}\cdot R_\mu{}^\alpha R_{\alpha\nu} + 2\, f_{R^2_m}\cdot R_{\mu\alpha\beta\gamma}R_\nu{}^{\alpha\beta\gamma} - \nabla_\alpha\nabla_\nu(R_\mu{}^\alpha f_{R^2_c}) \\ &- \nabla_\alpha\nabla_\mu(R_\nu{}^\alpha f_{R^2_c}) + \Box(R_{\mu\nu} f_{R^2_c}) + g_{\mu\nu}\nabla_\alpha\nabla_\beta(R^{\alpha\beta} f_{R^2_c}) + 4\,\nabla^\beta\nabla^\alpha(R_{\alpha\mu\beta\nu} f_{R^2_m})\,. \end{aligned} \tag{3.13}$$

Note that $\{f, f_R, f_{R^2_c}, f_{R^2_m}\}$ herein are all functions of $(R, R^2_c, R^2_m, \mathscr{L}_m)$, and $H^{(fR)}_{\mu\nu} = f_R R_{\mu\nu} + (g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu) f_R$ has been written down directly to facilitate comparison with GR and $f(R){+}2\kappa\mathscr{L}_m$ or $f(R, \mathscr{L}_m)$ gravity. Taking the trace of Eq.(3.12), the simple algebraic equality $R = -T$ (where $T = g^{\mu\nu}T_{\mu\nu}$) in GR is now generalized to the following differential relation,

$$-2f + f_R\, R + 2f_{R^2_c}\cdot R^2_c + 2\, f_{R^2_m}\cdot R^2_m + \Box\,(3f_R + f_{R^2_c}R) + 2\nabla_\alpha\nabla_\beta(R^{\alpha\beta} f_{R^2_c} + 2R^{\alpha\beta} f_{R^2_m}) \;=\; f_{\mathscr{L}_m}\,(\frac{1}{2}T - 2\mathscr{L}_m)\,. \tag{3.14}$$

Compared with Einstein's equation $R_{\mu\nu} - Rg_{\mu\nu}/2 = \kappa T_{\mu\nu}$ in GR, nonlinear terms and derivatives of the metric up to fourth order have come forth and been encoded into $\{H^{(fR)}_{\mu\nu}, H^{(fR^2_c)}_{\mu\nu}, H^{(fR^2_m)}_{\mu\nu}\}$ on the left hand side of Eq.(3.12). On the right hand side, the matter Lagrangian density $\mathscr{L}_m$ explicitly participates in the field equation as a consequence of the confrontation between nonminimal curvature-matter coupling in $f(R, R^2_c, R^2_m, \mathscr{L}_m)$ and the minimal-coupling definition of $T_{\mu\nu}$ in Eq.(3.10). Note that not all matter terms have been moved to the right hand side, because $-\frac{1}{2}f g_{\mu\nu}$ is still $\mathscr{L}_m$-dependent before a concrete $f(R, R^2_c, R^2_m, \mathscr{L}_m)$ model gets specified and rearranged.

Also, $f_{\mathscr{L}_m} = f_{\mathscr{L}_m}(R, R^2_c, R^2_m, \mathscr{L}_m)$ represents the gravitational coupling strength and never vanishes, so in vacuum one has $\mathscr{L}_m = 0$ and $T_{\mu\nu} = 0$, yet $f_{\mathscr{L}_m} \neq 0$. Such a generic coupling strength $f_{\mathscr{L}_m}$ will unavoidably violate Einstein's equivalence principle and the strong equivalence principle unless it reduces to a constant.

3.2.2 Field equation under minimal coupling

When the matter content is minimally coupled to the spacetime metric, the coupling coefficient $f_{\mathscr{L}_m}$ reduces to become a constant. In accordance with the gravitational coupling strength in GR, this constant is necessarily equal to Einstein's constant κ (and doubled just for scaling tradition). That is,

$$f_{\mathscr{L}_m} = \text{constant} \; = \; 2\kappa \quad , \quad f(R\,,R_c^2\,,R_m^2\,,\mathscr{L}_m) \; = \; \tilde{f}(R\,,R_c^2\,,R_m^2) + 2\kappa\,\mathscr{L}_m\,. \tag{3.15}$$

We have neglected the situation when $f_{\mathscr{L}_m}$ is a pointwise scalar field $\phi = \phi(x^\alpha)$, which should be treated as a scalar-tensor theory mixed with metric gravity: in fact, $\phi(x^\alpha)\,\mathscr{L}_m$ is also a type of nonminimal coupling, but it goes beyond the scope of this paper and will not be discussed here. Under minimal coupling as in Eq.(3.15), the field equation (3.12) becomes (with tildes on $\tilde{f}$ omitted)

$$-\frac{1}{2}f\,g_{\mu\nu} + f_R\,R_{\mu\nu} + (g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu)\,f_R + H_{\mu\nu}^{(fR_c^2)} + H_{\mu\nu}^{(fR_m^2)} \; = \; \kappa\,T_{\mu\nu}\,, \tag{3.16}$$

which coincides with the result in [8]. The weak field limit of this minimally coupled model has been systematically studied in [21].

3.2.3 Two types of nonminimal curvature-matter coupling

Apart from the $\mathscr{L} = f(R, R_c^2, R_m^2, \mathscr{L}_m)$ model under discussion, another type of curvature-matter coupling was introduced in [14] by the $\mathscr{L} = f(R,T) + 2\kappa\mathscr{L}_m$ model, where a curvature invariant was nonminimally coupled to the trace of the SEM tensor $T = g^{\mu\nu}T_{\mu\nu}$ rather than the matter Lagrangian density $\mathscr{L}_m$. In this spirit, we consider the following nonminimally coupled action,

$$\mathcal{S} \; = \; \int d^4x\,\sqrt{-g}\,\Big\{f(R\,,R_c^2\,,R_m^2\,,T) + 2\kappa\,\mathscr{L}_m\Big\}\,. \tag{3.17}$$

By the standard methods we find that its field equation is:

$$-\frac{1}{2}f\,g_{\mu\nu} + f_R\cdot R_{\mu\nu} + (g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu)\,f_R + H_{\mu\nu}^{(fR_c^2)} + H_{\mu\nu}^{(fR_m^2)} \; = -f_T\cdot(T_{\mu\nu} + \Theta_{\mu\nu}) + \kappa T_{\mu\nu}\,, \tag{3.18}$$

where $\{f, f_R, f_{R_c^2}, f_T\}$ are all functions of (R, R_c^2, R_m^2, T) , $H_{\mu\nu}^{(fR_c^2)} + H_{\mu\nu}^{(fR_m^2)}$ is given by Eq.(3.13), $-f_T\,(T_{\mu\nu} + \Theta_{\mu\nu})$ comes from the T-dependence in $f(R, R_c^2, R_m^2, T)$, and

$$\Theta_{\mu\nu} \; := \; \frac{g^{\alpha\beta}\,\delta T_{\alpha\beta}}{\delta g^{\mu\nu}}\,. \tag{3.19}$$

As will be extensively discussed in Section 5, for some matter sources $\mathscr{L}_m$ cannot be uniquely specified, and therefore the equations of continuity and motion based on Eq.(3.12) have to rely on the choice of $\mathscr{L}_m$. In such situations $T_{\mu\nu}$ is easier to set up than $\mathscr{L}_m$, so at first glance, it seems as if the new field equation (3.18) could avoid the flaws from nonminimal $\mathscr{L}_m$-coupling, at the cost of employing a supplementary matter tensor $\Theta_{\mu\nu}$. However, the definition of $\Theta_{\mu\nu}$ is still based on the relation $T_{\mu\nu} = \mathscr{L}_m g_{\mu\nu} - 2\delta\mathscr{L}_m/\delta g^{\mu\nu}$ in Eq.(3.11), and explicit calculations have revealed that [14]

$$\Theta_{\mu\nu} = -2T_{\mu\nu} + g_{\mu\nu}\mathscr{L}_m - 2g^{\alpha\beta}\frac{\partial^2\mathscr{L}_m}{\partial g^{\mu\nu}\partial g^{\alpha\beta}}\,. \tag{3.20}$$

Thus, both $\mathscr{L}_m$ and its second-order derivative with respect to the metric are hidden in $\Theta_{\mu\nu}$, and consequently, both $f(R, R_c^2, R_m^2, T) + 2\kappa\mathscr{L}_m$ and $f(R, R_c^2, R_m^2, \mathscr{L}_m)$ theories are sensitive to the $\mathscr{L}_m$ in use. The equations of continuity and nongeodesic motion will differ for different choices of $\mathscr{L}_m$ for the same matter source.

The $\mathscr{L} = f(R, R_c^2, R_m^2, \mathscr{L}_m)$ model and the $\mathscr{L} = f(R, R_c^2, R_m^2, T) + 2\kappa\mathscr{L}_m$ model are both reasonable realizations of nonminimal curvature-matter coupling, and in this paper we have adopted the former case as a generalization of the existing $\mathscr{L} = f(R, \mathscr{L}_m)$ [13] and $\mathscr{L} = f(R, R_c^2, R_m^2) + 2\kappa\mathscr{L}_m$ [8] theories. Also, it looks redundant and unnecessary to further consider the superposition of nonminimal $\mathscr{L}_m$- and T-couplings, which can be depicted by the action

$$\mathcal{S} = \int d^4x\sqrt{-g}\,f(R\,, R_c^2\,, R_m^2\,, \mathscr{L}_m\,, T)\,, \tag{3.21}$$

whose field equation is

$$-\frac{1}{2}f\,g_{\mu\nu} + f_R\cdot R_{\mu\nu} + (g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu)\,f_R + H_{\mu\nu}^{(fR_c^2)} + H_{\mu\nu}^{(fR_m^2)} = \frac{1}{2}f_{\mathscr{L}_m}\cdot(T_{\mu\nu} - \mathscr{L}_m\,g_{\mu\nu}) - f_T\cdot(T_{\mu\nu} + \Theta_{\mu\nu})\,. \tag{3.22}$$

Practically it is implicitly assumed in Eq.(3.21) that nonminimal couplings happen between $(R\,, R_c^2\,, R_m^2\,, \mathscr{L}_m)$ and $(R\,, R_c^2\,, R_m^2\,, T)$ respectively, and there is no matter-matter $\mathscr{L}_m$-T coupling which would cause severe theoretical complexity and physical ambiguity. In fact, $\mathscr{L}_m$ and T are not independent, as Eq.(3.11) implies that

$$T = g^{\alpha\beta}T_{\alpha\beta} = 4\mathscr{L}_m - 2g^{\alpha\beta}\frac{\delta\mathscr{L}_m}{\delta g^{\alpha\beta}}\,. \tag{3.23}$$

3.3 R^2-dependence, smooth transition to generalized Gauss-Bonnet gravity, and quadratic gravity

Generalized (Einstein-)Gauss-Bonnet gravity is perhaps the most popular and typical situation in which there is dependence on R and the quadratic invariants $\{R_c^2, R_m^2\}$ [7, 25]. However, to the best of our knowledge, there is no demonstration of how generic fourth-order model $f(R, R_c^2, R_m^2, \mathscr{L}_m)$ (or $f(R, R_c^2, R_m^2) + 2\kappa\mathscr{L}_m$ model if minimally coupled [8]) may be smoothly reduced into generalized Gauss-Bonnet theories. We tackle this problem by considering an explicit dependence on R^2 in $f(R, R_c^2, R_m^2, \mathscr{L}_m)$ gravity.

3.3.1 Two generic R^2-dependent models

Based on the $f(R, R_c^2, R_m^2, \mathscr{L}_m)$ gravity, we consider the following situation with an explicit dependence on R^2:

$$\mathscr{L} = f(R\,, R^2\,, R_c^2\,, R_m^2\,, \mathscr{L}_m)\,. \tag{3.24}$$

Here we have formally split the generic R-dependence of $f(R, R_c^2, R_m^2, \mathscr{L}_m)$ into an R- and R^2-dependence, $f_R\,\delta R \mapsto f_R\,\delta R + f_{R^2}\,\delta R^2$, to lay the foundation for subsequent discussion. However, this $f(R, R^2, R_c^2, R_m^2, \mathscr{L}_m)$ Lagrangian density is not more generic than $f(R, R_c^2, R_m^2, \mathscr{L}_m)$ by one more variable R^2. Absorbing f_{R^2} into

$\delta R^2 = 2R\,\delta R$ by the replacement $f_R \mapsto 2R\, f_{R^2}$ in Eq.(3.7), we learn that R^2-dependence would contribute to the field equation by

$$f_{R^2}\cdot\delta R^2 \;\cong\; \Big[2R\, f_{R^2}\cdot R_{\mu\nu} + 2\,(g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu)\,(R\cdot f_{R^2})\Big]\cdot\delta g^{\mu\nu} \;=:\; H^{(fR^2)}_{\mu\nu}\cdot\delta g^{\mu\nu}\,, \tag{3.25}$$

and a resubstitution of $f_R \mapsto f_R{+}2Rf_{R^2}$ into Eq.(3.12) directly yields the field equation for $f(R, R^2, R_c^2, R_m^2, \mathscr{L}_m)$ gravity,

$$-\frac{1}{2}f\, g_{\mu\nu} + f_R\, R_{\mu\nu} + (g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu)\, f_R + H^{(fR^2)}_{\mu\nu} + H^{(fR_c^2)}_{\mu\nu} + H^{(fR_m^2)}_{\mu\nu} \;=\; \frac{1}{2}f_{\mathscr{L}_m}\,(T_{\mu\nu} - \mathscr{L}_m\, g_{\mu\nu})\,, \tag{3.26}$$

where $\{f, f_R, f_{R^2}\}$ and the $\{f_{R_c^2}, f_{R_m^2}\}$ in $\{H^{(fR_c^2)}_{\mu\nu} + H^{(fR_m^2)}_{\mu\nu}\}$ are all functions of $(R, R^2, R_c^2, R_m^2, \mathscr{L}_m)$.

Here we have assumed no ambiguity between the R-dependence and the R^2-dependence in Eq.(3.24). To explicitly avoid this problem, one could consider a Lagrangian density of the form,

$$\mathscr{L} \;=\; \tilde{f}(R) + f(R^2\,, R_c^2\,, R_m^2\,, \mathscr{L}_m)\,. \tag{3.27}$$

However, potential coupling between R^2 and $\mathscr{L}_m$ can still be turned around and retreated as $R - \mathscr{L}_m$ coupling, so this $\tilde{f}(R) + f(R^2, R_c^2, R_m^2, \mathscr{L}_m)$ model is still equally generic with $f(R, R_c^2, R_m^2, \mathscr{L}_m)$ as well as the $f(R, R^2, R_c^2, R_m^2, \mathscr{L}_m)$ just above. Setting $f \mapsto \tilde{f} + f$ and $f_R \mapsto \tilde{f}_R + 2Rf_{R^2}$ in Eq.(3.12), we get the field equation for Eq.(3.27),

$$-\frac{1}{2}(\tilde{f} + f)\, g_{\mu\nu} + \tilde{f}_R\, R_{\mu\nu} + (g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu)\, \tilde{f}_R + H^{(fR^2)}_{\mu\nu} + H^{(fR_c^2)}_{\mu\nu} + H^{(fR_m^2)}_{\mu\nu} \;=\; \frac{1}{2}f_{\mathscr{L}_m}\,(T_{\mu\nu} - \mathscr{L}_m\, g_{\mu\nu})\,, \tag{3.28}$$

where $\tilde{f}_R = \tilde{f}_R(R)$, $f_{R^2} = f_{R^2}(R^2, R_c^2, R_m^2, \mathscr{L}_m)$, and $\{f_{R_c^2}, f_{R_m^2}\}$ remain dependent on $(R, R^2, R_c^2, R_m^2, \mathscr{L}_m)$. Moreover, Eq.(3.28) can instead be obtained from Eq.(3.26) by the replacement $f_R \mapsto \tilde{f}_R$.

For subsequent investigations, it will be sufficient to just employ the former model $\mathscr{L} = f(R, R^2, R_c^2, R_m^2, \mathscr{L}_m)$ and its field equation (3.26).

3.3.2 Reduced field equation with $f_{R^2} = f_{R_m^2} = -f_{R_c^2}/4$

Now recall that the second Bianchi identity $\nabla_\gamma R_{\alpha\mu\beta\nu} + \nabla_\nu R_{\alpha\mu\gamma\beta} + \nabla_\beta R_{\alpha\mu\nu\gamma} = 0$ implies the following simplifications, which rewrite the derivative of a high-rank curvature tensor into that of lower-rank curvature tensors plus nonlinear algebraic terms:

$$\nabla^\alpha R_{\alpha\mu\beta\nu} \;=\; \nabla_\beta R_{\mu\nu} - \nabla_\nu R_{\mu\beta} \tag{3.29}$$

$$\nabla^\alpha R_{\alpha\beta} \;=\; \frac{1}{2}\,\nabla_\beta R \tag{3.30}$$

$$\nabla^\beta\nabla^\alpha R_{\alpha\beta} \;=\; \frac{1}{2}\,\Box R \tag{3.31}$$

$$\nabla^\beta\nabla^\alpha R_{\alpha\mu\beta\nu} \;=\; \Box R_{\mu\nu} \;-\; \frac{1}{2}\nabla_\mu\nabla_\nu R + R_{\alpha\mu\beta\nu}R^{\alpha\beta} - R_\mu{}^\alpha R_{\alpha\nu} \tag{3.32}$$

$$\nabla^\alpha\nabla_\mu R_{\alpha\nu} + \nabla^\alpha\nabla_\nu R_{\alpha\mu} \;=\; \nabla_\mu\nabla_\nu R - 2R_{\alpha\mu\beta\nu}R^{\alpha\beta} + 2R_\mu{}^\alpha R_{\alpha\nu}\,, \tag{3.33}$$

along with the symmetry $\nabla^\beta\nabla^\alpha R_{\alpha\mu\beta\nu} = \nabla^\beta\nabla^\alpha R_{\alpha\nu\beta\mu}$ and $\nabla^\alpha\nabla_\mu R_{\alpha\nu} + \nabla^\alpha\nabla_\nu R_{\alpha\mu} = 2\,(\Box R_{\mu\nu} - \nabla^\beta\nabla^\alpha R_{\alpha\mu\beta\nu})$. Applying these relations to expand all the second-order covariant derivatives in Eq.(3.26), it turns out that:

Theorem: When the coefficients $\{f_{R^2}, f_{R_c^2}, f_{R_m^2}\}$ satisfy the following proportionality conditions,

$$f_{R^2} \;=\; f_{R_m^2} \;= -\frac{1}{4} f_{R_c^2} \;=:\; F\,, \tag{3.34}$$

where $F = F(R, R^2, R_c^2, R_m^2, \mathscr{L}_m)$, then the field equation (3.26) reduces to

$$-\frac{1}{2} f\, g_{\mu\nu} + f_R\, R_{\mu\nu} + (g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu)\, f_R + \mathcal{H}_{\mu\nu}^{(F)} \;=\; \frac{1}{2} f_{\mathscr{L}_m}\,(T_{\mu\nu} - \mathscr{L}_m\, g_{\mu\nu})\,, \tag{3.35}$$

where

$$\begin{aligned}
\mathcal{H}_{\mu\nu}^{(F)} \;:=\;& 2R f_{R^2}\cdot R_{\mu\nu} - 4 f_{R_m^2}\cdot R_\mu{}^\alpha R_{\alpha\nu} + (2 f_{R_c^2} + 4 f_{R_m^2})\cdot R_{\alpha\mu\beta\nu} R^{\alpha\beta} + 2 f_{R_m^2}\cdot R_{\mu\alpha\beta\gamma} R_\nu{}^{\alpha\beta\gamma} \\
&+ 2R(g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu)\, f_{R^2} - R_\mu{}^\alpha \nabla_\alpha\nabla_\nu f_{R_c^2} - R_\nu{}^\alpha\nabla_\alpha\nabla_\mu f_{R_c^2} + R_{\mu\nu}\Box f_{R_c^2} \\
&+ g_{\mu\nu}\cdot R^{\alpha\beta}\nabla_\alpha\nabla_\beta f_{R_c^2} + 4\, R_{\alpha\mu\beta\nu}\nabla^\beta\nabla^\alpha f_{R_m^2} \quad (f_{R^2} = f_{R_m^2} = -f_{R_c^2}/4) \\
\equiv\;& 2RF\cdot R_{\mu\nu} - 4F\cdot R_\mu{}^\alpha R_{\alpha\nu} - 4F\cdot R_{\alpha\mu\beta\nu}R^{\alpha\beta} + 2F\cdot R_{\mu\alpha\beta\gamma}R_\nu{}^{\alpha\beta\gamma} \\
&+ 2R(g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu)\, F + 4R_\mu{}^\alpha\nabla_\alpha\nabla_\nu F + 4R_\nu{}^\alpha\nabla_\alpha\nabla_\mu F \\
&- 4R_{\mu\nu}\Box F - 4g_{\mu\nu}\cdot R^{\alpha\beta}\nabla_\alpha\nabla_\beta F + 4\, R_{\alpha\mu\beta\nu}\nabla^\beta\nabla^\alpha F\,.
\end{aligned} \tag{3.36}$$

$\mathcal{H}_{\mu\nu}^{(F)}\delta g^{\mu\nu} = f_F\,\delta F$ and second-order-derivative operators $\{\Box, \nabla_\alpha\nabla_\nu, \text{etc}\}$ only act on the scalar functions $\{f_{R^2}, f_{R_c^2}, f_{R_m^2}\}$ in contrast to $H_{\mu\nu}^{(fR^2)} + H_{\mu\nu}^{(fR_c^2)} + H_{\mu\nu}^{(fR_m^2)}$ in Eq.(3.24)[2].

Note that similar techniques have been employed in [24] to finalize the field equation of the dilaton-Gauss-Bonnet model. The simplified field equation (3.35) after imposing the proportionality condition Eq.(3.34) to Eq.(3.26) will serve as a bridge connecting $f(R, R^2, R_c^2, R_m^2, \mathscr{L}_m)$ gravity to generalized Gauss-Bonnet gravity. We refer to the proportionality condition Eq.(3.34) as the *coherence condition* to highlight the fact that it aligns the behaviors of $\{f_{R^2}, f_{R_c^2}, f_{R_m^2}\}$, and call F therein the *coherence function*.

3.3.3 Generalized Gauss-Bonnet gravity with nonminimal coupling

Generic $\mathscr{L} = f(R, \mathcal{G}, \mathscr{L}_m)$ model

A nice way to realize the coherence condition Eq.(3.34) is to let $\{R^2, R_c^2, R_m^2\}$ participate in the action through the well-known Gauss-Bonnet invariant $\mathcal{G}$,

$$\mathcal{G} \;:=\; R^2 - 4R_c^2 + R_m^2\,. \tag{3.37}$$

In this case, Eq.(3.24) reduces to become the Lagrangian density of a generalized Gauss-Bonnet gravity model allowing nonminimal curvature-matter coupling,

$$\mathscr{L} \;=\; f(R\,, \mathcal{G}\,, \mathscr{L}_m)\,. \tag{3.38}$$

[2]This is also why we use the denotation $\mathcal{H}_{\mu\nu}^{(F)}$ rather than $H_{\mu\nu}^{(F)}$

Then the proportionality in Eq.(3.34) is naturally satisfied with the coherence function F recognized as $f_{\mathcal{G}} := \partial f/\partial\mathcal{G}$. Given $F \mapsto f_{\mathcal{G}}$, Eqs.(3.36) and (3.35) give rise to the field equation for $f(R,\mathcal{G},\mathscr{L}_m)$ gravity right away,

$$-\frac{1}{2}f\,g_{\mu\nu} + f_R\,R_{\mu\nu} + (g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu)\,f_R + \mathcal{H}^{(\mathrm{GB})}_{\mu\nu} \;=\; \frac{1}{2}\,f_{\mathscr{L}_m}\,(T_{\mu\nu} - \mathscr{L}_m\,g_{\mu\nu})\,, \tag{3.39}$$

where

$$\begin{aligned}\mathcal{H}^{(\mathrm{GB})}_{\mu\nu} := {}& 2f_{\mathcal{G}}\cdot RR_{\mu\nu} - 4f_{\mathcal{G}}\cdot R_\mu{}^\alpha R_{\alpha\nu} - 4f_{\mathcal{G}}\cdot R_{\alpha\mu\beta\nu}R^{\alpha\beta} + 2f_{\mathcal{G}}\cdot R_{\mu\alpha\beta\gamma}R_\nu{}^{\alpha\beta\gamma} + 2R\,(g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu)\,f_{\mathcal{G}}\\ & + 4R_\mu{}^\alpha\nabla_\alpha\nabla_\nu f_{\mathcal{G}} + 4R_\nu{}^\alpha\nabla_\alpha\nabla_\mu f_{\mathcal{G}} - 4R_{\mu\nu}\Box f_{\mathcal{G}} - 4g_{\mu\nu}\cdot R^{\alpha\beta}\nabla_\alpha\nabla_\beta f_{\mathcal{G}} + 4\,R_{\alpha\mu\beta\nu}\nabla^\beta\nabla^\alpha f_{\mathcal{G}}\,,\end{aligned} \tag{3.40}$$

and $\{f, f_R, f_{\mathcal{G}}\}$ are all functions of $(R,\mathcal{G},\mathscr{L}_m)$, and $\mathcal{H}^{(\mathrm{GB})}_{\mu\nu}\delta g^{\mu\nu} = f_{\mathcal{G}}\,\delta\mathcal{G}$.

No contributions from a pure Gauss-Bonnet term

As for the $\mathcal{G}$-dependence, Eqs.(3.39) and (3.40) are best simplified when $f_{\mathcal{G}} = \lambda$ =constant; that is to say, $\mathcal{G}$ joins $\mathscr{L}$ straightforwardly as a pure Gauss-Bonnet term, with Lagrangian density $\mathscr{L} = f(R,\mathscr{L}_m) + \lambda\mathcal{G}$, for which Eq.(3.39) gives rise to the field equation (with $f = f(R,\mathscr{L}_m)$, $f_R = f_R(R,\mathscr{L}_m)$):

$$\begin{aligned}&\lambda\cdot\Big(-\frac{1}{2}\mathcal{G}\,g_{\mu\nu} + 2R\,R_{\mu\nu} - 4R_\mu{}^\alpha R_{\alpha\nu} - 4R_{\alpha\mu\beta\nu}R^{\alpha\beta} + 2R_{\mu\alpha\beta\gamma}R_\nu{}^{\alpha\beta\gamma}\Big)\\ &-\frac{1}{2}f\,g_{\mu\nu} + f_R\,R_{\mu\nu} + (g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu)\,f_R = \frac{1}{2}f_{\mathscr{L}_m}\,(T_{\mu\nu} - \mathscr{L}_m\,g_{\mu\nu})\,.\end{aligned} \tag{3.41}$$

At first glance, it may seem that, after $\mathcal{G}$ decouples from $f(R,\mathcal{G},\mathscr{L}_m)$ to form a pure term $\lambda\,\mathcal{G}$, the isolated covariant density $\lambda\sqrt{-g}\,\mathcal{G}$ would still make a difference to the field equation by the $\lambda\cdot(\ldots)$ term in Eq.(3.41). This result conflicts our *a priori* anticipation that, since $\mathcal{G}$ is a topological invariant, variation of the Euler-Poincaré topological density $\sqrt{-g}\,\mathcal{G}$ should not change the gravitational field equation. In fact, by setting $f_{R^2} = f_{R_c^2} = f_{R_m^2} = 1$ in Eqs.(3.8), (3.9) and (3.25), one has

$$\delta R^2/\delta g^{\mu\nu} \;=\; 2R\,R_{\mu\nu} + 2\,(g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu)\,R\,, \tag{3.42}$$

$$\delta R_c^2/\delta g^{\mu\nu} \;=\; 2R_\mu{}^\alpha R_{\alpha\nu} - \nabla_\alpha\nabla_\nu R_\mu{}^\alpha - \nabla_\alpha\nabla_\mu R_\nu{}^\alpha + \Box R_{\mu\nu} + g_{\mu\nu}\cdot\nabla_\alpha\nabla_\beta R^{\alpha\beta}\,,\quad\text{and} \tag{3.43}$$

$$\delta R_m^2/\delta g^{\mu\nu} \;=\; 2\,R_{\mu\alpha\beta\gamma}R_\nu{}^{\alpha\beta\gamma} + 4\,\nabla^\beta\nabla^\alpha R_{\alpha\mu\beta\nu}\,, \tag{3.44}$$

which together with the Bianchi implications Eqs.(3.29)-(3.33) exactly lead to

$$\delta\,(\sqrt{-g}\,\mathcal{G})/\delta g^{\mu\nu} \;=\; -\frac{1}{2}\mathcal{G}\,g_{\mu\nu} + 2R\,R_{\mu\nu} - 4R_\mu{}^\alpha R_{\alpha\nu} - 4R_{\alpha\mu\beta\nu}R^{\alpha\beta} + 2R_{\mu\alpha\beta\gamma}R_\nu{}^{\alpha\beta\gamma}\,. \tag{3.45}$$

Thus one can recover the term $\lambda\cdot(\ldots)$ in Eq.(3.41) by directly varying the quadratic invariants comprising $\mathcal{G}$.

However, in four dimensions $\mathcal{G}$ is a most special invariant among all algebraic and differential Riemannian invariants $\mathcal{R} = \mathcal{R}(g_{\alpha\beta}, R_{\alpha\mu\beta\nu}, \nabla_\gamma R_{\alpha\mu\beta\nu}, \ldots, \nabla_{\gamma_1}\nabla_{\gamma_2}\ldots\nabla_{\gamma_n}R_{\alpha\mu\beta\nu})$ in the sense that it respects the Bach-Lanczos identity

$$\delta\int dx^4\,\sqrt{-g}\,\mathcal{G} \;\equiv\; 0\,, \tag{3.46}$$

which prevents the Gauss-Bonnet covariant density $\lambda\sqrt{-g}\,\mathcal{G}$ from contributing to the field equation. This identity can be verified by carrying out the variational derivative [19, 26]

$$\frac{\delta(\sqrt{-g}\,\mathcal{G})}{\delta g^{\mu\nu}} = \frac{\partial(\sqrt{-g}\,\mathcal{G})}{\partial g^{\mu\nu}} - \partial_\alpha \frac{\partial(\sqrt{-g}\,\mathcal{G})}{\partial(\partial_\alpha g^{\mu\nu})} + \partial_\alpha\partial_\beta \frac{\partial(\sqrt{-g}\,\mathcal{G})}{\partial(\partial_\alpha\partial_\beta g^{\mu\nu})} \equiv 0\,. \tag{3.47}$$

On the other hand, algebraic identities satisfied by the Riemann tensor also guarantee that $-\frac{1}{2}\mathcal{G}\,g_{\mu\nu} + 2R\,R_{\mu\nu} - 4R_\mu{}^\alpha R_{\alpha\nu} - 4R_{\alpha\mu\beta\nu}R^{\alpha\beta} + 2R_{\mu\alpha\beta\gamma}R_\nu{}^{\alpha\beta\gamma} = 0$ [19].

Hence, the $\lambda\cdot(\dots)$ term in Eq.(3.41), as a remnant of degrading the generic $f(R, \mathcal{G}, \mathcal{L}_m)$ gravity and all existing generalized Gauss-Bonnet theories, is removable, and Eq.(3.41) for $\mathcal{L} = f(R, \mathcal{L}_m) + \lambda\mathcal{G}$ gravity finally becomes

$$-\frac{1}{2} f\, g_{\mu\nu} + f_R\, R_{\mu\nu} + (g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu)\, f_R = \frac{1}{2}\, f_{\mathcal{L}_m}\,(T_{\mu\nu} - \mathcal{L}_m\, g_{\mu\nu})\,, \tag{3.48}$$

which coincides with the field equation of $\mathcal{L} = f(R, \mathcal{L}_m)$ gravity [13]. Although a pure Gauss-Bonnet term in the Lagrangian density cannot change the gravitational field equation $\delta(\sqrt{-g}\,\mathcal{L})/\delta g^{\mu\nu} = 0$, it does join the dynamical equation $\delta(\sqrt{-g}\,\mathcal{L})/\delta\phi = 0$ when $\mathcal{G}$ is coupled to a scalar field $\phi(x^a)$ (e.g. [24]), and can still cause nontrivial effects in other aspects (e.g. [17]).

Recovery of some typical models

$f(R, \mathcal{G}, \mathcal{L}_m)$ is the maximally generalized Gauss-Bonnet gravity when $\{R, \mathcal{G}, \mathcal{L}_m\}$ are the only scalar invariants taken into account, and all existing $(R, \mathcal{G}, \mathcal{L}_m)$-dependent models can be recovered as a specialized $f(R, \mathcal{G}, \mathcal{L}_m)$ gravity. For example,

Reference	Lagrangian density	Specialization
[7]	$R/(2\kappa^2) + f(\mathcal{G}) + \mathcal{L}_m$	$f_R \mapsto 1/(2\kappa^2)\,,\ f_\mathcal{G} \mapsto f_\mathcal{G}\,,\ f_{\mathcal{L}_m} \mapsto 1$
[12]	$R/2 + \mathcal{L}_m + \lambda\, f(\mathcal{G})\,\mathcal{L}_m$	$f_R \mapsto 1/2\,,\ f_\mathcal{G} \mapsto \lambda\mathcal{L}_m f_\mathcal{G}\,,\ f_{\mathcal{L}_m} \mapsto 1 + \lambda f(\mathcal{G})$
[12]	$R/2 + f(\mathcal{G}) + \mathcal{L}_m + \lambda\, F(\mathcal{G})\,\mathcal{L}_m$	$f_R \mapsto 1/2\,,\ f_\mathcal{G} \mapsto f_\mathcal{G} + \lambda\mathcal{L}_m F_\mathcal{G}\,,\ f_{\mathcal{L}_m} \mapsto 1 + \lambda F(\mathcal{G})$
[25]	$f(R, \mathcal{G}) + 2\kappa\mathcal{L}_m$	$f_R \mapsto f_R\,,\ f_\mathcal{G} \mapsto f_\mathcal{G}\,,\ f_{\mathcal{L}_m} \mapsto 2\kappa$

For a detailed review of generalized Gauss-Bonnet gravity, see [6] in which various types of nonminimal coupling are also extensively discussed.

3.3.4 Quadratic gravity

Following the discussion of (generalized) Gauss-Bonnet gravity, we would like to revisit the simplest case with R_c^2-dependence (and R_m^2-dependence), the so-called quadratic gravity (e.g. [17]):

$$\begin{aligned}\mathscr{L} &= R + \tilde{a}\cdot R^2 + \tilde{b}\cdot R_c^2 + \tilde{c}\cdot R_m^2 + \tilde{d}\cdot R_S^2 + \tilde{e}\cdot C^2 + 2\kappa\mathscr{L}_m \qquad (3.49)\\ &= R + (\tilde{a} - \tilde{c} - \tilde{d}/4 - 2\tilde{e}/3)\cdot R^2 + (\tilde{b} + 4\tilde{c} + \tilde{d} + 2\tilde{e})\cdot R_c^2 + (\tilde{c} + \tilde{e})\cdot\mathcal{G} + 2\kappa\mathscr{L}_m\\ &\cong R + a\cdot R^2 + b\cdot R_c^2 + 2\kappa\mathscr{L}_m\,. \qquad (3.50)\end{aligned}$$

The first row is a general linear superposition of some popular quadratic invariants $\{R^2, R_c^2, R_m^2, R_S^2, C^2\}$ with constant coefficients $\{\tilde{a}, \tilde{b}, \ldots\}$, where $\{R_S^2 = R_c^2 - R^2/4\,, C^2 = R_m^2 - 2R_c^2 + R^2/3\}$ respectively denote the square of traceless Ricci tensor and Weyl tensor (see the next subsection). In Eq.(3.50) the pure Gauss-Bonnet term $(\tilde{c} + \tilde{d})\cdot\mathcal{G}$ has been neglected for reasons indicated above. Substitution of

$$f_R \mapsto 1\,, \quad f_{R^2} \mapsto a\,, \quad f_{R_c^2} \mapsto b\,, \quad f_{R_m^2} \mapsto 0 \text{ and } \quad f_{\mathscr{L}_m} \mapsto 2\kappa \qquad (3.51)$$

into Eq.(3.26) and Eq.(3.13) yields the field equation for the quadratic Lagrangian density Eq.(3.50),

$$-\frac{1}{2}(R + a\cdot R^2 + b\cdot R_c^2)\, g_{\mu\nu} + (1 + 2aR)\, R_{\mu\nu} + 2a\,(g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu)\, R + H_{\mu\nu}^{(\text{QRc})} = \kappa\, T_{\mu\nu}\,, \qquad (3.52)$$

where

$$H_{\mu\nu}^{(\text{QRc})} = b\cdot\Big(2R_\mu{}^\alpha R_{\alpha\nu} - \nabla_\alpha\nabla_\nu R_\mu{}^\alpha - \nabla_\alpha\nabla_\mu R_\nu{}^\alpha + \Box R_{\mu\nu} + g_{\mu\nu}\nabla_\alpha\nabla_\beta R^{\alpha\beta}\Big). \qquad (3.53)$$

Moreover, via the Bianchi implications Eq.(3.31) and Eq.(3.33), $H_{\mu\nu}^{(\text{QRc})}$ can be rewritten as

$$H_{\mu\nu}^{(\text{QRc})} = b\cdot\Big(2R_{\alpha\mu\beta\nu}R^{\alpha\beta} + (\frac{1}{2}\, g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu)\, R + \Box R_{\mu\nu}\Big). \qquad (3.54)$$

Using this to rewrite Eq.(3.52), we obtain the commonly used form of the field equation [17, 18].

On the other hand, one can instead drop the Ricci square in favor of the Kretschmann scalar, and accordingly manipulate Eq.(3.49) via

$$\begin{aligned}\mathscr{L} &= R + (\tilde{a} + \tilde{b}/4 - \tilde{e}/6)\cdot R^2 + (\tilde{b}/4 + \tilde{c} + \tilde{d}/4 + 2\tilde{e})/2\cdot R_m^2 - (\tilde{b}/4 + \tilde{d}/4 - \tilde{e}/2)\cdot\mathcal{G} + 2\kappa\mathscr{L}_m\\ &\cong R + a\cdot R^2 + b\cdot R_m^2 + 2\kappa\mathscr{L}_m\,. \qquad (3.55)\end{aligned}$$

Now, substitute $f_R \mapsto 1$, $f_{R^2} \mapsto a$, $f_{R_c^2} \mapsto 0$, $f_{R_m^2} \mapsto b$ and $f_{\mathscr{L}_m} \mapsto 2\kappa$ into Eqs.(3.26) and (3.13) to obtain

$$-\frac{1}{2}(R + a\cdot R^2 + b\cdot R_m^2)\, g_{\mu\nu} + (1 + 2aR)\, R_{\mu\nu} + 2b\,(g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu)\, R + H_{\mu\nu}^{(\text{QRm})} = \kappa\, T_{\mu\nu}\,, \qquad (3.56)$$

where

$$H_{\mu\nu}^{(\text{QRm})} = b\cdot\Big(2R_{\mu\alpha\beta\gamma}R_\nu{}^{\alpha\beta\gamma} + 4\nabla^\beta\nabla^\alpha R_{\alpha\mu\beta\nu}\Big), \qquad (3.57)$$

and $H_{\mu\nu}^{(\text{QRm})}$ can be recast by the Bianchi property Eq.(3.33) into

$$H_{\mu\nu}^{(\text{QRm})} = b\cdot\Big(2R_{\mu\alpha\beta\gamma}R_\nu{}^{\alpha\beta\gamma} + 4R_{\alpha\mu\beta\nu}R^{\alpha\beta} - 4R_\mu{}^\alpha R_{\alpha\nu} + 4\Box R_{\mu\nu} - 2\nabla_\mu\nabla_\nu R\Big). \qquad (3.58)$$

3.3.5 Field equations with traceless Ricci and Riemann squares

It is worthwhile to mention that, as is well known in Riemann geometry, many other tensors can be built algebraically out of $\{R^2, R_{\alpha\beta}, R_{\alpha\mu\beta\nu}\}$ with their squares recast into $\{R, R_c^2, R_m^2\}$, such as the traceless Ricci tensor, traceless Riemann tensor (Weyl tensor), Schouten tensor, Plebanski tensor, Bel-Robinson tensor, etc. It can be convenient or sometimes preferable for specific purposes to employ these tensors in the field equation, so in this subsection we will take a quick look at how the squares of these tensors in the Lagrangian density contribute to the gravitational field equation. It is unnecessary to exhaust all these tensors here and we will just consider the squares of traceless Ricci tensor and Weyl tensor as an example.

Traceless Ricci square

The traceless counterpart of Ricci tensor $S_{\alpha\beta}$ ($g^{\alpha\beta}S_{\alpha\beta}=0$) and its square (denoted as R_S^2) is,

$$S_{\alpha\beta} \;=\; R_{\alpha\beta} - \frac{1}{4} R\, g_{\alpha\beta} \quad\Rightarrow\quad R_S^2 \;\coloneqq\; S_{\alpha\beta}S^{\alpha\beta} = R_c^2 - \frac{1}{4} R^2\,. \tag{3.59}$$

Consider $f(\ldots, R_S^2)$ as a generic function of R_S^2, where $\ldots$ collects the dependence on all other possible scalar invariants, and the variation $\delta f(\ldots, R_S^2) = \delta f(\ldots, R_c^2 - R^2/4)$ yields

$$f_{R_S^2}\cdot \delta R_S^2 \;=\; f_{R_S^2}\cdot\Big(\frac{\partial R_S^2}{\partial R_c^2}\,\delta R_c^2 + \frac{\partial R_S^2}{\partial R}\,\delta R\Big) \;=\; f_{R_S^2}\cdot\Big(\delta R_c^2 - \frac{1}{2} R\,\delta R\Big). \tag{3.60}$$

Absorbing $f_{R_S^2}$ into δR_c^2 by replacing $f_{R_c^2}$ with $f_{R_S^2}$ in Eq.(3.8), merging $R\,f_{R_S^2}$ into δR by replacing f_R with $R\,f_{R_S^2}$ in Eq.(3.7), and finally replacing all Ricci tensors in $f_{R_S^2}\delta R_c^2$ and $R\,f_{R_S^2}\,\delta R$ by their traceless counterparts $R_{\alpha\beta} = S_{\alpha\beta} + R g_{\alpha\beta}/4$, then $f_{R_S^2}\cdot\big(\delta R_c^2 - \frac{1}{2}R\,\delta R\big) = f_{R_S^2}\cdot\delta R_S^2$ becomes

$$\begin{aligned} f_{R_S^2}\cdot\delta R_S^2 \;=\; &\Big[2 f_{R_S^2}\, S_\mu{}^\alpha S_{\alpha\nu} - \frac{1}{2} R\, f_{R_S^2}\, S_{\mu\nu} - \nabla_\alpha\nabla_\nu(S_\mu{}^\alpha f_{R_S^2}) \\ &-\nabla_\alpha\nabla_\mu(S_\nu{}^\alpha f_{R_S^2}) + \Box(S_{\mu\nu} f_{R_S^2}) + g_{\mu\nu}\nabla_\alpha\nabla_\beta(S^{\alpha\beta} f_{R_S^2})\Big]\cdot\delta g^{\mu\nu} \eqqcolon H_{\mu\nu}^{(fR_S^2)}\cdot\delta g^{\mu\nu}\,, \end{aligned} \tag{3.61}$$

which is consistent with the field equation in [22]. Thus, for a Lagrangian density dependent on the traceless Ricci square $\mathscr{L} = f(\ldots, R_S^2)$, the contributions of $f_{R_S^2}\cdot\delta R_S^2$ to the field equation is just $H_{\mu\nu}^{(fR_S^2)}$ as in Eq.(3.61).

Weyl square

Being the totally traceless part of the Riemann tensor in the Ricci decomposition, the Weyl conformal tensor $C_{\alpha\beta\gamma\delta}$ ($g^{\alpha\gamma}g^{\beta\delta}C_{\alpha\beta\gamma\delta}=0$) and its square (denoted as C^2) are respectively

$$C_{\alpha\beta\gamma\delta} \;=\; R_{\alpha\beta\gamma\delta} + \frac{1}{2}\Big(g_{\alpha\delta}R_{\beta\gamma} - g_{\alpha\gamma}R_{\beta\delta} + g_{\beta\gamma}R_{\alpha\delta} - g_{\beta\delta}R_{\alpha\gamma}\Big) + \frac{1}{6}\Big(g_{\alpha\gamma}g_{\beta\delta} - g_{\alpha\delta}g_{\beta\gamma}\Big)R\,, \quad\text{and} \tag{3.62}$$

$$C^2 \;\coloneqq\; C_{\alpha\mu\beta\nu}C^{\alpha\mu\beta\nu} \;=\; R_m^2 - 2R_c^2 + \frac{1}{3}R^2 \;=\; R_m^2 - 2R_S^2 - \frac{1}{6}R^2 \;=\; \mathcal{G} + 2R_c^2 - \frac{2}{3}R^2\,. \tag{3.63}$$

Given a function $f(\dots,C^2) = f(\dots,R_m^2 - 2R_c^2 + R^2/3) = f(\dots,R_m^2 - 2R_S^2 - R^2/6) = f(\dots,\mathcal{G} + 2R_c^2 - 2R^2/3)$, the variation $\delta f(\dots,C^2)$ yields

$$f_{C^2}\cdot\delta C^2 \;=\; f_{C^2}\cdot\Big(\delta R_m^2 - 2\,\delta R_c^2 + \frac{2}{3}\,R\,\delta R\Big) \;=\; f_{C^2}\cdot\Big(\delta R_m^2 - 2\,\delta R_S^2 - \frac{1}{3}\,R\,\delta R\Big) \;=\; f_{C^2}\cdot\Big(\delta\mathcal{G} + 2\,\delta R_c^2 - \frac{4}{3}\,R\,\delta R\Big)\,. \tag{3.64}$$

Which of these expressions is most convenient to use will depend on which other Riemann invariants are involved in the Lagrangian density. As such we stop at this stage: the exact expression of $H_{\mu\nu}^{(fC^2)}\delta g^{\mu\nu} := f_{C^2}\delta C^2$ depends on which expansion we choose for C^2.

3.4 Nonminimal coupling and energy-momentum divergence

From this section on, we switch our attention to another important aspect of $\mathscr{L} = f(R, R_c^2, R_m^2, \mathscr{L}_m)$ gravity: the stress-energy-momentum-conservation problem. Taking the contravariant derivative of the field equation (3.12), we find

$$f_{\mathscr{L}_m}\nabla^\mu T_{\mu\nu} \;=\; (\mathscr{L}_m\, g_{\mu\nu} - T_{\mu\nu})\,\nabla^\mu f_{\mathscr{L}_m} - f_R\nabla_\nu R - f_{R_c^2}\nabla_\nu R_c^2 - f_{R_m^2}\nabla_\nu R_m^2 + 2\nabla^\mu H_{\mu\nu}^{(fR)} + 2\nabla^\mu H_{\mu\nu}^{(fR_c^2)} + 2\nabla^\mu H_{\mu\nu}^{(fR_m^2)}\,, \tag{3.65}$$

where $\{f, f_R, f_{R_c^2}, f_{R_m^2}\}$ remain as functions of the invariants $(R, R_c^2, R_m^2, \mathscr{L}_m)$, and $\{H_{\mu\nu}^{(fR)}, H_{\mu\nu}^{(fR_c^2)}, H_{\mu\nu}^{(fR_m^2)}\}$ have already been concretized in Eqs.(3.7)-(3.9). However, despite the extended variable-dependence in $f_R(R, R_c^2, R_m^2, \mathscr{L}_m)$ as opposed to $f(R) + 2\kappa\mathscr{L}_m$ gravity, we still have[3]

$$\frac{1}{2}\Big(-f_R\nabla_\nu R + 2\nabla^\mu H_{\mu\nu}^{(fR)}\Big) \;=\; -f_R\,\nabla^\mu\Big(\frac{1}{2}\,R\,g_{\mu\nu}\Big) + \nabla^\mu(\,f_R\cdot R_{\mu\nu}\,) + (\nabla_\nu\Box - \Box\nabla_\nu)\,f_R \;=\; 0\,. \tag{3.66}$$

It vanishes as a consequence of the contracted Bianchi identity $\nabla^\mu(R_{\mu\nu} - Rg_{\mu\nu}/2) = 0$ and the third-order-derivative commutation relation $(\Box\nabla_\nu - \nabla_\nu\Box)f_R = R_{\mu\nu}\nabla^\nu f_R$. Thus, Eq.(3.65) further reduces to

$$f_{\mathscr{L}_m}\nabla^\mu T_{\mu\nu} \;=\; (\mathscr{L}_m\, g_{\mu\nu} - T_{\mu\nu})\,\nabla^\mu f_{\mathscr{L}_m} - f_{R_c^2}\nabla_\nu R_c^2 - f_{R_m^2}\nabla_\nu R_m^2 + 2\nabla^\mu H_{\mu\nu}^{(fR_c^2)} + 2\nabla^\mu H_{\mu\nu}^{(fR_m^2)}\,, \tag{3.67}$$

which constitutes the equation of energy-momentum divergence in $f(R, R_c^2, R_m^2, \mathscr{L}_m)$ gravity. It can be regarded as a generalization of the following divergence equation in $f(R, \mathscr{L}_m)$ gravity [13],

$$\nabla^\mu T_{\mu\nu} \;=\; (\mathscr{L}_m\, g_{\mu\nu} - T_{\mu\nu})\,\nabla^\mu \ln f_{\mathscr{L}_m}\,, \tag{3.68}$$

with $\nabla^\mu \ln f_{\mathscr{L}_m} \equiv f_{\mathscr{L}_m}^{-1}\nabla^\mu f_{\mathscr{L}_m}$, which in turn can be recovered from Eq.(3.67) by setting $f_{R_c^2} = 0 = f_{R_m^2}$.

In standard GR, $\nabla^\mu T_{\mu\nu} = 0$ is the mathematical expression of conservation of stress-energy-momentum. However for our models it is clear that this does not vanish and so this fundamental conservation law does not hold in the standard form. Then, how to understand the energy-momentum nonconservation/divergence equation (3.67)? Is it further reducible and how does it influence the equations of continuity and motion given concrete matter sources? We will investigate these questions in a more generic framework.

[3] This is actually the stress-energy-momentum conservation condition of $f(R)$ gravity with Lagrangian density $\mathscr{L} = f(R) + 2\kappa\mathscr{L}_m$ and field equation $-f(R)\,g_{\mu\nu}/2 + f_R R_{\mu\nu} + (g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu)f_R = \kappa T_{\mu\nu}$, except that $f_R = f_R(R)$.

3.4.1 Automatic energy-momentum conservation under minimal coupling

Consider a generic gravitational Lagrangian $\mathscr{L}_G = f(\mathcal{R})$ where $f(\mathcal{R})$ is an arbitrary function of an $(n+2)$-order algebraic ($n = 0$) or differential ($n \geq 1$) Riemannian invariant $\mathcal{R}$:

$$\mathcal{R} = \mathcal{R}(g_{\alpha\beta}\,, R_{\alpha\mu\beta\nu}\,, \nabla_\gamma R_{\alpha\mu\beta\nu}\,, \ldots\,, \nabla_{\gamma_1}\nabla_{\gamma_2}\ldots\nabla_{\gamma_n} R_{\alpha\mu\beta\nu})\,, \tag{3.69}$$

so that variational derivative of the covariant density $\sqrt{-g}\,\mathscr{L}_G$ will lead to a $(2n+4)$-order model of gravity. Such an $\mathscr{L}_G = f(\mathcal{R})$ is still a covariant invariant for which Noether's conservation law would yield [27]

$$\nabla^\mu \left(\frac{1}{\sqrt{-g}} \frac{\delta\left(\sqrt{-g}\,f(\mathcal{R})\right)}{\delta g^{\mu\nu}} \right) = 0\,, \tag{3.70}$$

which can be expanded into

$$f_\mathcal{R}(\mathcal{R}) \cdot \nabla_\nu \mathcal{R} = 2\nabla^\mu H_{\mu\nu}^{(f\mathcal{R})} \quad \text{with} \quad H_{\mu\nu}^{(f\mathcal{R})} \cdot \delta g^{\mu\nu} := f_\mathcal{R} \cdot \delta\mathcal{R}\,, \tag{3.71}$$

where $H_{\mu\nu}^{(f\mathcal{R})}$ is defined the same way as $\{H_{\mu\nu}^{(fR)}, H_{\mu\nu}^{(fR_c^2)}, H_{\mu\nu}^{(fR_m^2)}\}$ in Eqs.(3.7)-(3.9). It absorbs $f_\mathcal{R}$ into $\delta\mathcal{R}$ and collects all nonlinear and higher-order terms generated by $f_\mathcal{R} \cdot \delta\mathcal{R}$.

These results can be directly generalized to the situation where $\mathscr{L}_G$ relies on multiple Riemannian invariants, $\mathscr{L}_G = f(\mathcal{R}_1, \mathcal{R}_2, \ldots, \mathcal{R}_p) \equiv \mathscr{L}_G(g_{\alpha\beta}, R_{\alpha\mu\beta\nu}, \nabla_\gamma R_{\alpha\mu\beta\nu}, \ldots, \nabla_{\gamma_1}\nabla_{\gamma_2}\ldots\nabla_{\gamma_q} R_{\alpha\mu\beta\nu})$, and we have

$$\sum_i f_{\mathcal{R}_i}\, \nabla_\nu \mathcal{R}_i = 2\sum_i \nabla^\mu H_{\mu\nu}^{(f\mathcal{R}_i)} \quad \text{with} \quad H_{\mu\nu}^{(f\mathcal{R}_i)} \cdot \delta g^{\mu\nu} := f_{\mathcal{R}_i} \cdot \delta\mathcal{R}_i\,, \tag{3.72}$$

where $f_{\mathcal{R}_i} = f_{\mathcal{R}_i}(\mathcal{R}_1\,, \mathcal{R}_2\,, \ldots\,, \mathcal{R}_p)$, with each $\mathcal{R}_i$ given by Eq.(3.69) to certain order derivatives of Riemann tensor, and $H_{\mu\nu}^{(f\mathcal{R}_i)} = H_{\mu\nu}^{(f\mathcal{R}_i)}(\mathcal{R}_1\,, \mathcal{R}_2\,, \ldots\,, \mathcal{R}_p)$ absorbs $f_{\mathcal{R}_i}$ into $\delta\mathcal{R}_i$.

Since $f(\mathcal{R}_1, \mathcal{R}_2, \ldots, \mathcal{R}_p)$ is a purely geometric entity solely dependent on the metric and derivatives of Riemann tensor, Eqs.(3.71) and (3.72) arising from Noether's theorem are also called the "generalized (contracted) Bianchi identities" [27, 28]. As the simplest example, when $f(\mathcal{R}_1, \mathcal{R}_2, \ldots, \mathcal{R}_p) = R$, Eq.(3.71) or Eq.(3.72) immediately reproduces the standard contracted Bianchi identity $\nabla^\mu(R_{\mu\nu} - Rg_{\mu\nu}/2) = 0$ which is often used in GR.

On the other hand, for the matter Lagrangian density $\mathscr{L}_m$, Noether's conservation law yields

$$\nabla^\mu \left(\frac{1}{\sqrt{-g}} \frac{\delta\left(\sqrt{-g}\,\mathscr{L}_m\right)}{\delta g^{\mu\nu}} \right) = 0 = -\frac{1}{2}\nabla^\mu T_{\mu\nu} \quad \text{with} \quad T_{\mu\nu} := \frac{-2}{\sqrt{-g}} \frac{\delta\left(\sqrt{-g}\,\mathscr{L}_m\right)}{\delta g^{\mu\nu}}\,, \tag{3.73}$$

where $T_{\mu\nu}$ is the standard stress-energy-momentum (SEM) tensor as in Eq.(3.10). This way of defining $T_{\mu\nu}$ from Noether's law therefore naturally guarantees energy-momentum conservation $\nabla^\mu T_{\mu\nu} = 0$. Moreover, in the case of minimal coupling, it is unnecessary to consider a covariant matter density of the form $\sqrt{-g}\,h(\mathscr{L}_m)$, since $h(\mathscr{L}_m)$ can always be treated as a whole, $h(\mathscr{L}_m) \mapsto \tilde{\mathscr{L}}_m$.

Hence, for a generic Lagrangian density where $\mathscr{L}_m$ is minimally coupled to the spacetime geometry:

$$\mathscr{L} = \mathscr{L}_G + 2\kappa\mathscr{L}_m = f(\mathcal{R}_1\,, \mathcal{R}_2\,, \ldots\,, \mathcal{R}_p) + 2\kappa\mathscr{L}_m\,, \tag{3.74}$$

and whose field equation arises from extremizing the action or equivalently $\frac{1}{\sqrt{-g}}\frac{\delta(\sqrt{-g}\,\mathscr{L})}{\delta g^{\mu\nu}}=0$:

$$-\frac{1}{2}f g_{\mu\nu}+\sum_i H^{(f\mathcal{R}_i)}_{\mu\nu} \;=\; \kappa T_{\mu\nu}\,, \tag{3.75}$$

the generalized Bianchi identities Eq.(3.72) for pure geometric $\mathscr{L}_G$ together with the Noether-type definition of $T_{\mu\nu}$ in Eq.(3.73) yield that contravariant derivatives of the left (geometry) and right (matter) - hand side of the field equation (3.75) vanish *independently*[4]. This ensures automatic fulfillment of energy-momentum conservation in any minimally coupled gravity theories of the form Eqs.(3.74) and (3.75), such as $\mathscr{L}=f(R,R_c^2,R_m^2)+2\kappa\mathscr{L}_m$ gravity and $\mathscr{L}=f(R,\mathcal{G})+2\kappa\mathscr{L}_m$ gravity.

3.4.2 Divergence of SEM tensor under nonminimal coupling

Now consider a generic Lagrangian density $\mathscr{L}=f(\mathcal{R}_1,\ldots,\mathcal{R}_p,\mathscr{L}_m)$ which allows nonminimal coupling between $\mathscr{L}_m$ and Riemannian invariants $\mathcal{R}_i$. Noether's law yields the following equation for the divergence of the energy-momentum tensor,

$$\nabla^\mu\left(\frac{1}{\sqrt{-g}}\frac{\delta\left(\sqrt{-g}\,f(\mathcal{R}_1,\ldots,\mathcal{R}_p,\mathscr{L}_m)\right)}{\delta g^{\mu\nu}}\right)=0\,, \tag{3.77}$$

with expansion

$$f_{\mathscr{L}_m}\nabla^\mu T_{\mu\nu}=(\mathscr{L}_m\,g_{\mu\nu}-T_{\mu\nu})\,\nabla^\mu f_{\mathscr{L}_m}-\sum_i f_{\mathcal{R}_i}\nabla_\nu\mathcal{R}_i+2\sum_i\nabla^\mu H^{(f\mathcal{R}_i)}_{\mu\nu}\,, \tag{3.78}$$

where $\{f_{\mathscr{L}_m},\,f_{\mathcal{R}_i}\}$ are all dependent on $(\mathcal{R}_1\ldots,\mathcal{R}_p,\mathscr{L}_m)$, and $H^{(f\mathcal{R}_i)}_{\mu\nu}\delta g^{\mu\nu}:=f_{\mathcal{R}_i}\delta\mathcal{R}_i$ as usual. Note that, "conservation" of $\sqrt{-g}\,f(,\ldots,\mathcal{R}_p,\mathscr{L}_m)$ yields an unavoidable "divergence" term $(\mathscr{L}_m g_{\mu\nu}-T_{\mu\nu})\nabla^\mu f_{\mathscr{L}_m}$ essentially because of how $T_{\mu\nu}$ was defined; that is to say, for the nonminimally coupled $\mathscr{L}=f(\mathcal{R}_1,\ldots,\mathcal{R}_p,\mathscr{L}_m)$ under discussion, we have continued to use the definition of $T_{\mu\nu}$ from Eq.(3.73) which was adapted to minimal coupling. Also, for $\mathscr{L}=f(R,\mathcal{R}_1,\ldots,\mathcal{R}_p,\mathscr{L}_m)$ gravity where the first invariant is identified as the Ricci scalar, the same argument as Eq.(3.66) yields that $-f_R\nabla_\nu R+H^{(fR)}_{\mu\nu}=0$ for $f_R=f_R(R,\mathcal{R}_1,\ldots,\mathcal{R}_p,\mathscr{L}_m)$.

For the moment, we cannot directly use Eq.(3.72) to eliminate $-\sum_i f_{\mathcal{R}_i}\nabla_\nu\mathcal{R}_i$ by $2\sum_i\nabla^\mu H^{(f\mathcal{R}_i)}_{\mu\nu}$ in Eq.(3.78) as they are no longer purely geometric entities. In principle, the coefficient $f_{\mathcal{R}_i}=f_{\mathcal{R}_i}(\mathcal{R}_1,\ldots,\mathcal{R}_p,\mathscr{L}_m)$ allows for arbitrary dependence on $\mathscr{L}_m$, and this complexity gets even further promoted after taking the contravariant derivative of the effective tensor $H^{(f\mathcal{R}_i)}_{\mu\nu}(f_{\mathcal{R}_i})$. Also, note that, for the Lagrangian density $\mathscr{L}=f(R,R_c^2,R_m^2,\mathscr{L}_m)$ and $\mathscr{L}=f(R,\mathscr{L}_m)$, the generic result Eq.(3.78) soon recovers Eqs.(3.65) and (3.68), which were obtained in an alternative way from directly taking contravariant derivatives of their field equation.

As we have already learned, in Eq.(3.78) the term $(\mathscr{L}_m g_{\mu\nu}-T_{\mu\nu})\nabla^\mu f_{\mathscr{L}_m}$ originates from the contradiction

[4] Instead of directly starting from Eq.(3.10), one can consider $T_{\mu\nu}$ from the perspective of diffeomorphism (or gauge) invariance by requiring that the total action $\mathcal{S}_G+\mathcal{S}_m$ be invariant under an arbitrary and infinitesimal active transformation $g_{\mu\nu}\mapsto g_{\mu\nu}+\delta_\zeta g_{\mu\nu}=g_{\mu\nu}+\nabla_\mu\zeta_\nu+\nabla_\nu\zeta_\mu$, where ζ^μ vanishes at the boundary.

$$\delta\mathcal{S}_m=-\frac{1}{2}\delta\int d^4x\sqrt{-g}\,T_{\mu\nu}\,\delta g^{\mu\nu}=-\delta\int d^4x\sqrt{-g}\,T_{\mu\nu}\,\nabla^\mu\zeta^\nu\;\cong\;\delta\int d^4x\sqrt{-g}\,(\nabla^\mu T_{\mu\nu})\,\zeta^\nu\,. \tag{3.76}$$

Now the automatic conservation $\nabla^\mu T_{\mu\nu}=0$ would become a consequence of the (generalized) Bianchi identities which arise from the diffeomorphism invariance of $\mathcal{S}_G$. Both ways trace back to Noether's law.

between the nonminimal $\mathcal{R}_i$–$\mathscr{L}_m$ coupling and the minimal definition of $T_{\mu\nu}$. However, how can we understand the other divergence terms $-\sum_i f_{\mathcal{R}_i}\nabla_\nu\mathcal{R}_i$ and $2\sum_i \nabla^\mu H^{(f\mathcal{R}_i)}_{\mu\nu}$? Fortunately, investigations of $\mathscr{L}=\tilde{f}(\mathcal{R})+2\kappa\mathscr{L}_m+f(\mathcal{R})\,\mathscr{L}_m$ gravity shed some light on this question.

3.4.3 Lessons from $\tilde{f}(\mathcal{R}_i)+2\kappa\mathscr{L}_m+f(\mathcal{R}_i)\mathscr{L}_m$ model

Now, consider a further specialized model with Lagrangian density

$$\mathscr{L} = \tilde{f}(\mathcal{R}_1,\ldots,\mathcal{R}_p) + 2\kappa\mathscr{L}_m + f(\mathcal{R}_1,\ldots,\mathcal{R}_q)\cdot\mathscr{L}_m\,. \tag{3.79}$$

Sec. 3.4.1 has shown us that, energy-momentum conservation (divergence-freeness) is automatically satisfied for the minimally coupled component $\tilde{f}(\mathcal{R}_1,\ldots,\mathcal{R}_p)+2\kappa\mathscr{L}_m$, so we just need to concentrate on the nonminimally coupled term $f(\mathcal{R}_1,\ldots,\mathcal{R}_q)\cdot\mathscr{L}_m$. Following the discussion in Sec. 3.4.2 just above, treat $f(\mathcal{R}_1,\ldots,\mathcal{R}_q)\cdot\mathscr{L}_m$ as an invariant, so that Noether conservation of the covariant Lagrangian density $\sqrt{-g}\,f(\mathcal{R}_1,\ldots,\mathcal{R}_q)\cdot\mathscr{L}_m$ yields

$$\nabla^\mu\left(\frac{1}{\sqrt{-g}}\,\frac{\delta\left(\sqrt{-g}\,f(\mathcal{R}_1,\ldots,\mathcal{R}_q)\cdot\mathscr{L}_m\right)}{\delta g^{\mu\nu}}\right) = 0\,, \tag{3.80}$$

which in turn implies that

$$f\,\nabla^\mu T_{\mu\nu} = (\mathscr{L}_m\,g_{\mu\nu}-T_{\mu\nu})\,\nabla^\mu f - \sum_i f_{\mathcal{R}_i}(\mathcal{R}_1,\ldots,\mathcal{R}_q)\cdot\nabla_\nu\mathcal{R}_i + 2\sum_i\nabla^\mu\left(\frac{\mathscr{L}_m f_{\mathcal{R}_i}\cdot\delta\mathcal{R}_i}{\delta g^{\mu\nu}}\right). \tag{3.81}$$

Note that in the last term, $\mathscr{L}_m f_{\mathcal{R}_i}(\mathcal{R}_1,\ldots,\mathcal{R}_q)\cdot\delta\mathcal{R}_i$ acts as a unity rather than a triple multiplication and *cannot* be expanded via the product rule when acted upon by ∇^μ: In fact, $\mathscr{L}_m f_{\mathcal{R}_i}(\mathcal{R}_1,\ldots,\mathcal{R}_q)\cdot\delta\mathcal{R}_i =: H^{(\mathscr{L}_m f\mathcal{R}_i)}_{\mu\nu}\cdot\delta g^{\mu\nu}$ and thus $\mathscr{L}_m f_{\mathcal{R}_i}$ is merged into $\delta\mathcal{R}_i$.

Now recall that, based on the Petrov and Serge classifications, there are fourteen independent algebraic Riemannian invariants $\mathcal{I}=\mathcal{I}(g_{\alpha\beta},R_{\alpha\mu\beta\nu})$ characterizing a four-dimensional spacetime [15, 16], among which nine are of even parity and five are of odd parity, though this minimum set can be slightly expanded after considering the matter content. As a special example of Eq.(3.81), energy-momentum divergence of the nonminimally coupled Lagrangian $f(\mathcal{I}_1,\ldots,\mathcal{I}_9)\cdot\mathscr{L}_m$ was studied in [23], where $\{\mathcal{I}_1,\ldots,\mathcal{I}_9\}$ refer to the nine parity-even algebraic Riemannian invariants. Explicit calculations of $H^{(\mathscr{L}_m f\mathcal{I}_i)}_{\mu\nu}$ and $\nabla^\mu H^{(\mathscr{L}_m f\mathcal{I}_i)}_{\mu\nu}$ show that [23], for each individual $\mathcal{I}_i$ in $\mathscr{L}=f(\mathcal{I}_i,\mathscr{L}_m)$,

$$-f_{\mathcal{I}_i}(\mathcal{I}_i)\cdot\nabla_\nu\mathcal{I}_i + 2\nabla^\mu\left(\frac{\mathscr{L}_m f_{\mathcal{I}_i}(\mathcal{I}_i)\cdot\delta\mathcal{I}_i}{\delta g^{\mu\nu}}\right) = 0\,, \tag{3.82}$$

and most generally for $f(\mathcal{I}_1,\ldots,\mathcal{I}_9)\cdot\mathscr{L}_m$ with an arbitrary multiple dependence of these nine invariants,

$$-\sum_i f_{\mathcal{I}_i}(\mathcal{I}_1,\ldots,\mathcal{I}_9)\cdot\nabla_\nu\mathcal{I}_i + 2\sum_i\nabla^\mu\left(\frac{\mathscr{L}_m f_{\mathcal{I}_i}(\mathcal{I}_1,\ldots,\mathcal{I}_9)\cdot\delta\mathcal{I}_i}{\delta g^{\mu\nu}}\right) = 0\,. \tag{3.83}$$

Hence, the equation of energy-momentum divergence for $\mathscr{L}=\tilde{f}(\mathcal{I}_1,\ldots,\mathcal{I}_9)+2\kappa\mathscr{L}_m+f(\mathcal{I}_1,\ldots,\mathcal{I}_9)\cdot\mathscr{L}_m$ gravity finally becomes

$$f(\mathcal{I}_1,\ldots,\mathcal{I}_9)\cdot\nabla^\mu T_{\mu\nu} = (\mathscr{L}_m\,g_{\mu\nu}-T_{\mu\nu})\cdot\nabla^\mu f(\mathcal{I}_1,\ldots,\mathcal{I}_9)\,. \tag{3.84}$$

3.4.4 Conjecture for energy-momentum divergence

Now, let's summarize the facts we have confirmed so far:

1. In the simplest $\mathscr{L} = f(R, \mathscr{L}_m)$ gravity [13], one has $-f_R \nabla_\nu R + 2\nabla^\mu H^{(fR)}_{\mu\nu} = 0$, so R-dependence in $\mathscr{L} = f$ makes no contribution and $(\mathscr{L}_m\, g_{\mu\nu} - T_{\mu\nu})\,\nabla^\mu f_{\mathscr{L}_m}$ is the only energy-momentum divergence term;
2. In $\mathscr{L} = f(R, \mathcal{R}_1, \mathcal{R}_2, \ldots, \mathcal{R}_p, \mathscr{L}_m)$ gravity, $-f_R \nabla_\nu R + 2\nabla^\mu H^{(fR)}_{\mu\nu} = 0$ for $f_R = f_R(R, \mathcal{R}_1, \mathcal{R}_2, \ldots, \mathcal{R}_p, \mathscr{L}_m)$;
3. In $\mathscr{L} = \tilde{f}(\mathcal{I}_1, \ldots, \mathcal{I}_9) + 2\kappa \mathscr{L}_m + f(\mathcal{I}_1, \ldots, \mathcal{I}_9) \cdot \mathscr{L}_m$ gravity [23], one has individually $-f_{\mathcal{I}_i}(\mathcal{I}_i) \cdot \nabla_\nu \mathcal{I}_i + 2\nabla^\mu H^{(\mathscr{L}_m f \mathcal{I} i)}_{\mu\nu} = 0$ and collectively $-\sum_i f_{\mathcal{I}}(\mathcal{I}_i) \cdot \nabla_\nu \mathcal{I}_i + 2\sum_i \nabla^\mu H^{(\mathscr{L}_m f \mathcal{I} i)}_{\mu\nu} = 0$, so $(\mathscr{L}_m\, g_{\mu\nu} - T_{\mu\nu})\,\nabla^\mu f_{\mathscr{L}_m}$ is the only nonconservation term, while $\mathcal{I}_i$-dependence in $f \cdot \mathscr{L}_m$ makes no contribution;
4. In the case of minimal coupling, all algebraic and differential Riemannian invariants $\mathcal{R}_i$ act equally and indiscriminately in front of Noether's conservation law and generalized Bianchi identities.

Starting with these results, the belief that for the situation of generic nonminimal curvature-matter coupling all Riemannian invariants continue to play equal roles in energy-momentum nonconservation/divergence leads us to propose the following:

Weak conjecture: Consider a Lagrangian density allowing generic nonminimal coupling between the matter density $\mathscr{L}_m$ and Riemannian invariants $\mathcal{R}$,

$$\mathscr{L} \;=\; f(\mathcal{R}_1\,, \mathcal{R}_2 \ldots, \mathcal{R}_n\,, \mathscr{L}_m)\,, \tag{3.85}$$

where

$$\mathcal{R}_i \;=\; \mathcal{R}_i\left(g_{\alpha\beta}\,, R_{\alpha\mu\beta\nu}\,, \nabla_\gamma R_{\alpha\mu\beta\nu}\,, \ldots\,, \nabla_{\gamma_1}\nabla_{\gamma_2} \ldots \nabla_{\gamma_m} R_{\alpha\mu\beta\nu}\right).$$

Then contributions from the $\mathcal{R}_i$-dependence of $\mathscr{L} = f$ in the Noether-induced divergence equation cancel out collectively,

$$-\sum_i f_{\mathcal{R}_i} \cdot \nabla_\nu \mathcal{R}_i + 2\sum_i \nabla^\mu H^{(f\mathcal{R}_i)}_{\mu\nu} \;=\; 0\,, \tag{3.86}$$

and the equation of energy-momentum conservation/divergence takes the form[5]

$$f_{\mathscr{L}_m} \cdot \nabla^\mu T_{\mu\nu} \;=\; (\mathscr{L}_m\, g_{\mu\nu} - T_{\mu\nu})\,\nabla^\mu f_{\mathscr{L}_m}\,, \tag{3.87}$$

where $H^{(f\mathcal{R}_i)}_{\mu\nu} := \dfrac{f_{\mathcal{R}_i}(\mathcal{R}_1, \ldots, \mathscr{L}_m) \cdot \delta \mathcal{R}_i}{\delta g^{\mu\nu}}$, $f_{\mathcal{R}_i} = f_{\mathcal{R}_i}(\mathcal{R}_1, \ldots, \mathscr{L}_m)$, and $f_{\mathscr{L}_m} = f_{\mathscr{L}_m}(\mathcal{R}_1, \ldots, \mathcal{R}_n, \mathscr{L}_m)$.

Moreover, inspired by the behavior of R in Eq.(3.66) that $-f_R \nabla_\nu R + 2\nabla^\mu H^{(fR)}_{\mu\nu} = 0$ in spite of $f_R = f_R(R, R_c^2, R_m^2, \mathscr{L}_m)$, we further promote the weak conjecture to the following:

[5] When talking about its nontrivial divergence, $T_{\mu\nu}$ can be understood as the $T^{(\mathrm{NC})}_{\mu\nu}$ which comes from the $\mathscr{L}_m$ under nonminimal coupling, because the contribution $T^{(\mathrm{MC})}_{\mu\nu}$ to the total SEM tensor by an isolated (i.e. minimally coupled) covariant matter density $\sqrt{-g}\,\mathscr{L}_m$ automatically satisfies the standard stress-energy-momentum conservation.

Strong conjecture: For every invariant $\mathcal{R}_i$ in $\mathscr{L} = f(\mathcal{R}_1, \mathcal{R}_2 \ldots, \mathcal{R}_n, \mathscr{L}_m)$, the divergence terms arising from each $\mathcal{R}_i$-dependence in $\mathscr{L} = f$ cancel out *individually*,

$$-f_{\mathcal{R}_i} \cdot \nabla_\nu \mathcal{R}_i + 2\nabla^\mu H_{\mu\nu}^{(f\mathcal{R}_i)} \;=\; 0\,, \tag{3.88}$$

and the equation of energy-momentum conservation/divergence remains the same as in Eq.(3.87),

$$f_{\mathscr{L}_m} \cdot \nabla^\mu T_{\mu\nu} \;=\; (\mathscr{L}_m\, g_{\mu\nu} - T_{\mu\nu})\, \nabla^\mu f_{\mathscr{L}_m}\,.$$

Specifically, when the possible nonminimal coupling reduces to ordinary minimal coupling, Eq.(3.85) will be specialized into $\mathscr{L} = f(\mathcal{R}_1, \ldots, \mathcal{R}_n) + 2\kappa\mathscr{L}_m$ as in Eq.(3.74), so Eqs.(3.86) and (3.88) in the weak conjecture are naturally satisfied because of the generalized Bianchi identities Eqs.(3.71) and (3.72). Also, if the conjecture were correct, then the generalized Bianchi indentities Eqs.(3.71) and (3.72) could be generalized again, and they cannot serve as a sufficient condition for judging minimal coupling.

Furthermore, reading left to right the nonconservation equation (3.87) clearly shows that the energy-momentum divergence is transformed into the gradient of nonminimal gravitational coupling strength $f_{\mathscr{L}_m}$. On the other hand, if the weak or even the strong conjecture were true, does it mean that differences between the set of Riemannian invariants which the Lagrangian density depends on are trivial? The answer is of course no, because the gradient $\nabla^\mu f_{\mathscr{L}_m}$ is superposed by the gradient of $\mathscr{L}_m$ and the gradients of all characteristic Riemannian invariants $\mathcal{R}_i$ used in $\mathscr{L} = f$:

$$f_{\mathscr{L}_m} \cdot \nabla^\mu T_{\mu\nu} \;=\; (\mathscr{L}_m\, g_{\mu\nu} - T_{\mu\nu}) \cdot \Big(f_{\mathscr{L}_m \mathscr{L}_m} \cdot \nabla^\mu \mathscr{L}_m + \sum_i f_{\mathscr{L}_m \mathcal{R}_i} \cdot \nabla^\mu \mathcal{R}_i \Big), \tag{3.89}$$

where $f_{\mathscr{L}_m \mathscr{L}_m} = \partial f_{\mathscr{L}_m} / \partial \mathscr{L}_m$, $f_{\mathscr{L}_m \mathcal{R}_i} = \partial f_{\mathscr{L}_m} / \partial \mathcal{R}_i$. Note that, if we adopt Eq.(3.89) rather than Eq.(3.87) as the final form of nonconservation equation, the coefficient $(\mathscr{L}_m\, g_{\mu\nu} - T_{\mu\nu}) = 2\delta\mathscr{L}_m / \delta g^{\mu\nu}$ associated to the divergences $\{\nabla^\mu \mathscr{L}_m\,, \nabla^\mu \mathcal{R}_i\}$ helps to clarify that they exclusively come from the $\mathscr{L}_m$-dependence in $\mathscr{L} = f$.

Following the weak conjecture, we now formally rewrite the divergence equation (3.67) for $f(R, R_c^2, R_m^2, \mathscr{L}_m)$ gravity into

$$f_{\mathscr{L}_m} \cdot \nabla^\mu T_{\mu\nu} \;=\; (\mathscr{L}_m\, g_{\mu\nu} - T_{\mu\nu})\, \nabla^\mu f_{\mathscr{L}_m} + \mathcal{E}_\nu\,, \tag{3.90}$$

where

$$\mathcal{E}_\nu \;\coloneqq\; -f_{R_c^2} \nabla_\nu R_c^2 - f_{R_m^2} \nabla_\nu R_m^2 + 2\nabla^\mu H_{\mu\nu}^{(fR_c^2)} + 2\nabla^\mu H_{\mu\nu}^{(fR_m^2)}\,, \tag{3.91}$$

and $\mathcal{E}_\nu$ is expected to vanish by the weak conjecture, while $\mathcal{E}_\nu \equiv 0$ trivially holds under minimal coupling because of generalized Bianchi identities. Since we have not yet proved that $\mathcal{E}_\nu = 0$, we preserve $\mathcal{E}_\nu$ in the divergence equation (3.90) and proceed to use it to check the equations of continuity and motion with different matter sources.

3.5 Equations of continuity and nongeodesic motion

Once the matter content in the spacetime is known, Eq.(3.90) can be concretized in accordance with the particular forms of $T_{\mu\nu}$, which would imply the equations of continuity of the energy-matter content and the equation of (nongeodesic) motion for a test particle[6]. This topic will be studied in this section, and note that $T_{\mu\nu}$ and $\mathscr{L}_m$ will be adapted to the $(-,+++)$ metric signature.

3.5.1 Perfect fluid

The stress-energy-momentum (SEM) tensor of a perfect fluid (no internal viscosity, no shear stresses, and zero thermal-conductivity coefficients) with mass-energy density $\rho=\rho(x^\alpha)$, isotropic pressure $P=P(x^\alpha)$ and equation of state $P=w\,\rho$, is given by [20]

$$\begin{aligned} T^{(\mathrm{PF})}_{\mu\nu} &= (\rho+P)\,u_\mu u_\nu + P\,g_{\mu\nu} \\ &= \rho\,u_\mu u_\nu + P\,(g_{\mu\nu}+u_\mu u_\nu) \\ &= \rho\,u_\mu u_\nu + P\,h_{\mu\nu}\,, \end{aligned} \tag{3.92}$$

where u^μ is the four-velocity along the worldline, satisfying $u_\mu u^\mu=-1$ and $u_\mu\nabla_\nu u^\mu=0$; $h_{\mu\nu}$ is the projected spatial 3-metric, $h_{\mu\nu}:=g_{\mu\nu}+u_\mu u_\nu$ with inverse $h^{\mu\nu}=g^{\mu\nu}+u^\mu u^\nu$, $h^{\mu\nu}u_\mu=0$, and $h^{\mu\nu}h_{\mu\nu}=3$. Substituting Eq.(3.92) into Eq.(3.90) and multiplying both sides by u^ν, we get

$$u^\mu\,\nabla_\mu\rho + (\rho+P)\,\nabla^\mu u_\mu \;=\; -(\mathscr{L}_m+\rho)\,u^\mu\,\nabla_\mu \ln f_{\mathscr{L}_m} - f^{-1}_{\mathscr{L}_m}\,u^\nu\mathcal{E}_\nu\,, \tag{3.93}$$

which generalizes the original continuity equation of perfect fluid in GR, $u^\mu\nabla_\mu\rho+(\rho+P)\nabla^\mu u_\mu=0$.

On the other hand, after putting Eq.(3.92) back to Eq.(3.90), use $h^{\xi\nu}$ to project the free index ν, and it follows that

$$(\rho+P)\cdot u^\mu\nabla_\mu u^\xi = -h^{\xi\mu}\cdot\nabla_\mu P + h^{\xi\mu}\cdot(\mathscr{L}_m-P)\,\nabla_\mu\ln f_{\mathscr{L}_m} + f^{-1}_{\mathscr{L}_m}\,h^{\xi\nu}\mathcal{E}_\nu\,, \tag{3.94}$$

where we have employed the properties $h^{\xi\nu}\cdot u_\mu\nabla^\mu u_\nu = g^{\xi\nu}\cdot u_\mu\nabla^\mu u_\nu = u_\mu\nabla^\mu u^\xi$. In general, $\rho+P\neq 0$ (in fact $\rho+P\geq 0$ by all four energy conditions in GR, and equality happens only for matters with large negative pressure). Thus we obtain the following absolute derivative along u^ξ as the equation of motion:

$$\frac{Du^\xi}{D\tau} \;\equiv\; \frac{du^\xi}{d\tau} + \Gamma^\xi_{\alpha\beta}u^\alpha u^\beta \;=\; a^\xi_{(\mathrm{PF})} + a^\xi_{(f_{\mathscr{L}_m})} + a^\xi_{(\mathcal{E})}\,, \tag{3.95}$$

where τ is an affine parameter (e.g. proper time) for the timelike worldline along which $dx^\alpha=u^\alpha d\tau$, and the three proper accelerations are given by

$$\begin{cases} a^\xi_{(\mathrm{PF})} &\equiv -h^{\xi\mu}\cdot(\rho+P)^{-1}\,\nabla_\mu P \\ a^\xi_{(f_{\mathscr{L}_m})} &\equiv -h^{\xi\mu}\cdot(\rho+P)^{-1}\,(P-\mathscr{L}_m)\,\nabla_\mu\ln f_{\mathscr{L}_m} \\ a^\xi_{(\mathcal{E})} &\equiv -h^{\xi\nu}\cdot(\rho+P)^{-1}\,f^{-1}_{\mathscr{L}_m}\,\mathcal{E}_\nu\,. \end{cases} \tag{3.96}$$

Thus, three proper accelerations are responsible for the nongeodesic motion. $a^\xi_{(\mathrm{PF})}$ is the standard acceleration from the pressure of fluid as in GR [20], $a^\xi_{(f_{\mathscr{L}_m})}$ comes from the curvature-matter coupling, while $a^\xi_{(\mathcal{E})}$ is a collaborative effect of the $\{R^2_c$-, R^2_m-$\}$dependence in the action and their generic nonminimal coupling to $\mathscr{L}_m$. This is consistent with the result in [11] in the absence of $\{R^2_c, R^2_m\}$. Also, all three accelerations are orthogonal

[6] The method and discussion in this section are also valid for a generic $\mathscr{L}=f(\mathcal{R}_1,\mathcal{R}_2\ldots,\mathcal{R}_n,\mathscr{L}_m)$ gravity as in Eq.(3.86), and we just need to define the effective 1-form $\tilde{\mathcal{E}}_\nu=-\sum_i f_{\mathcal{R}_i}(\mathcal{R}_1\ldots\mathscr{L}_m)\cdot\nabla_\nu\mathcal{R}_i+2\sum_i\nabla^\mu H^{(f\mathcal{R}_i)}_{\mu\nu}$ in place of the $\mathcal{E}_\nu$ for $f(R,R^2_c,R^2_m,\mathscr{L}_m)$ gravity. Specifically, $\tilde{\mathcal{E}}_\nu\equiv 0$ under minimal coupling, and furthermore $\tilde{\mathcal{E}}_\nu$ vanishes universality if the weak conjecture were correct.

to the worldline with tangent u^ξ, since

$$a^\xi_{(\mathrm{PF})} u_\xi \;=\; 0 \quad , \quad a^\xi_{(f_{\mathscr{L}_m})} u_\xi \;=\; 0 \quad , \quad a^\xi_{(\mathcal{E})} u_\xi \;=\; 0\,. \tag{3.97}$$

Both Eq.(3.93) and Eqs.(3.95) and (3.96) depend on the choice of the perfect-fluid matter Lagrangian density. If $\mathscr{L}_m = -\rho$ [20, 29], the continuity equation (3.93) becomes

$$u^\mu\,\nabla_\mu\rho + (\rho + P)\,\nabla_\mu u^\mu \;=\; -f^{-1}_{\mathscr{L}_m}\,u^\nu \mathcal{E}_\nu\,, \tag{3.98}$$

which is free from the gradient of the geometry-matter coupling strength $f^{-1}_{\mathscr{L}_m}\,u^\mu\nabla_\mu f_{\mathscr{L}_m}$, while $a^\xi_{(f_{\mathscr{L}_m})}$ reduces to

$$a^\xi_{(f_{\mathscr{L}_m})} \;\equiv -h^{\xi\mu}\cdot\nabla_\mu \ln f_{\mathscr{L}_m}\,, \tag{3.99}$$

which does not rely on the equation of state $P = w\,\rho$.

On the other hand, for the choice $\mathscr{L}_m = P$ [29, 30], Eq.(3.93) and Eq.(3.96) respectively yields

$$u^\mu\,\nabla_\mu\rho + (\rho + P)\,\nabla^\mu u_\mu \;=\; -(\rho + P)\,u^\mu\,\nabla_\mu \ln f_{\mathscr{L}_m} - f^{-1}_{\mathscr{L}_m}\,u^\mu \mathcal{E}_\mu\,, \tag{3.100}$$

and

$$a^\xi_{(f_{\mathscr{L}_m})} \;\equiv\; 0\,. \tag{3.101}$$

Although the continuity equation (3.100) looks pretty ordinary, the proper acceleration $a^\xi_{(f_{\mathscr{L}_m})}$ vanishes identically for $\mathscr{L}_m = P$ and consequently the nongeodesic motion in the gravitational field of the perfect fluid becomes independent of the gradient of the nonminimal coupling strength $u^\mu\nabla_\mu f_{\mathscr{L}_m}$.

As shown in [31], both $\mathscr{L}_m = P$ and $\mathscr{L}_m = -\rho$ are correct matter densities and both lead to the SEM tensor given in Eq.(3.92). Differences of physical effects only occur in the situation of nonminimal coupling, where $\mathscr{L}_m$ becomes a direct and explicit input in the energy-momentum divergence equation. In fact, as for the matter Lagrangian density $\mathscr{L}_m$ for a perfect fluid, one can also adopt the following ansatz,

$$\mathscr{L}_m \;=\; (a\rho + bP)\cdot g^{\alpha\beta} u_\alpha u_\beta + (c\rho + dP)\cdot g^{\alpha\beta} g_{\alpha\beta} \;=\; (4c - a)\,\rho + (4d - b)\,P\,. \tag{3.102}$$

Applying this to Eq.(3.11), the equality with Eq.(3.92) yields $a = -1/2 = b$ and $c = -1/4 = -d$, so

$$\mathscr{L}_m \;=\; \left(-\frac{1}{2}\rho - \frac{1}{2}P\right)\cdot g^{\alpha\beta} u_\alpha u_\beta + \left(-\frac{1}{4}\rho + \frac{1}{4}P\right)\cdot g^{\alpha\beta} g_{\alpha\beta} \;=\; -\frac{1}{2}\rho + \frac{3}{2}P\,. \tag{3.103}$$

This density makes Eqs.(3.93), (3.95) and (3.96) act normally, losing the aforementioned extraordinary properties associated with $\mathscr{L}_m = -\rho$ and $\mathscr{L}_m = P$.

3.5.2 (Timelike) Dust

The (timelike) dust source with mass-energy density ρ has SEM tensor [20, 30]

$$T^{(\mathrm{Dust})}_{\mu\nu} \;=\; \rho\,u_\mu u_\nu\,, \tag{3.104}$$

where $u_\mu = g_{\mu\nu}u^\nu$ with u^ν being the tangent vector field along the worldline of a timelike dust particle. One can still introduce the spatial metric $h_{\mu\nu} \equiv g_{\mu\nu} + u_\mu u_\nu$ orthogonal to u^μ, with $\{u_\mu\,, h_{\mu\nu}\}$ sharing all those properties as in the case of perfect fluid, so dust acts just like a perfect fluid with zero pressure, $P = 0$. Substituting Eq.(3.104) back into Eq.(3.90) and multiplying by u^ν on both its sides yields

$$u^\mu\,\nabla_\mu\rho + \rho\,\nabla^\mu u_\mu \;=\; -(\mathscr{L}_m + \rho)\,u^\nu\nabla_\nu\ln f_{\mathscr{L}_m} - f_{\mathscr{L}_m}^{-1}\,u^\nu\mathcal{E}_\nu\,, \tag{3.105}$$

which modifies the continuity equation of dust $\nabla_\mu(\rho u^\mu) = 0$ in GR. Meanwhile, projection of the free index ν by $h^{\xi\nu}$ in $\nabla^\mu T^{(\text{Dust})}_{\mu\nu}$ gives rise to the modified equation of motion

$$\frac{Du^\xi}{D\tau} \;\equiv\; \frac{du^\xi}{d\tau} + \Gamma^\xi_{\alpha\beta}u^\alpha u^\beta \;=\; \hat{a}^{\,\xi}_{(f_{\mathscr{L}_m})} + \hat{a}^{\,\xi}_{(\mathcal{E})}\,, \tag{3.106}$$

where

$$\begin{cases} \hat{a}^{\,\xi}_{(f_{\mathscr{L}_m})} \;\equiv\; h^{\xi\mu}\cdot\rho^{-1}\,\mathscr{L}_m\,\nabla_\mu\ln f_{\mathscr{L}_m} \\ \hat{a}^{\,\xi}_{(\mathcal{E})} \;\equiv -h^{\xi\nu}\cdot\rho^{-1}\,f_{\mathscr{L}_m}^{-1}\,\mathcal{E}_\nu\,. \end{cases} \tag{3.107}$$

Being pressureless, the dust inherits just the two extra accelerations $\hat{a}^{\,\xi}_{(f_{\mathscr{L}_m})}$ and $\hat{a}^{\,\xi}_{(\mathcal{E})}$, and both remain orthogonal to the worldline with tangent u^ξ,

$$\hat{a}^{\,\xi}_{(f_{\mathscr{L}_m})}u_\xi \;=\; 0 \quad , \quad \hat{a}^{\,\xi}_{(\mathcal{E})}u_\xi \;=\; 0\,. \tag{3.108}$$

3.5.3 Null dust

The SEM tensor for null dust with energy density ϱ is (e.g. [30])

$$T^{(\text{ND})}_{\mu\nu} \;=\; \varrho\,\ell_\mu\ell_\nu\,, \tag{3.109}$$

where $\ell_\mu = g_{\mu\nu}\ell^\nu$ with ℓ^ν being the tangent vector field along the worldline of a null dust particle, $\ell_\mu\ell^\mu = 0$. $T^{(\text{ND})}_{\mu\nu}$ together with the energy-momentum divergence equation (3.90) yields

$$\ell_\nu\,\ell^\mu\nabla_\mu\varrho + \varrho\,\ell^\mu\nabla_\mu\ell_\nu + \varrho\,\ell_\nu\nabla_\mu\ell^\mu \;=\; (\mathscr{L}_m\,g_{\mu\nu} - \varrho\,\ell_\mu\ell_\nu)\,\nabla^\mu\ln f_{\mathscr{L}_m} + f_{\mathscr{L}_m}^{-1}\,\mathcal{E}_\nu\,. \tag{3.110}$$

Multiplying both sides with ℓ^ν, $\ell^\nu\ell_\nu = 0$, $\ell_\nu\nabla_\mu\ell^\nu = 0$, we obtain the following constraint:

$$f_{\mathscr{L}_m}\,\ell^\nu\nabla_\nu f_{\mathscr{L}_m} \;=\; -\ell^\nu\mathcal{E}_\nu\,. \tag{3.111}$$

Now, introduce an auxiliary null vector field n^μ as null normal to ℓ^μ such that $n^\mu n_\mu = 0$, $\ell^\mu n_\mu = -1$, which induces the two-dimensional spatial metric $g_{\mu\nu} = -\ell_\mu n_\nu - n_\mu\ell_\nu + q_{\mu\nu}$, satisfying the conditions

$$q_{\mu\nu}q^{\mu\nu} = 2 \quad , \quad q_{\mu\nu}\ell^\nu = 0 = q_{\mu\nu}n^\nu \quad , \quad \ell^\alpha\nabla_\alpha q_{\mu\nu} = 0\,. \tag{3.112}$$

Multiplying Eq.(3.110) by n^ν, and with $n^\nu\nabla_\mu\ell_\nu = -\ell^\nu\nabla_\mu n_\nu$, we get the continuity equation

$$\ell^\mu\nabla_\mu\varrho + \varrho\,\nabla_\mu\ell^\mu + \varrho\ell^\nu\ell^\mu\nabla_\mu n_\nu \;=\; -(\mathscr{L}_m\,n^\mu + \varrho\,\ell^\mu)\,\nabla_\mu\ln f_{\mathscr{L}_m} - f_{\mathscr{L}_m}^{-1}\,n^\nu\mathcal{E}_\nu\,, \tag{3.113}$$

while projecting Eq.(3.110) with $h^{\xi\nu}$ gives rise to the equation of motion along ℓ^ξ,

$$\varrho\, \ell^\mu \nabla_\mu \ell^\xi \;=\; \varrho\, \ell^\xi \ell^\nu \ell^\mu \nabla_\mu n_\nu + h^{\xi\nu}\, \mathscr{L}_m\, \nabla_\nu \ln f_{\mathscr{L}_m} + f_{\mathscr{L}_m}^{-1}\, h^{\xi\nu} \mathcal{E}_\nu\,, \tag{3.114}$$

$$\frac{D\ell^\xi}{D\lambda} \;\equiv\; \frac{d\ell^\xi}{d\lambda} + \Gamma^\xi_{\alpha\beta} \ell^\alpha \ell^\beta \;=\; \check{a}^\xi_{(\mathrm{ND})} + \check{a}^\xi_{(f_{\mathscr{L}_m})} + \check{a}^\xi_{(\mathcal{E})}\,, \tag{3.115}$$

where λ is an affine parameter for the null worldline along which $dx^\alpha = \ell^\alpha d\xi$, and the three proper accelerations are respectively

$$\begin{cases} \check{a}^\xi_{(\mathrm{ND})} & \equiv \quad \ell^\xi \ell^\nu \ell^\mu \nabla_\mu n_\nu \\ \check{a}^\xi_{(f_{\mathscr{L}_m})} & \equiv \quad h^{\xi\mu} \cdot \varrho^{-1} \mathscr{L}_m\, \nabla_\nu \ln f_{\mathscr{L}_m} \\ \check{a}^\xi_{(\mathcal{E})} & \equiv \quad h^{\xi\nu} \cdot \varrho^{-1}\, f_{\mathscr{L}_m}^{-1}\, \mathcal{E}_\nu\,. \end{cases} \tag{3.116}$$

As we can see, compared with timelike dust, one more proper acceleration $\check{a}^\xi_{(\mathrm{ND})}$ shows up in the case of null dust, and we will refer to it the *affine* acceleration or *inaffinity* acceleration.

3.5.4 Scalar field

The matter Lagrangian density and SEM tensor of a massive scalar field $\phi(x^\alpha)$ with mass m in a potential $V(\phi)$ are respectively given by

$$\begin{aligned} \mathscr{L}_m \;&=\; -\frac{1}{2}(\nabla_\alpha \phi \nabla^\alpha \phi + m^2 \phi^2) + V(\phi)\,, \\ T_{\mu\nu} \;&=\nabla_\mu \phi \nabla_\nu \phi - \frac{1}{2} g_{\mu\nu} \left(\nabla_\alpha \phi \nabla^\alpha \phi + m^2 \phi^2 - 2V(\phi)\right), \end{aligned} \tag{3.117}$$

thus $\mathscr{L}_m\, g_{\mu\nu} - T_{\mu\nu} = -\nabla_\mu \phi \nabla_\nu \phi$. For the ν component, the equations of continuity and motion are both given by

$$\left(\Box\phi - m^2\phi + V_\phi\right) \cdot \nabla_\nu \phi \;=\; -\nabla_\nu \phi \cdot \nabla_\mu \phi\, \nabla^\mu \ln f_{\mathscr{L}_m} + f_{\mathscr{L}_m}^{-1}\, \mathcal{E}_\nu\,. \tag{3.118}$$

Specifically, by setting $V(\phi) = 0$ and under minimal coupling ($f_{\mathscr{L}_m}$ =constant, $\mathcal{E}_\nu$=0), we get

$$\Box\phi - m^2\phi \;=\; 0\,, \tag{3.119}$$

which is the standard covariant Klein-Gordon equation for spin-zero particles in GR.

3.6 Further physical implications of nonminimal coupling

We have seen that under nonminimal curvature-matter coupling, the divergence of the standard SEM density tensor is equal to the gradient of the coupling strength $\nabla^\mu f_{\mathscr{L}_m}$ which, in general, will be nonvanishing. As such, the usual energy-momentum conservation laws for particular matter fields will be modified as compared to the corresponding fields in general relativity. At the same time, as is discussed in the Appendix , nonminimal coupling also affects the energy conditions. The standard energy energy conditions of general relativity are phrased in terms of the stress-energy tensor and require positive energies (null and strong) and causal flows of matter (dominant). However, in applications these conditions are generally used to constrain the Riemann tensor and so the allowed geometries of spacetime and structures like singularities or horizons. For standard general relativity the two approaches are essentially equivalent but for modified gravity they are not: if the Einstein equations are modified then the bounds on the Ricci tensor that achieve the desired effects generally do not translate into the usual restrictions on the stress-energy-momentum. Thus one is faced with a choice: either keep the standard GR results and give up the usual energy conditions or keep the usual energy conditions but lose those results.

In this section we consider some immediate physical consequences of this choice. All of these are consequences of the Raychaudhuri equations for null and timelike geodesic congruences and so the difference between the standard energy conditions and those needed to enforce the focussing theorems is crucial to these discussions. These are considered in some detail in the Appendix and in the following $T^{(\text{eff})}_{\mu\nu}$ refers to an effective stress-energy tensor for which the standard form of the energy conditions will leave those theorems intact.

3.6.1 Black hole physics

Many results in black hole physics follow from understanding a black hole horizon as a congruence of null geodesics whose evolution is governed by the (twist-free) Raychaudhuri equation:

$$\frac{d\theta_{(\ell)}}{d\lambda} = \kappa_{(\ell)}\theta_{(\ell)} - \frac{1}{2}\,\theta^2_{(\ell)} - \sigma^{(\ell)}_{\mu\nu}\sigma^{\mu\nu}_{(\ell)} - R_{\mu\nu}\ell^\mu\ell^\nu\,, \tag{3.120}$$

where $\ell^\mu = \left(\frac{\partial}{\partial\lambda}\right)^\mu$ is a null tangent to the horizon, and $\kappa_{(\ell)}$, $\theta_{(\ell)}$ and $\sigma^{(\ell)}_{\mu\nu}$ are respectively the associated acceleration/inaffinity, expansion and shear.

The second law of black hole mechanics follows from this equation along with the requirement that the congruence of null curves that rules the event horizon have no future endpoints (see, for example, the discussion [20]). Now choosing an affine parameterization for the congruence $\kappa_{(\ell)} = 0$ it is straightforward to see that the righthand side of (3.120) is nonpositive as long as $R_{\mu\nu}\ell^\mu\ell^\nu \geq 0$. In standard GR this follow from the null energy condition: $T_{\mu\nu}\ell^\mu\ell^\nu \geq 0$. It then almost immediately follows that $\theta_{(\ell)}$ must be everywhere nonnegative. Else $\theta_{(\ell)} \to -\infty$ and the congruence focuses. However, for modified gravity we will usually lose the equivalence $T_{\mu\nu}\ell^\mu\ell^\nu \geq 0 \Leftrightarrow R_{\mu\nu}\ell^\mu\ell^\nu \geq 0$ and so we will be faced with a modified area increase theorem if we require the standard energy conditions.

By similar arguments, again involving the null Raychaudhuri equation, the energy conditions play a crucial role in the theorems that require trapped surfaces to be contained in black holes and singularities to lie in their causal future [20]. Thus for black hole physics, modifications of the energy conditions are a serious business which can affect core results and intuitions.

3.6.2 Wormholes

On the other hand, for those interested in faster-than-light travel changing the energy conditions would be a boon. Introducing the nonminimal gravitational coupling strength $f_{\mathscr{L}_m}$ brings new flexibility and the possibility of supporting wormholes, as shown in [32] and [33] for a $\lambda R \cdot \mathscr{L}_m$ coupling term. More generally for the $\mathscr{L} = f(R, \mathcal{R}_1, \ldots, \mathcal{R}_n, \mathscr{L}_m)$ gravity, based on the generalized null and weak energy conditions developed in the Appendix, it proves possible to defocus null and timelike congruences and form wormholes by violating these generalized conditions, while having the standard energy conditions in GR [20] maintained to exclude the need for exotic matters. It also leads to an extra constraint $f_{\mathscr{L}_m}/f_R \geq 0$ as in Eq.(3.138).

From Eq.(3.139) in the Appendix, for a null congruence ℓ^μ, one can maintain the standard null energy condition $T_{\mu\nu}\ell^\mu\ell^\nu \geq 0$ while violating $T^{(\text{eff})}_{\mu\nu}\ell^\mu\ell^\nu \leq 0$ (and so evade the focusing theorems) if

$$0 \leq T_{\mu\nu}\,\ell^\mu\ell^\nu \leq 2\,f^{-1}_{\mathscr{L}_m}\Big(\sum_i H^{(f\mathcal{R}i)}_{\mu\nu}\ell^\mu\ell^\nu - \ell^\nu\ell^\mu\nabla_\mu\nabla_\nu\,f_R\Big). \tag{3.121}$$

Similarly for a timelike congruence, one has $T_{\mu\nu}\,u^\mu u^\nu \geq 0$ while $T^{(\text{eff})}_{\mu\nu}\,u^\mu u^\nu \leq 0$, and Eq.(3.140) leads to

$$0 \leq T_{\mu\nu}u^\mu u^\nu \leq f^{-1}_{\mathscr{L}_m}\Big(f - R\,f_R + 2\sum_i H^{(f\mathcal{R}i)}_{\mu\nu}u^\mu u^\nu - 2\,(u^\mu u^\nu\nabla_\mu\nabla_\nu + \Box)\,f_R\Big) - \mathscr{L}_m\,. \tag{3.122}$$

Specifically for $\mathscr{L} = f(R, R^2_c, R^2_m, \mathscr{L}_m)$ gravity, these two conditions are concretized as

$$0 \leq T_{\mu\nu}\,\ell^\mu\ell^\nu \leq 2\,f^{-1}_{\mathscr{L}_m}\Big(H^{(fR^2_c)}_{\mu\nu}\ell^\mu\ell^\nu + H^{(fR^2_m)}_{\mu\nu}\ell^\mu\ell^\nu - \ell^\nu\ell^\mu\nabla_\mu\nabla_\nu\,f_R\Big) \quad \text{and} \tag{3.123}$$

$$0 \leq T_{\mu\nu}u^\mu u^\nu \leq f^{-1}_{\mathscr{L}_m}\Big(f - R\,f_R + 2H^{(fR^2_c)}_{\mu\nu}u^\mu u^\nu + 2H^{(fR^2_m)}_{\mu\nu}u^\mu u^\nu - 2\,(u^\mu u^\nu\nabla_\mu\nabla_\nu + \Box)\,f_R\Big) - \mathscr{L}_m\,, \tag{3.124}$$

where $\{H^{(fR^2_c)}_{\mu\nu},\, H^{(fR^2_m)}_{\mu\nu}\}$ have been given in Eqs.(3.8) and (3.9).

Moreover, Eqs.(3.121)(3.122) indicate that in the case without dependence on Riemannian invariants beyond R, i.e. $\mathscr{L} = f(R, \mathscr{L}_m)$, a wormhole can be solely supported by the nonminimal-coupling effect if

$$0 \leq T_{\mu\nu}\,\ell^\mu\ell^\nu \leq -2\,f^{-1}_{\mathscr{L}_m}\,\ell^\nu\ell^\mu\nabla_\mu\nabla_\nu\,f_R \quad \text{and} \tag{3.125}$$

$$0 \leq T_{\mu\nu}u^\mu u^\nu \leq -\mathscr{L}_m + f^{-1}_{\mathscr{L}_m}\Big(f - Rf_R - 2(u^\mu u^\nu\nabla_\mu\nabla_\nu + \Box)f_R\Big). \tag{3.126}$$

For example, let $\mathscr{L} = f(R, \mathscr{L}_m) = R + 2\kappa\mathscr{L}_m + \lambda\,R\mathscr{L}_m$, and the field equation (3.48) becomes

$$R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} + \lambda\cdot\Big(\mathscr{L}_m R_{\mu\nu} + (g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu)\mathscr{L}_m\Big) = (\kappa + \frac{1}{2}\lambda R)T_{\mu\nu} \tag{3.127}$$

To have a quick realization of Eq.(3.125), we further assume $\lambda = 1$, $T_{\mu\nu} = \text{diag}[-\rho(r), P(r), P(r), P(r)]$, $\mathscr{L}_m = P(r)$ (recall Sec. 3.5.1), and adopt the following simplest wormhole metric,

$$ds^2 = -dt^2 + dr^2 + (r^2 + L^2)\cdot\Big(d\theta^2 + \sin^2\theta\,d\phi^2\Big), \tag{3.128}$$

with minimum throat scale L and outgoing radial null vector field $\ell^\mu\partial_\mu = (-1, 1, 0, 0)$. Then the condition Eq.(3.125) reduces to become

$$0 \leq -\rho + 3P \leq \Big(1 + \frac{r^2}{L^2}\Big)\partial_r\partial_r P\,, \tag{3.129}$$

which clearly shows that the standard null energy condition remains valid while spatial inhomogeneity of the pressure $\partial_r\partial_r P$ supports the wormhole.

Finally, note that it remains to be carefully checked whether solutions exist that meet these conditions.

3.7 Conclusions

In this paper, we have derived the field equation for $\mathscr{L} = f(R, R_c^2, R_m^2, \mathscr{L}_m)$ fourth-order gravity allowing for participation of the Ricci square R_c^2 and Riemann square R_m^2 in the Lagrangian density and nonminimal coupling between the curvature invariants and $\mathscr{L}_m$ as compared to GR. It turned out that $\mathscr{L}_m$ appears explicitly in the field equation because of confrontation between the nonminimal coupling and the traditional minimal definition of the SEM tensor $T_{\mu\nu}$. When $f_{\mathscr{L}_m} = \text{constant} = 2\kappa$, we recover the minimally coupled $\mathscr{L} = f(R, R_c^2, R_m^2) + 2\kappa\mathscr{L}_m$ model. Also, we have showed that both the curvature-$\mathscr{L}_m$ nonminimal coupling and the curvature-T coupling are sensitive to the concrete forms of $\mathscr{L}_m$.

Secondly, by considering an explicit R^2-dependence, we have found the smooth transition from $f(R, R_c^2, R_m^2, \mathscr{L}_m)$ gravity to the $\mathscr{L} = f(R, \mathcal{G}, \mathscr{L}_m)$ generalized Gauss-Bonnet gravity by imposing the coherence condition $f_{R^2} = f_{R_m^2} = -f_{R_c^2}/4$. When $f(R, \mathcal{G}, \mathscr{L}_m)$ reduces to the case $f(R, \mathscr{L}_m) + \lambda\mathcal{G}$ where $\mathcal{G}$ appears as a pure Gauss-Bonnet term, an extra term $\lambda\,(-\frac{1}{2}\mathcal{G}\,g_{\mu\nu} + 2R\,R_{\mu\nu} - 4R_\mu{}^\alpha R_{\alpha\nu} - 4R_{\alpha\mu\beta\nu}R^{\alpha\beta} + 2R_{\mu\alpha\beta\gamma}R_\nu{}^{\alpha\beta\gamma})$ is left behind in the field equation representing the contribution from the covariant density $\lambda\sqrt{-g}\mathcal{G}$. We have shown that this term actually vanishes and thus $\lambda\mathcal{G}$ makes no difference to the gravitational field equation.

After studying the Gauss-Bonnet limit of $f(R, R_c^2, R_m^2, \mathscr{L}_m)$ gravity, we moved on to more generic theories focusing on how the the standard stress-energy-momentum conservation equation $\nabla^\mu T_{\mu\nu} = 0$ in GR is violated. Under minimal coupling with $\mathscr{L} = f(\mathcal{R}_1, \ldots, \mathcal{R}_p) + 2\kappa\mathscr{L}_m$, we commented that the generalized Bianchi identities and the Noether-induced definition of SEM tensor lead to automatic energy-momentum conservation. Under nonminimal coupling with $\mathscr{L} = f(\mathcal{R}_1, \ldots, \mathcal{R}_p, \mathscr{L}_m)$, we have proposed a weak conjecture and a strong one which state that the gradient of the nonminimal gravitational coupling strength $\nabla^\mu f_{\mathscr{L}_m}$ is the only divergence term balancing $f_{\mathscr{L}_m}\nabla^\mu T_{\mu\nu}$, while contributions from $\mathcal{R}_i$-dependence in the divergence equation all cancel out. Using the energy-momentum nonconservation equation specialized for $f(R, R_c^2, R_m^2, \mathscr{L}_m)$ gravity, we have derived the equations of continuity and nongeodesic motion in the matter sources for perfect fluids, (timelike) dust, null dust, and massive scalar fields. These equations directly generalize those in $f(\mathcal{R}_1, \ldots, \mathcal{R}_p, \mathscr{L}_m)$ gravity.

Also, within $f(\mathcal{R}_1, \ldots, \mathcal{R}_p, \mathscr{L}_m)$ gravity, we have considered some implications of nonminimal coupling and $\mathcal{R}_i$-dependence for black hole and wormhole physics. Moreover, it is expected that the $\mathscr{L} = f(R, R_c^2, R_m^2, \mathscr{L}_m)$ model can provide many more possibilities to realize the late-time phase transition from cosmic deceleration to acceleration, and the energy-momentum nonconservation relation $f_{\mathscr{L}_m}\cdot\nabla^\mu T_{\mu\nu} = (\mathscr{L}_m g_{\mu\nu} - T_{\mu\nu})\nabla^\mu f_{\mathscr{L}_m}$ under nonminimal coupling can cause interesting consequences in early-era cosmic evolution and compact astrophysical objects if is effective as a high-energy phenomenon. These topics will be extensively investigated in prospective studies.

Acknowledgement

This work was financially supported by the Natural Sciences and Engineering Research Council of Canada.

Appendix: Generalized energy conditions for $f(R, \mathcal{R}_1, \ldots, \mathcal{R}_n, \mathscr{L}_m)$ gravity

For the generic $\mathscr{L} = f(R, \mathcal{R}_1, \ldots, \mathcal{R}_n, \mathscr{L}_m)$ gravity introduced in Section 4, the variational principle or equivalently $\dfrac{1}{\sqrt{-g}}\dfrac{\delta(\sqrt{-g}\,\mathscr{L})}{\delta g^{\mu\nu}} = 0$ yields the field equation:

$$-\frac{1}{2} f g_{\mu\nu} + f_R R_{\mu\nu} + (g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu) f_R + \sum_i H_{\mu\nu}^{(f\mathcal{R}_i)} = \frac{1}{2} f_{\mathscr{L}_m} \cdot (T_{\mu\nu} - \mathscr{L}_m g_{\mu\nu}), \tag{3.130}$$

where $H_{\mu\nu}^{(f\mathcal{R}_i)} \cdot \delta g^{\mu\nu} := f_{\mathcal{R}_i} \cdot \delta\mathcal{R}_i$. An immediate and very useful implication of this field equation is a group of generalized null, weak, strong and dominant energy conditions (abbreviated into NEC, WEC, SEC and DEC respectively), which has been employed in Sec. 3.6.2 in studying effects of nonminimal coupling in supporting wormholes.

Recall that in a (region of) spacetime filled by a null or a timelike congruence, the expansion rate along the null tangent ℓ^μ or the timelike tangent u^μ is given by the respective Raychaudhuri equation [20]:

$$\ell^\mu \nabla_\mu \theta_{(\ell)} = \frac{d\theta_{(\ell)}}{d\lambda} = \kappa_{(\ell)}\theta_{(\ell)} - \frac{1}{2}\theta_{(\ell)}^2 - \sigma_{\mu\nu}^{(\ell)}\sigma_{(\ell)}^{\mu\nu} + \omega_{\mu\nu}^{(\ell)}\omega_{(\ell)}^{\mu\nu} - R_{\mu\nu}\ell^\mu\ell^\nu \quad \text{and} \tag{3.131}$$

$$u^\mu \nabla_\mu \theta_{(u)} = \frac{d\theta_{(u)}}{d\tau} = \kappa_{(u)}\theta_{(u)} - \frac{1}{3}\theta_{(u)}^2 - \sigma_{\mu\nu}^{(u)}\sigma_{(u)}^{\mu\nu} + \omega_{\mu\nu}^{(u)}\omega_{(u)}^{\mu\nu} - R_{\mu\nu}u^\mu u^\nu\,. \tag{3.132}$$

Under affine parametrizations one has $\kappa_{(\ell)} = 0 = \kappa_{(u)}$, for hypersurface-orthogonal congruences the twist vanishes $\omega_{\mu\nu}\omega^{\mu\nu} = 0$, and the shear as a spatial tensor ($\sigma_{\mu\nu}^{(\ell)}\ell^\mu = 0$, $\sigma_{\mu\nu}^{(u)}u^\mu = 0$) always satisfies $\sigma_{\mu\nu}\sigma^{\mu\nu} \geq 0$. Thus, to ensure $d\theta_{(\ell)}/d\lambda \leq 0$ and $d\theta_{(u)}/d\tau \leq 0$ under all conditions so that "gravity always gravitates" and the congruence focuses, the following geometric nonnegativity conditions should hold:

$$R_{\mu\nu}\ell^\mu\ell^\nu \geq 0 \quad \text{(NEC)} \quad , \quad R_{\mu\nu}u^\mu u^\nu \geq 0 \quad \text{(SEC)}\,. \tag{3.133}$$

On the other hand, the field equation (3.12) can be recast into a compact GR form,

$$G_{\mu\nu} \equiv R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} = \kappa\, T_{\mu\nu}^{(\text{eff})}\,, \qquad R = -\kappa\, T^{(\text{eff})}\,, \qquad R_{\mu\nu} = \kappa\Big(T_{\mu\nu}^{(\text{eff})} - \frac{1}{2}g_{\mu\nu}T^{(\text{eff})}\Big), \tag{3.134}$$

where all terms beyond GR ($G_{\mu\nu} = \kappa T_{\mu\nu}$) in Eq.(3.130) have been packed into the effective SEM tensor $T_{\mu\nu}^{(\text{eff})}$,

$$T_{\mu\nu}^{(\text{eff})} = \frac{1}{2\kappa}\frac{f_{\mathscr{L}_m}}{f_R}\Big(T_{\mu\nu} - \mathscr{L}_m g_{\mu\nu}\Big) + \frac{1}{2\kappa}\frac{f_{\mathscr{L}_m}}{f_R}\Big((f - R f_R)\, g_{\mu\nu} + 2(\nabla_\mu\nabla_\nu - g_{\mu\nu}\Box) f_R - 2\sum_i H_{\mu\nu}^{(f\mathcal{R}i)}\Big). \tag{3.135}$$

The purely *geometric* conditions Eq.(3.133) can be translated into *matter* nonnegativity conditions through Eq.(3.134),

$$T_{\mu\nu}^{(\text{eff})}\,\ell^\mu\ell^\nu \geq 0 \quad \text{(NEC)} \quad , \quad T_{\mu\nu}^{(\text{eff})}u^\mu u^\nu \geq \frac{1}{2}T^{(\text{eff})}u_\mu u^\mu \quad \text{(SEC)} \quad , \quad T_{\mu\nu}^{(\text{eff})}\,u^\mu u^\nu \geq 0 \quad \text{(WEC)}\,, \tag{3.136}$$

where $u_\mu u^\mu = -1$ in SEC for the signature $(-,+++)$ used in this paper. Then the generalized NEC in

Eq.(3.136) is expanded into (as $\kappa > 0$)

$$\frac{f_{\mathscr{L}_m}}{f_R} T_{\mu\nu} \ell^\mu \ell^\nu + \frac{2}{f_R} \Big(\ell^\nu \ell^\mu \nabla_\mu \nabla_\nu f_R - \sum_i H_{\mu\nu}^{(f\mathcal{R}i)} \ell^\mu \ell^\nu \Big) \geq 0 \,, \tag{3.137}$$

which is the simplest one with $\mathscr{L}_m$ absent. Now, consider a special situation where f_R =constant and $H_{\mu\nu}^{(f\mathcal{R}i)} = 0$ (i.e. dropping all dependence on $\mathcal{R}_i$ in f), so Eq.(3.137) reduces to $\big(f_{\mathscr{L}_m}/f_R\big) \cdot T_{\mu\nu}\ell^\mu\ell^\nu \geq 0$; since $T_{\mu\nu}\ell^\mu\ell^\nu \geq 0$ due to the standard NEC in GR, which continues to hold here as exotic matters are unfavored, we obtain an extra constraint

$$\frac{f_{\mathscr{L}_m}}{f_R} \geq 0 \,, \tag{3.138}$$

with which Eq.(3.137) becomes

$$T_{\mu\nu} \ell^\mu \ell^\nu + 2 f_{\mathscr{L}_m}^{-1} \Big(\ell^\nu \ell^\mu \nabla_\mu \nabla_\nu f_R - \sum_i H_{\mu\nu}^{(f\mathcal{R}i)} \ell^\mu \ell^\nu \Big) \geq 0 \,, \tag{3.139}$$

and the WEC in Eq.(3.136) can be expanded into

$$T_{\mu\nu} u^\mu u^\nu + \mathscr{L}_m + f_{\mathscr{L}_m}^{-1} \Big(R f_R - f + 2(u^\mu u^\nu \nabla_\mu \nabla_\nu + \Box) f_R - 2 \sum_i H_{\mu\nu}^{(f\mathcal{R}i)} u^\mu u^\nu \Big) \geq 0 \,. \tag{3.140}$$

In general, the pointwise nonminimal coupling strength $f_{\mathscr{L}_m}$ can take either positive or negative values. However, recall that within $f(R) + 2\kappa\mathscr{L}_m$ gravity, physically viable models specializing $f(R)$ should satisfy $f_R > 0$ and $f_{RR} > 0$ [5]; if this were still true in $f(R, \mathcal{R}_1, \ldots, \mathcal{R}_n, \mathscr{L}_m)$ gravity, we would get $f_{\mathscr{L}_m} > 0$ by the extra constraint Eq.(3.138), which would be in strong agreement with the case of minimal coupling when $f_{\mathscr{L}_m} = 2\,\kappa > 0$.

Applying Eqs.(3.135), (3.139) and (3.140) to the Lagrangian density $\mathscr{L} = f(R, R_c^2, R_m^2, \mathscr{L}_m)$, we immediately obtain

$$T_{\mu\nu}^{(\text{eff})} = \frac{1}{2\kappa} \frac{f_{\mathscr{L}_m}}{f_R} \Big(T_{\mu\nu} - \mathscr{L}_m \, g_{\mu\nu} \Big) + \frac{1}{2\kappa} \frac{f_{\mathscr{L}_m}}{f_R} \Big((f - R\, f_R)\, g_{\mu\nu} + 2(\nabla_\mu \nabla_\nu - g_{\mu\nu}\Box)\, f_R - 2H_{\mu\nu}^{(fR_c^2)} - 2H_{\mu\nu}^{(fR_m^2)} \Big). \tag{3.141}$$

as the effective SEM tensor for for $f(R, R_c^2, R_m^2, \mathscr{L}_m)$ gravity. Then relative to the standard SEM tensor the generalized null and weak energy conditions respectively become

$$T_{\mu\nu} \ell^\mu \ell^\nu + 2 f_{\mathscr{L}_m}^{-1} \Big(\ell^\nu \ell^\mu \nabla_\mu \nabla_\nu f_R - H_{\mu\nu}^{(fR_c^2)} \ell^\mu \ell^\nu - H_{\mu\nu}^{(fR_m^2)} \ell^\mu \ell^\nu \Big) \geq 0 \quad \text{and} \tag{3.142}$$

$$T_{\mu\nu} u^\mu u^\nu + \mathscr{L}_m + f_{\mathscr{L}_m}^{-1} \Big(R f_R - f + 2(u^\mu u^\nu \nabla_\mu \nabla_\nu + \Box) f_R - 2H_{\mu\nu}^{(fR_c^2)} u^\mu u^\nu - 2H_{\mu\nu}^{(fR_m^2)} u^\mu u^\nu \Big) \geq 0 \,, \tag{3.143}$$

where $\{H_{\mu\nu}^{(fR_c^2)},\, H_{\mu\nu}^{(fR_m^2)}\}$ have been given in Eqs.(3.8) and (3.9).

Also, with Eq.(3.135) one can directly obtain the concrete forms SEC and DEC for $\mathscr{L} = f(R, \mathcal{R}_1, \ldots, \mathcal{R}_n, \mathscr{L}_m)$ gravity, which however will not be listed here.

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Chapter 4. Friedmann equations from nonequilibrium thermodynamics of the Universe: A unified formulation for modified gravity

[*Phys. Rev. D* **90** (2014), 104042]

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Abstract

Inspired by the Wald-Kodama entropy $S = A/(4G_{\text{eff}})$ where A is the horizon area and G_{eff} is the effective gravitational coupling strength in modified gravity with field equation $R_{\mu\nu} - Rg_{\mu\nu}/2 = 8\pi G_{\text{eff}} T^{(\text{eff})}_{\mu\nu}$, we develop a unified and compact formulation in which the Friedmann equations can be derived from thermodynamics of the Universe. The Hawking and Misner-Sharp masses are generalized by replacing Newton's constant G with G_{eff}, and the unified first law of equilibrium thermodynamics is supplemented by a nonequilibrium energy dissipation term $\mathcal{E}$ which arises from the revised continuity equation of the perfect-fluid effective matter content and is related to the evolution of G_{eff}. By identifying the mass as the total internal energy, the unified first law for the interior and its smooth transit to the apparent horizon yield both Friedmann equations, while the nonequilibrium Clausius relation with entropy production for an isochoric process provides an alternative derivation on the horizon. We also analyze the equilibrium situation $G_{\text{eff}} = G =$ constant, provide a viability test of the generalized geometric masses, and discuss the continuity/conservation equation. Finally, the general formulation is applied to the FRW cosmology of minimally coupled $f(R)$, generalized Brans-Dicke, scalar-tensor-chameleon, quadratic, $f(R, \mathcal{G})$ generalized Gauss-Bonnet and dynamical Chern-Simons gravity. In these theories we also analyze the $f(R)$-Brans-Dicke equivalence, find that the chameleon effect causes extra energy dissipation and entropy production, geometrically reconstruct the mass $\rho_m V$ for the physical matter content, and show the self-inconsistency of $f(R, \mathcal{G})$ gravity in problems involving G_{eff}.

PACS numbers: 04.20.Cv , 04.50.Kd , 98.80.Jk

4.1 Introduction

Ever since the discovery of black hole thermodynamics [1], physicists have been searching for more and deeper connections between relativistic gravity and fundamental laws of thermodynamics. One avenue of investigation by Gibbons and Hawking [2] found that the event horizon with radius ℓ for the de Sitter spacetime also produces Hawking radiation of temperature $1/(2\pi\ell)$. Jacobson [3] further showed within general

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relativity (GR) that on any local Rindler horizon, the entropy $S = A/4G$ and the Clausius relation $TdS = \delta Q$ could reproduce Einstein's field equation, with δQ and T being the energy flux and the Unruh temperature [4].

Besides global and quasilocal black-hole horizons [5, 6] and the local Rindler horizon, another familiar class of horizons are the various cosmological horizons. Frolov and Kofman [7] showed that for the flat quasi-de Sitter inflationary universe, $dE = TdS$ yields the Friedmann equation for the rolling inflaton field, and with metric and entropy perturbations it reproduces the linearized Einstein equations. By studying the heat flow during an infinitesimal time interval on the apparent horizon of the FRW universe within GR, Cai and Kim [8] showed that the Clausius thermal relation $TdS = \delta Q = -A\psi$ yields the second Friedmann gravitational equation with any spatial curvature, from which the first Friedmann equation can be directly recovered via the continuity/conservation equation of the perfect-fluid matter content. This work soon attracted much interest, and cosmology in different dark-energy content and gravity theories came into attention.

In [9] it was found that extensions of this formulation from GR to $f(R)$ and scalar-tensor theories are quite nontrivial, and the entropy formulas $S = Af_R/4G$ and $S = Af(\phi)/4G$ for black-hole horizons prove inconsistent in recovering Friedmann equations. In the meantime, Eling et al. [10] studied nonequilibrium thermodynamics of spacetime and found that $f(R)$ gravity indeed corresponds to a nonequilibrium description and therefore needs an entropy production term to balance the energy supply; the nonequilibrium Clausius relation $\delta Q = T(dS + d_pS)$ with $S = Af_R/(4G)$ then recovers the Friedmann equations. This nonequilibrium picture has been widely accepted, and relativistic gravity theories with nontrivial coefficient for $R_{\mu\nu}$ or equivalently $T^{(m)}_{\mu\nu}$ (hence nontrivial gravitational coupling strength G_{eff}) in their field equations always require a nonequilibrium description. Following [10], Friedmann equations are recovered from nonequilibrium thermodynamics within scalar-tensor gravity with horizon entropy $S = Af(\phi)/(4G)$ [11]. Besides the most typical $f(R)$ [9, 10] and scalar-tensor [9, 11] gravity, Friedmann equations from the Clausius relation are also studied in higher-dimensional gravity models like Lovelock gravity [8, 11] and Gauss-Bonnet gravity [8].

In the early investigations within modified and alternative theories of gravity, the standard definition of the Misner-Sharp mass [12] was used. However, the interesting fact that higher-order geometrical term or extra physical degrees of freedom beyond GR act like an effective matter content encourages the attempts to generalize such geometric definitions of mass in modified gravity. [13] generalized the Misner-Sharp mass in $f(R)$ gravity, and also for the FRW universe in the scalar-tensor gravity. In [14], a masslike function was employed in place of the standard Misner-Sharp mass, so that for $f(R)$ and scalar-tensor gravity the Friedmann equations on the apparent horizon could be recovered from the equilibrium Clausius relation $TdS = \delta Q$ without the nonequilibrium correction of [10]. Moreover, the opposite process of [8] to inversely rewrite the Friedmann equations into the thermodynamic relations has been investigated as well. For example, [15] studies such reverse process for GR, Lovelock and Gauss-Bonnet gravity, [16] for $f(R)$ gravity, [17] for the braneworld scenario, and [18] for generic $f(R, \phi, \nabla_\alpha\phi\nabla^\alpha\phi)$ gravity. Also, the field equations of various modified gravity are recast into the form of the Clausius relation in [19]. One should carefully distinguish the problem of "thermodynamics to Friedmann equations" with "Friedmann equations to thermodynamics", to avoid falling into the trap of cyclic logic.

Considering the discreteness of these works following [8] and the not-so-consistent setups of thermodynamic quantities therein, we are pursuing a simpler and more concordant mechanism hiding behind them: the purpose of this paper is to develop a unified formulation which derives the Friedmann equations from the (non)equilibrium thermodynamics of the FRW universe within all relativistic gravity with field equation $R_{\mu\nu} - Rg_{\mu\nu}/2 = 8\pi G_{\rm eff} T^{\rm (eff)}_{\mu\nu}$ with a possibly dynamical $G_{\rm eff}$. These theories include fourth-order modified theories of gravity in the metric approach (as opposed to Palatini) (eg. [20, 21]) with Lagrangian densities like $\mathscr{L} = f(R) + 16\pi G\mathscr{L}_m$ [22], $\mathscr{L} = f(R, \mathcal{G}) + 16\pi G\mathscr{L}_m$ [23] ($\mathcal{G}$ denoting the Gauss-Bonnet invariant), $\mathscr{L} = f(R, R_{\mu\nu}R^{\mu\nu}, R_{\mu\alpha\nu\beta}R^{\mu\alpha\nu\beta}) + 16\pi G\mathscr{L}_m$ [24] and quadratic gravity [25]; alternative theories of gravity[1] like Brans-Dicke [26] and scalar-tensor-chameleon [27] in the Jordan frame; typical dark-energy models $\mathscr{L} = R + f(\phi\,, \nabla_\alpha\phi\nabla^\alpha\phi) + 16\pi G\mathscr{L}_m$ [28], and even generic mixed models like $\mathscr{L} = f(R\,, \phi\,, \nabla_\alpha\phi\nabla^\alpha\phi) + 16\pi G\mathscr{L}_m$ (eg. [18]). All have minimal geometry-matter coupling with isolated matter Lagrangian density $\mathscr{L}_m$. The situation with nonminimal curvature-matter coupling terms [29, 30] like $R\mathscr{L}_m$ will not be considered in this paper, although the nonminimal chameleon coupling $\phi\mathscr{L}_m$ [27, 31] in scalar-tensor gravity is still analyzed.

This paper is organized as follows. Sec. 4.2 makes necessary preparations by locating the marginally inner trapped horizon as the apparent horizon of the FRW universe, revising the continuity equation for effective perfect fluids, and introducing the energy dissipation term $\mathcal{E}$ for modified gravity with field equation $R_{\mu\nu} - Rg_{\mu\nu}/2 = 8\pi G_{\rm eff} T^{\rm (eff)}_{\mu\nu}$. In Sec. 4.3, we generalize the geometric definitions of mass using $G_{\rm eff}$, supplement the unified first law of thermodynamics into $dE = A\boldsymbol{\psi} + WdV + \mathcal{E}$ by $\mathcal{E}$, and match the transverse gradient of the geometric mass with the change of total internal energy to directly obtain both Friedmann equations. We continue to study the thermodynamics of the apparent horizon by taking the smooth limit from the interior to the horizon in Sec. 4.4, and alternatively obtain the Friedmann equation from the nonequilibrium Clausius relation $T(dS + d_pS) = \delta Q = -(A\boldsymbol{\psi}_t + \mathcal{E})$, where d_pS represents entropy production which is generally nontrivial unless $G_{\rm eff} = \text{constant}$. After developing the generic theories, Sec. 4.5 provides a viability test for the generalized geometric masses, discusses the continuity equation, and analyzes the equilibrium case of $G_{\rm eff} = G = \text{constant}$ with vanishing dissipation $\mathcal{E} = 0$ and entropy production $d_pS = 0$. Finally in Sec. 4.6, the theory is applied to $f(R)$, generalized Brans-Dicke, scalar-tensor-chameleon, quadratic, $f(R, \mathcal{G})$ generalized Gauss-Bonnet and dynamical Chern-Simons gravity, with comments on existing treatment in $f(R)$ and scalar-tensor theories. Throughout this paper, especially for Sec. 4.6, we adopt the sign convention $\Gamma^\alpha_{\delta\beta} = \Gamma^\alpha{}_{\delta\beta}$, $R^\alpha{}_{\beta\gamma\delta} = \partial_\gamma\Gamma^\alpha_{\delta\beta} - \partial_\delta\Gamma^\alpha_{\gamma\beta}\cdots$ and $R_{\mu\nu} = R^\alpha{}_{\mu\alpha\nu}$ with the metric signature $(-, +\,+\,+)$.

4.2 Preparations and setups

4.2.1 FRW cosmology and location of the apparent horizon

The Friedman-Robertson-Walker (FRW) metric provides the most general solution describing a spatially homogeneous and isotropic Universe. It is not just a theoretical construct: it matches with observations. As such it must, a priori, be a solution of any aspiring modified or alternative theory of gravity [20]. In the comoving coordinates (t, r, θ, φ) the line element reads (eg. [8])

$$\begin{aligned} ds^2 &= -dt^2 + \frac{a(t)^2}{1-kr^2}\,dr^2 + a(t)^2r^2\left(d\theta^2 + \sin^2\theta\, d\varphi^2\right) \\ &= h_{\alpha\beta}\,dx^\alpha dx^\beta + \Upsilon^2\left(d\theta^2 + \sin^2\theta\, d\varphi^2\right), \end{aligned} \tag{4.1}$$

[1] For brevity, we will use the terminology "modified gravity" to denote both modified and alternative theories of relativistic gravity without discrimination whenever appropriate.

where the curvature index k is normalized to one of $\{-1\,,0\,,+1\}$ which correspond to closed, flat and open universes, respectively; the metric function $a(t)$ is the scale factor, which is an arbitrary function of the comoving time and is to be determined by the particular gravitational field equations. $h_{\alpha\beta} := \mathrm{diag}[-1\,, \frac{a(t)^2}{1-kr^2}]$ is the transverse two-metric spanned by $x^\alpha = (t, r)$, and $\Upsilon := a(t)\,r$ is the astrophysical circumference/areal radius. Although observations currently support a flat universe with $k = 0$, we will allow for all three situations $k = \{0\,, \pm1\}$ of spatial homogeneity and isotropy throughout this paper.

This solution is spherically symmetric and so in studying its physical and geometric properties it is convenient to work with a null tetrad[2] adapted to this symmetry:

$$\ell^\mu = \left(1\,, \frac{\sqrt{1-kr^2}}{a}\,, 0\,, 0\right) \quad , \quad n^\mu = \frac{1}{2}\left(1\,, -\frac{\sqrt{1-kr^2}}{a}\,, 0\,, 0\right) \quad , \quad m^\mu = \frac{1}{\sqrt{2}\,\Upsilon}\left(0, 0, 1, \frac{i}{\sin\theta}\right), \tag{4.2}$$

where the null vectors ℓ^μ and n^μ have respectively been adapted to the outgoing and ingoing null directions. The tetrad obeys the cross normalization $\ell_\mu n^\mu = -1$ and $m_\mu \bar{m}^a = 1$, and thus the inverse metric satisfies $g^{\mu\nu} = -\ell^\mu n^\nu - n^\mu \ell^\nu + m^\mu \bar{m}^\nu + \bar{m}^\mu m^\nu$. In this tetrad, the outward and inward expansions of radial null flow are found to be

$$\theta_{(\ell)} = -(\rho_{\mathrm{NP}} + \bar{\rho}_{\mathrm{NP}}) = \frac{2r\dot{a} + 2\sqrt{1-kr^2}}{a\,r} = 2H + 2\Upsilon^{-1}\sqrt{1 - \frac{k\Upsilon^2}{a^2}} \tag{4.3}$$

and

$$\theta_{(n)} = \mu_{\mathrm{NP}} + \bar{\mu}_{\mathrm{NP}} = \frac{r\dot{a} - \sqrt{1-kr^2}}{a\,r} = H - \Upsilon^{-1}\sqrt{1 - \frac{k\Upsilon^2}{a^2}}\,, \tag{4.4}$$

where $\rho_{\mathrm{NP}} := -m^\mu \bar{m}^\nu \nabla_\nu \ell_\mu$ and $\mu_{\mathrm{NP}} := \bar{m}^\mu m^\nu \nabla_\nu n_\mu$ are two Newman-Penrose spin coefficients, and H is Hubble's parameter

$$H := \frac{\dot{a}}{a}\,, \tag{4.5}$$

with the overdot denoting the derivative with respect to the comoving time t. In our universe in which $\dot{a} > 0$ and $H > 0$ the outward expansion $\theta_{(\ell)}$ is always positive while $\theta_{(n)}$ can easily be seen to vanish when

$$r_{\mathrm{A}} = \frac{1}{\sqrt{\dot{a}^2 + k}} \qquad \Leftrightarrow \qquad \Upsilon_{\mathrm{A}} = \frac{1}{\sqrt{H^2 + \dfrac{k}{a^2}}}\,. \tag{4.6}$$

On this surface

$$\theta_{(\ell)} = 4H > 0\,, \tag{4.7}$$

and thus $\Upsilon = \Upsilon_{\mathrm{A}}$ is a marginally inner trapped horizon [5] with $\theta_{(n)} < 0$ for $\Upsilon < \Upsilon_{\mathrm{A}}$ and $\theta_{(n)} > 0$ for $\Upsilon > \Upsilon_{\mathrm{A}}$. It is identified as the apparent horizon of the FRW universe[3]. Unlike the cosmological event horizon $\Upsilon_{\mathrm{E}} := a\int_t^\infty a^{-1}dt$ [33], which is the horizon of *absolute causality* and relies on the entire future

[2]The null tetrad formalism and all Newman-Penrose quantities in use here are adapted to the metric signature $(-,+++)$, which is the preferred convention for quasilocal black hole horizons (see eg. the Appendix B of [6]). Also, the tetrad can be rescaled by $\ell^\mu \mapsto e^f \ell^\mu$ and $n^\mu \mapsto e^{-f} n^\mu$ for an arbitrary function f, and consequently $\theta_{(\ell)} \mapsto e^f \theta_{(\ell)}$ and $\theta_{(n)} \mapsto e^{-f}\theta_{(n)}$.

[3]By the original definition [32] an apparent horizon is always marginally outer trapped with $\theta_{(\ell)} = 0$. However in this paper we follow the more general cosmological vernacular convention which defines an apparent horizon to be either a marginally outer trapped or marginally inner trapped surface. In a contracting universe with $\dot{a} < 0$ and $H < 0$, however, we would have a more standard marginally outer trapped horizon with $\theta_{(\ell)} = 0$ and $\theta_{(n)} = 2H < 0$ at $\Upsilon = \Upsilon_{\mathrm{A}}$.

history of the universe, the geometrically defined apparent horizon $\Upsilon_{\rm A}$ is the horizon of *relative causality* and is observer-dependent: if we center our coordinate system on any observer comoving with the universe, then $r_{\rm A}$ is the coordinate location of the apparent horizon relative to that observer. $\Upsilon_{\rm A}$ is practically more useful and realistic in observational cosmology as it can be identified by local observations in short duration. In fact, it has been found that [34] for an accelerating universe driven by scalarial dark energy with a possibly varying equation of state, the first and second laws of thermodynamics hold on $\Upsilon_{\rm A}$ but break down on $\Upsilon_{\rm E}$. Moreover for black holes, Hajicek [35] has argued that Hawking radiation happens on the apparent horizon rather than the event horizon. Hence in this paper we will focus on the cosmological apparent horizon $\Upsilon_{\rm A}$. Note that in spherical symmetry $\Upsilon_{\rm A}$ can equivalently be specified by setting $g^{\mu\nu}\partial_\mu\Upsilon\partial_\nu\Upsilon= h^{\alpha\beta}\partial_\alpha\Upsilon\partial_\beta\Upsilon = 0$, which locates the hypersurface on which $\partial_\alpha\Upsilon$ becomes a null vector. Hereafter, quantities related to or evaluated on the apparent horizon $\Upsilon = \Upsilon_{\rm A}$ will be highlighted by the subscript A.

In some calculations we will find it useful to work with the metric with radial coordinate Υ rather than r. To that end note that the total derivative of the physical radius $\Upsilon = a(t)r$ yields

$$adr \;=\; d\Upsilon - H\Upsilon dt\,, \tag{4.8}$$

so the FRW metric Eq.(4.1) can be rewritten into

$$ds^2 \;=\Big(1-\frac{k\Upsilon^2}{a^2}\Big)^{-1}\left(-\Big(1-\frac{\Upsilon^2}{\Upsilon_{\rm A}^2}\Big)dt^2-2H\Upsilon\, dt d\Upsilon+d\Upsilon^2\right)+\Upsilon^2\Big(d\theta^2+\sin^2\theta\, d\varphi^2\Big)\,. \tag{4.9}$$

For Eqs.(4.1) and (4.9), the coordinate singularity $r^2 = 1/k$ or $\Upsilon^2 = a^2/k$ can be removed in the isotropic radial coordinate $\bar r$ with $r := \bar r\,(1+\frac{k\bar r^2}{4})^{-1}$. Following Eq.(4.9) and keeping in mind that t is not orthogonal to Υ in the $(t\,,\Upsilon\,,\theta\,,\varphi)$ coordinates, the transverse component of the tetrad can be rebuilt as as

$$\ell^\mu \;=\left(1\,,H\Upsilon+\sqrt{1-\frac{k\Upsilon^2}{a^2}}\,,0\,,0\right)\quad,\quad n^\mu \;=\;\frac{1}{2}\left(1\,,H\Upsilon-\sqrt{1-\frac{k\Upsilon^2}{a^2}}\,,0\,,0\right)\,, \tag{4.10}$$

with which we obtain the same expansion rates $\{\theta_{(\ell)}\,,\theta_{(n)}\}$ and the horizon location $\Upsilon_{\rm A}$ as from the previous tetrad Eq.(4.2).

4.2.2 Modified gravity and energy dissipation

For modified theories of relativistic gravity such as $f(R)$, $f(R,\mathcal{G})$ and $f(R,R_{\mu\nu}R^{\mu\nu},R_{\mu\alpha\nu\beta}R^{\mu\alpha\nu\beta})$ classes of fourth-order gravity, and alternative theories such as Brans-Dicke and generic scalar-tensor-chameleon gravity, the field equations can be recast into the following compact GR form,

$$G_{\mu\nu}\equiv R_{\mu\nu}-\frac{1}{2}Rg_{\mu\nu} \;=\; 8\pi G_{\rm eff}\,T^{\rm (eff)}_{\mu\nu}\quad \text{with}\quad T^{\rm (eff)}_{\mu\nu} \;=\; T^{(m)}_{\mu\nu}+T^{\rm (MG)}_{\mu\nu}\,, \tag{4.11}$$

where the effective gravitational coupling strength $G_{\rm eff}$ relies on the specific gravity model and can be directly recognized from the coefficient of the stress-energy-momentum (SEM) density tensor $T^{(m)}_{\mu\nu}$ for the physical matter content, which is defined from extremizing the matter action functional $\delta\mathcal{I}_m = -\frac{1}{2}\int d^4x\sqrt{-g}T_{\mu\nu}\delta g^{\mu\nu}$. For example, as will be extensively discussed later in Sec. 4.6, we have $G_{\rm eff} = G/f_R$ for $f(R)$ gravity, $G_{\rm eff} = G/\phi$ for Brans-Dicke, $G_{\rm eff} = G/(1+2aR)$ for quadratic gravity, $G_{\rm eff} = G/(f_R+2Rf_{\mathcal{G}})$ for $f(R,\mathcal{G})$ generalized

Gauss-Bonnet gravity, and $G_{\rm eff} = G$ for dynamical Chern-Simons gravity. All terms beyond GR ($G_{\mu\nu} = 8\pi G T^{(m)}_{\mu\nu}$) have been packed into $G_{\rm eff}$ and $T^{(\rm MG)}_{\mu\nu}$, which together with $T^{(m)}_{\mu\nu}$ comprises the total effective SEM tensor $T^{(\rm eff)}_{\mu\nu}$. Furthermore, we assume a perfect-fluid-type content, which in the metric-independent form is

$$T^{\mu\,(\rm eff)}_{\ \nu} = {\rm diag}\,[\,-\rho_{\rm eff}, P_{\rm eff}, P_{\rm eff}, P_{\rm eff}] \quad , \quad \rho_{\rm eff} = \rho_m + \rho_{(\rm MG)} \quad , \quad P_{\rm eff} = P_m + P_{(\rm MG)}\ , \tag{4.12}$$

so that $T^{\mu(m)}_{\ \nu} = {\rm diag}[-\rho_m, P_m, P_m, P_m]$ and $T^{\mu\,(\rm MG)}_{\ \nu} = {\rm diag}[-\rho_{(\rm MG)}, P_{(\rm MG)}, P_{(\rm MG)}, P_{(\rm MG)}]$. Here ρ_m and P_m respectively collect the energy densities and pressures of all matter components in the universe, say $\rho_m = \rho_m(\text{baryon dust}) + \rho_m(\text{radiation}) + \rho_m(\text{dark energy}) + \rho_m(\text{dark matter}) + \cdots$ and the same for P_m, while the effects of modified gravity have been encoded into $G_{\rm eff}$, $\rho_{(\rm MG)}$ and $P_{(\rm MG)}$. For the spatially homogeneous and isotropic FRW universe of maximal spatial symmetry, the coupling strength $G_{\rm eff}$, the energy densities $\{\rho_{\rm eff}\,, \rho_m\,, \rho_{(\rm MG)}\}$ and the pressures $\{P_{\rm eff}\,, P_m\,, P_{(\rm MG)}\}$, are all functions of the comoving time t only.

If we take the covariant derivative of the field equation (4.11), then it follows from the contracted Bianchi identities that the generalized stress-energy-momentum conservation $\nabla_\mu G^\mu_{\ \ \nu} = 0 = 8\pi\nabla_\mu\Big(G_{\rm eff}\, T^{\mu\,(\rm eff)}_{\ \nu}\Big)$ holds for *all* modified gravity. With respect to the FRW metric Eq.(4.1), only the t-component of this conservation equation is nontrivial and leads to the universal relation

$$\dot\rho_{\rm eff} + 3H\Big(\rho_{\rm eff} + P_{\rm eff}\Big) = -\frac{\dot G_{\rm eff}}{G_{\rm eff}}\,\rho_{\rm eff}\ , \tag{4.13}$$

which serves as the generalized continuity equation for the perfect fluid of Eq.(4.12). Compared with the continuity equation of a cosmological perfect fluid $\dot\rho_m + 3H(\rho_m + P_m) = 0$ within GR, the extra term $-(\dot G_{\rm eff}/G_{\rm eff})\,\rho_{\rm eff}$ shows up in Eq.(4.13) to balance the energy flow. Since it has the same dimension as the effective density flow $\dot\rho_{\rm eff}$, we introduce the following differential energy by multiplying $Vdt = \frac{4}{3}\pi\,\Upsilon^3\,dt$ to it,

$$\mathcal{E} \coloneqq -\frac{4}{3}\pi\,\Upsilon^3\,\frac{\dot G_{\rm eff}}{G_{\rm eff}}\,\rho_{\rm eff}\,dt\ . \tag{4.14}$$

and call it the term of *nonequilibrium energy dissipation*. Note that at this stage in Eq.(4.14) for $\mathcal{E}$, the $\frac{4}{3}\pi\,\Upsilon^3\,\rho_{\rm eff}$ should not be combined into some kind of physically defined mass $V\rho_{\rm eff} = \mathcal{M}_{\rm eff}$ as its meaning is not clear yet (this is just an issue for security to avoid cyclic logic).

$\mathcal{E}$ is related to the temporal evolution of $G_{\rm eff}$ and its coupling to $\rho_{\rm eff}$. Whether $\mathcal{E}$ drives the evolution of $G_{\rm eff}$ or contrarily is produced by the evolution of $G_{\rm eff}$ is however not yet certain. Also, as will be seen later, $\mathcal{E}$ plays an important role below in supplementing the unified first law of equilibrium thermodynamics and calculating the entropy production. .

4.3 Thermodynamics inside the apparent horizon

For the FRW universe as a solution to the generic field equation (4.11), we substitute the effective gravitational coupling strength $G_{\rm eff}$ for Newton's constant G and thus generalize the Hawking mass $M_{\rm Hk}$ [39] for twist-free spacetimes into

$$\begin{aligned} M_{\rm Hk} &:= \frac{1}{4\pi G_{\rm eff}}\left(\int\frac{dA}{4\pi}\right)^{\frac{1}{2}}\int\Big(-\Psi_2-\sigma_{\rm NP}\lambda_{\rm NP}+\Phi_{11}+\Lambda_{\rm NP}\Big)\,dA \\ &\equiv \frac{1}{4\pi G_{\rm eff}}\left(\int\frac{dA}{4\pi}\right)^{\frac{1}{2}}\left(2\pi-\int\rho_{\rm NP}\,\mu_{\rm NP}\,dA\right). \end{aligned} \tag{4.15}$$

Since we are dealing with spherical symmetry, $M_{\rm Hk}$ can equivalently be written as

$$M_{\rm MS} := \frac{\Upsilon}{2G_{\rm eff}}\Big(1-h^{\alpha\beta}\partial_\alpha\Upsilon\partial_\beta\Upsilon\Big)\,, \tag{4.16}$$

which similarly generalizes the Misner-Sharp mass $M_{\rm MS}$ [12]. As will be shown later in Sec. 4.5.1, the geometric definitions Eqs.(4.15) and (4.16) fully reflect the spirit of geometrodynamics that the effective matter content $\rho_{\rm eff}=\rho_m+\rho_{\rm (MG)}$ curves the space homogeneously and isotropically through the field equation (4.11) to form the FRW universe. Moreover, the Misner-Sharp mass of black holes in Brans-Dicke gravity with $G_{\rm eff}=1/\phi$ has been found to satisfy Eq.(4.16) [36], which also encourages us to make the extensions in Eqs.(4.15) and (4.16). Note that the Hawking and Misner-Sharp masses restrict their attentions to the mass of the matter content and do not include the energy of gravitational field.

With $\Psi_2=\sigma_{\rm NP}=\lambda_{\rm NP}=0$, $\Phi_{11}=-\big(\dot H-\frac{k}{a^2}\big)/4$, $\Lambda_{\rm NP}=\big(\dot H+2H^2+\frac{k}{a^2}\big)/4$ or $\rho_{\rm NP}\,\mu_{\rm NP}=-\theta_{(\ell)}\theta_{(n)}/4$ in the tetrad Eq.(4.2), and $h^{\alpha\beta}=\text{diag}[-1\,,\frac{a^2}{1-kr^2}]$ for the transverse two-metric in Eq.(4.1), either Eq.(4.15) and Eq.(4.16) yield that the mass enveloped by a standard sphere of physical radius Υ in the FRW universe is

$$M = \frac{\Upsilon^3}{2G_{\rm eff}}\left(H^2+\frac{k}{a^2}\right). \tag{4.17}$$

Immediately, the total derivative or the transverse gradient of $M=M(t,r)$ is

$$\begin{aligned} dM &= \frac{\Upsilon^3 H}{2G_{\rm eff}}\left(2\dot H+3H^2+\frac{k}{a^2}\right)dt+\frac{3\Upsilon^2}{2G_{\rm eff}}\left(H^2+\frac{k}{a^2}\right)adr-\frac{\Upsilon^3\dot G_{\rm eff}}{2G_{\rm eff}^2}\left(H^2+\frac{k}{a^2}\right)dt && (4.18)\\ &= \frac{\Upsilon^3 H}{G_{\rm eff}}\left(\dot H-\frac{k}{a^2}\right)dt+\frac{3\Upsilon^2}{2G_{\rm eff}}\left(H^2+\frac{k}{a^2}\right)d\Upsilon-\frac{\Upsilon^3\dot G_{\rm eff}}{2G_{\rm eff}^2}\left(H^2+\frac{k}{a^2}\right)dt\,, && (4.19) \end{aligned}$$

where Eq.(4.8) has been used to reexpress Eq.(4.18) into Eq.(4.19) in terms of the $(t\,,\Upsilon)$ normal coordinates.

Hayward derived a unified first law of equilibrium thermodynamics [37, 38] for the differential element of energy change within GR under spherical symmetry, which however will be taken as a *first principle* in our work. For modified gravity of the form Eq.(4.11), we supplement Hayward's result by the energy dissipation term $\mathcal{E}$ introduced in Eq.(4.14), so that the change of energy along the outgoing null normal ℓ^μ across a sphere of radius Υ with surface area $A=4\pi\Upsilon^2$ and volume $V=4\pi\Upsilon^3/3$ is

$$dE = A\boldsymbol{\psi}+WdV+\mathcal{E}\,, \tag{4.20}$$

where the covector invariant $\boldsymbol{\psi}$ is the energy/heat flux density, the scalar invariant W is the work density, and $WdV=WAd\Upsilon$. We formally inherit the original definitions of $\{\boldsymbol{\psi}\,,W\}$ [37] but make use of the total effective

SEM tensor $T^{(\text{eff})}_{\mu\nu}$ rather than just $T^{(m)}_{\mu\nu}$ as in GR:

$$\psi_\alpha \;:=\; T_{\alpha\,(\text{eff})}^{\;\;\beta}\,\partial_\beta\Upsilon + W\,\partial_\alpha\Upsilon \quad \text{with} \quad W \;:=\; -\frac{1}{2}\,T^{\alpha\beta}_{(\text{eff})}\,h_{\alpha\beta}\;, \tag{4.21}$$

where $T^{(\text{eff})}_{\alpha\beta}$ denote the components of $T^{(\text{eff})}_{\mu\nu}$ along the transverse directions. Note that the definitions of $\boldsymbol{\psi}$ and W also guarantee that they are independent of the coordinate systems or observers and the choice of metric signature. Moreover, with the matter content of effective perfect fluid assumed in Eq.(4.12), $\boldsymbol{\psi}$ and W explicitly become

$$W = \frac{1}{2}\left(\rho_{\text{eff}} - P_{\text{eff}}\right) \quad \text{and} \tag{4.22}$$

$$\begin{aligned} \boldsymbol{\psi} \;&=\; -\frac{1}{2}\left(\rho_{\text{eff}} + P_{\text{eff}}\right) H\Upsilon\,dt + \frac{1}{2}\left(\rho_{\text{eff}} + P_{\text{eff}}\right) a\,dr \\ &=\; -\;\left(\rho_{\text{eff}} + P_{\text{eff}}\right) H\Upsilon\,dt + \frac{1}{2}\left(\rho_{\text{eff}} + P_{\text{eff}}\right) d\Upsilon\;, \end{aligned} \tag{4.23}$$

where W no longer preserves the generalized energy conditions[4] as opposed to the situation of GR [37] unless G_{eff} is positive definite. Hence, the unified first law Eq.(4.20) leads to

$$dE \;=\; -A\Upsilon H\,P_{\text{eff}}\,dt + A\,\rho_{\text{eff}}\,adr - \frac{4}{3}\pi\,\Upsilon^3\,\frac{\dot{G}_{\text{eff}}}{G_{\text{eff}}}\,\rho_{\text{eff}}\,dt \tag{4.24}$$

$$\;=\; -A\left(\rho_{\text{eff}} + P_{\text{eff}}\right) H\Upsilon\,dt + A\,\rho_{\text{eff}}\,d\Upsilon - \frac{4}{3}\pi\,\Upsilon^3\,\frac{\dot{G}_{\text{eff}}}{G_{\text{eff}}}\,\rho_{\text{eff}}\,dt\,. \tag{4.25}$$

Hence, by identifying the geometrically defined mass M as the *total internal energy*, matching the coefficients of dt and dr in Eqs.(4.18) and (4.24) or the coefficients of dt and $d\Upsilon$ in Eqs.(4.19) and (4.25), we obtain

$$H^2 + \frac{k}{a^2} \;=\; \frac{8\pi G_{\text{eff}}}{3}\,\rho_{\text{eff}} \quad \text{and} \tag{4.26}$$

$$\dot{H} - \frac{k}{a^2} = -4\pi G_{\text{eff}}\left(\rho_{\text{eff}} + P_{\text{eff}}\right) \qquad \text{or} \qquad 2\dot{H} + 3H^2 + \frac{k}{a^2} \;=\; -8\pi G_{\text{eff}} P_{\text{eff}}\;, \tag{4.27}$$

where we have recognized the last term in Eqs.(4.18) and (4.19) for dM equal to the dissipation $\mathcal{E}$ in dE as they are both relevant to the evolution of G_{eff}.

In fact, by substituting the FRW metric Eq.(4.1) into the field equation (4.11), it can be verified that Eqs.(4.26) and (4.27) are exactly the first and the second Friedmann equations governing the dynamics of the scale factor $a(t)$ for the FRW cosmology. Hence, the gravitational equations (4.26) and (4.27) have been derived from the unified first law of nonequilibrium thermodynamics $dE = A\boldsymbol{\psi} + WdV + \mathcal{E}$ instead of the field equation (4.11), and this is not a result of cyclic logic as Eqs.(4.26) and (4.27) are preassumed as unknown.

[4]For the field equation (4.11) along with $R = -8\pi G_{\text{eff}}\,T^{(\text{eff})}$ and $R_{\mu\nu} = 8\pi G_{\text{eff}}\,(T^{(\text{eff})}_{\mu\nu} - \frac{1}{2}g_{\mu\nu}T^{(\text{eff})})$, the Raychaudhuri equations ([32] or the appendix of [21]) imply the following null, weak and strong energy conditions (abbreviated into NEC, WEC and SEC respectively):

$$G_{\text{eff}}T^{(\text{eff})}_{\mu\nu}\,\ell^\mu\ell^\nu \;\geq\; 0 \quad (\text{NEC}) \quad , \quad G_{\text{eff}}T^{(\text{eff})}_{\mu\nu}\,u^\mu u^\nu \;\geq\; 0 \quad (\text{WEC}) \quad , \quad G_{\text{eff}}T^{(\text{eff})}_{\mu\nu}u^\mu u^\nu \;\geq\; \frac{1}{2}\,G_{\text{eff}}T^{(\text{eff})}u_\mu u^\mu \quad (\text{SEC})\,,$$

where $u_\mu u^\mu = -1$ in the SEC for the metric signature $(-,+++)$ used in this paper. All energy conditions require $G_{\text{eff}}\,(\rho_{\text{eff}} - P_{\text{eff}}) \geq 0$ for the effective matter content Eq.(4.12).

By the way, for the two versions of the second Friedmann equation in Eq.(4.27), the former is generally more preferred than the latter, because the former directly reflects the evolution of the Hubble parameter H (especially for $k = 0$ of the observed universe), and in numerical simulations the values of $\dot{H}$ and H^2 can differ dramatically (eg. [7] with $H^2 \gg \dot{H}$) and thus be problematic to work with when put together.

Once one of the Friedmann equations is known, the other one can be obtained using the continuity equation (4.13). For example, taking the time derivative of the first Friedmann equation $H^2+k/a^2 = 8\pi G_{\text{eff}}\,\rho_{\text{eff}}/3$,

$$2H\left(\dot{H} - \frac{k}{a^2}\right) = \frac{8\pi}{3}\left(\dot{G}_{\text{eff}}\rho_{\text{eff}} + G_{\text{eff}}\,\dot{\rho}_{\text{eff}}\right), \tag{4.28}$$

and applying the continuity equation

$$\dot{G}_{\text{eff}}\,\rho_{\text{eff}} + G_{\text{eff}}\,\dot{\rho}_{\text{eff}} + 3G_{\text{eff}}\,H\left(\rho_{\text{eff}} + P_{\text{eff}}\right) = 0\,,$$

one recovers the second Friedmann equation $\dot{H} - k/a^2 = -4\pi G_{\text{eff}}\,(\rho_{\text{eff}} + P_{\text{eff}})$. Inversely, integration of the second Friedmann equation with the continuity equation leads to the first Friedmann equation by neglecting an integration constant or otherwise treat it as a cosmological constant [8] and incorporate it into ρ_{eff}.

4.4 Thermodynamics On the apparent horizon

Having derived the Friedmann equations from the thermodynamics of the FRW universe inside the apparent horizon $\Upsilon < \Upsilon_{\text{A}}$, we will continue to study this thermodynamics-gravity correspondence on the horizon $\Upsilon = \Upsilon_{\text{A}}$, and in the meantime require consistency between the interior and the horizon. In fact, existing papers about this problem almost exclusively focus on the horizon alone [8, 9, 11, 14], as a companion to the thermodynamics of black-hole and Rindler horizons. In this section, the apparent horizon $\Upsilon = \Upsilon_{\text{A}}$ will be studied via two methods: (1) Following Sec.4.3, applying the nonequilibrium unified first law $dE = A\boldsymbol{\psi} + WdV + \mathcal{E}$ and $dE = dM$ in the smooth limit $\Upsilon \to \Upsilon_{\text{A}}$; (2) Using the nonequilibrium Clausius relation $T(dS + d_pS) = \delta Q = -(A\boldsymbol{\psi} + \mathcal{E})$ with entropy production d_pS and the continuity equation (4.13).

4.4.1 Method 1: Unified first law and $dE \hat{=} dM$

As shown by Eq.(4.6) in Sec.4.2, the cosmological apparent horizon, in this case a marginally inner trapped horizon of the expanding FRW universe locates at $\Upsilon_{\text{A}} = 1/\sqrt{H^2 + k/a^2}$, and according to Eq.(4.17), the mass within the horizon is $M_{\text{A}} = \Upsilon_{\text{A}}/(2G_{\text{eff}})$. Following Sec. 4.2.2 and taking the smooth limit $\Upsilon \to \Upsilon_{\text{A}}$ from the interior to the horizon, Eqs.(4.18) and (4.24) yield in the $(t\,, r)$ comoving transverse coordinates that

$$dM \;\hat{=}\; \frac{\Upsilon_{\text{A}}^3 H}{2G_{\text{eff}}}\left(2\dot{H} + 3H^2 + \frac{k}{a^2}\right)dt + \frac{3a}{2G_{\text{eff}}}\,dr - \frac{\Upsilon_{\text{A}}\dot{G}_{\text{eff}}}{2G_{\text{eff}}^2}\,dt \tag{4.29}$$

$$dE \;\hat{=}\; -A_{\text{A}}\Upsilon_{\text{A}}H\,P_{\text{eff}}\,dt + A_{\text{A}}\,\rho_{\text{eff}}\,a dr - \frac{4}{3}\pi\,\Upsilon_{\text{A}}^3\frac{\dot{G}_{\text{eff}}}{G_{\text{eff}}}\rho_{\text{eff}}\,dt\,, \tag{4.30}$$

while Eqs.(4.19) and (4.25) in the $(t\,,\Upsilon)$ coordinates give rise to

$$dM \hat{=} \frac{\Upsilon_A^3 H}{G_{\text{eff}}}\left(\dot{H}-\frac{k}{a^2}\right)dt+\frac{3}{2G_{\text{eff}}}\,d\Upsilon \quad - \quad \frac{\Upsilon_A \dot{G}_{\text{eff}}}{2G_{\text{eff}}^2}\,dt \tag{4.31}$$

$$dE \hat{=} -A_A\left(\rho_{\text{eff}}+P_{\text{eff}}\right)H\Upsilon_A\,dt+A_A\,\rho_{\text{eff}}\,d\Upsilon \quad - \quad \frac{4}{3}\pi\,\Upsilon_A^3\frac{\dot{G}_{\text{eff}}}{G_{\text{eff}}}\rho_{\text{eff}}\,dt\,, \tag{4.32}$$

where the symbol $\hat{=}$ will be employed hereafter to denote "equality on the apparent horizon", a standard denotation widely used for equality on quasilocal black-hole horizons (eg. [6]). Note that for the dr components in Eqs.(4.29) and (4.30) as well as the $d\Upsilon$ components in Eqs.(4.31) and (4.32), one just needs to evaluate their coefficients in the limit $\Upsilon \to \Upsilon_A$; although both horizon radii $r_A = r_A(t)$ and $\Upsilon_A = \Upsilon_A(t)$ are functions of t according to Eq.(4.6), the differentials dr and $d\Upsilon$ should not be replaced by $\dot{r}_A dt$ and $\dot{\Upsilon}_A dt$ for $\Upsilon \to \Upsilon_A$, because the horizon is not treated as a thermodynamical system alone by itself. As expected, in the limit $\Upsilon \to \Upsilon_A$ the equality $dM \hat{=} dE$ recovers the Friedmann equations again,

$$H^2+\frac{k}{a^2}\hat{=}\frac{8\pi G_{\text{eff}}}{3}\rho_{\text{eff}} \quad \text{and} \quad \dot{H}-\frac{k}{a^2}\hat{=}-4\pi G_{\text{eff}}\left(\rho_{\text{eff}}+P_{\text{eff}}\right) \quad \text{or} \quad 2\dot{H}+3H^2+\frac{k}{a^2}\hat{=}-8\pi G_{\text{eff}}P_{\text{eff}}\,.$$

Specifically note note from Eqs.(4.31) and (4.32) that on the horizon the dissipation term satisfies

$$\frac{4}{3}\pi\,\Upsilon_A^3\frac{\dot{G}_{\text{eff}}}{G_{\text{eff}}}\rho_{\text{eff}} \hat{=} \frac{1}{2}\Upsilon_A\frac{\dot{G}_{\text{eff}}}{G_{\text{eff}}^2}\,, \tag{4.33}$$

which, without being further simplified, will be used in the next subsection to reduce the expression of the on-horizon entropy production.

4.4.2 Method 2: Nonequilibrium Clausius relation

The modified theories of gravity under our consideration with the field equation (4.11) are all diffeomorphism invariant, and therefore we can obtain the Wald-Kodama dynamical entropy of the FRW apparent horizon by Wald's Noether-charge method [41, 42, 38] as

$$S := \int \frac{dA}{4G_{\text{eff}}} \hat{=} \frac{A_A}{4G_{\text{eff}}} \hat{=} \frac{\pi\Upsilon_A^2}{G_{\text{eff}}}\,, \tag{4.34}$$

with $G_{\text{eff}} = G_{\text{eff}}(t)$. In fact, the field equations of modified and alternative gravity have been deliberately rearranged into the form of Eq.(4.11) with an effective gravitational coupling strength G_{eff} to facilitate the definition of the horizon entropy Eq.(4.34). Moreover, the absolute temperature of the horizon is assumed to be [8]

$$T \equiv \frac{1}{2\pi\Upsilon_A}\,, \tag{4.35}$$

which agrees with the temperature of the semiclassical thermal spectrum [40] for the matter tunneling into the region $\Upsilon < \Upsilon_A$ from the exterior $\Upsilon > \Upsilon_A$, as measured by a Kodama observer using the line element Eq.(4.9). In fact, if the dynamical surface gravity [43] for the FRW spacetime is defined as $\kappa := -\frac{1}{2}\partial_\Upsilon \Xi$ with $\Xi := h^{\alpha\beta}\partial_\alpha\Upsilon\partial_\beta\Upsilon \equiv 1-\Upsilon^2(H^2+\frac{k}{a^2}) = 1-\Upsilon^2/\Upsilon_A^2$, then $\kappa = \Upsilon/\Upsilon_A^2 \hat{=} 1/\Upsilon_A$ and the temperature ansatz Eq.(4.35) satisfies $T = \kappa/(2\pi)$. This formally matches the Hawking temperature of (quasi-)stationary black holes in terms of the traditional definition of surface gravity [1] based on Killing vectors and Killing horizons. Hence it follows from Eqs.(4.34) and (4.35) that

$$TdS \hat{=} \frac{\dot{\Upsilon}_A}{G_{\text{eff}}}dt - \frac{1}{2}\Upsilon_A \frac{\dot{G}_{\text{eff}}}{G_{\text{eff}}^2}dt \qquad \text{with} \qquad \dot{\Upsilon}_A = -H\Upsilon_A^3\left(\dot{H} - \frac{k}{a^2}\right) . \tag{4.36}$$

Assuming that at the moment $t = t_0$ the apparent horizon locates at Υ_{A0}, then during the infinitesimal time interval dt the horizon will move to[5] $\Upsilon_{A0} + \dot{\Upsilon}_{A0}dt$. In the meantime, for the *isochoric* process ($d\Upsilon = 0$) for the volume of constant radius Υ_{A0}, the amount of energy across the horizon $\Upsilon = \Upsilon_{A0}$ during this dt is just $dE \hat{=} A_A\boldsymbol{\psi}_t + \mathcal{E}_A$ evaluated at $t = t_0$, as has been calculated in Eq.(4.32) with the $d\Upsilon$ component removed.

Compare $dE \hat{=} A_A\boldsymbol{\psi}_t + \mathcal{E}_A$ with Eq.(4.36), and it turns out the Clausius relation $TdS \hat{=} \delta Q \hat{=} -dE$ for equilibrium thermodynamics does not hold. To balance the energy change, we have to introduce an extra entropy production term d_pS [10] (subscript p being short for "production") so that

$$TdS + Td_pS \hat{=} -dE \hat{=} -(A_A\boldsymbol{\psi}_t + \mathcal{E}_A) . \tag{4.37}$$

Hence, it follows from Eqs.(4.32) and (4.36) that

$$\begin{aligned} Td_pS &\hat{=} -TdS - A_A\boldsymbol{\psi}_t - \mathcal{E}_A \\ &\hat{=} -\left(\frac{\dot{\Upsilon}_A}{G_{\text{eff}}}dt + A_A\boldsymbol{\psi}\right) + \frac{1}{2}\Upsilon_A\frac{\dot{G}_{\text{eff}}}{G_{\text{eff}}^2}dt - \mathcal{E}_A \\ &\hat{=} -\left(\frac{\dot{\Upsilon}_A}{G_{\text{eff}}} - A_A\left(\rho_{\text{eff}} + P_{\text{eff}}\right)H\Upsilon_A\right)dt + \frac{1}{2}\Upsilon_A\frac{\dot{G}_{\text{eff}}}{G_{\text{eff}}^2} + \frac{4}{3}\pi\,\Upsilon_A^3\frac{\dot{G}_{\text{eff}}}{G_{\text{eff}}}\rho_{\text{eff}}\,dt . \end{aligned} \tag{4.38}$$

We have combined the $\dot{\Upsilon}_A$ component of TdS in Eq.(4.36) with $A_A\boldsymbol{\psi}_t$, which reproduces the second Friedmann equation

$$\frac{\dot{\Upsilon}_A}{G_{\text{eff}}} - A_A\left(\rho_{\text{eff}} + P_{\text{eff}}\right)H\Upsilon_A \hat{=} 0 \qquad \Rightarrow \qquad \dot{H} - \frac{k}{a^2} \hat{=} -4\pi G\Big(\rho_{\text{eff}} + P_{\text{eff}}\Big) , \tag{4.39}$$

while the $\dot{G}_{\text{eff}}$ component of TdS in Eq.(4.36) and the energy dissipation $\mathcal{E}_A$ add up together and give rise to the entropy production

$$Td_pS \hat{=} \frac{1}{2}\Upsilon_A\frac{\dot{G}_{\text{eff}}}{G_{\text{eff}}^2}dt + \frac{4}{3}\pi\,\Upsilon_A^3\frac{\dot{G}_{\text{eff}}}{G_{\text{eff}}}\rho_{\text{eff}}\,dt \qquad \text{and} \qquad d_pS \hat{=} \pi\Upsilon_A^2\frac{\dot{G}_{\text{eff}}}{G_{\text{eff}}^2}dt + \frac{8}{3}\pi^2\,\Upsilon_A^4\frac{\dot{G}_{\text{eff}}}{G_{\text{eff}}}\rho_{\text{eff}}\,dt . \tag{4.40}$$

Hence, for the Wald-Kodama dynamical entropy Eq.(4.34), TdS manifests its effects in two aspects: the $\dot{\Upsilon}_A$ bulk term is the equilibrium part related to the expansion of the universe and the apparent horizon, while the $\dot{G}_{\text{eff}}$ term is the nonequilibrium part associated to the evolution of the coupling strength. The former balances the energy flux $A\boldsymbol{\psi}_t$ and leads to the Friedmann equation (4.39), while the latter, together with the generic energy dissipation $\mathcal{E}$ evaluated on the horizon, constitute the two sources shown up in Eq.(4.40)

[5] The second Friedmann equation (4.27) can be rewritten into the evolution equation for the apparent-horizon radius Υ_A:

$$\dot{\Upsilon}_A = 4\pi\,H\Upsilon_A^3G_{\text{eff}}\left(\rho_{\text{eff}} + P_{\text{eff}}\right),$$

which shows that for an expanding universe ($H > 0$), Υ_A can be either expanding, contracting or even static, depending on the values of G_{eff} and the effective equation of state parameter $w_{\text{eff}} = P_{\text{eff}}/\rho_{\text{eff}}$.

responsible for the entropy production.

As discussed before in Sec. 4.3, the first Friedmann equation $H^2 + k/a^2 \hat{=} 8\pi G_{\text{eff}}\,\rho_{\text{eff}}/3$ can be obtained from Eq.(4.39) with the help of the continuity equation (4.13). For the consistency between the horizon and the interior in the relation $dE \hat{=} dM \hat{=} -T(dS + d_pS)$, we have adjusted the thermodynamic sign convention into $T(dS + d_pS) \hat{=} \delta Q \hat{=} -dE \hat{=} -(A_A \boldsymbol{\psi}_t + \mathcal{E}_A)$.

In this paper, following the spirit of [10], primarily we call the modified gravity an equilibrium or nonequilibrium theory from the thermodynamic point of view depending on whether the equilibrium Clausius relation $TdS \hat{=} \delta Q \hat{=} -dE \hat{=} -A_A \boldsymbol{\psi}_t$ or its nonequilibrium extension with entropy production $TdS + Td_pS \hat{=} -dE \hat{=} -(A_A \boldsymbol{\psi}_t + \mathcal{E}_A)$ works on the apparent horizon. Moreover, Eq.(4.40) clearly shows that both sources for the nonequilibrium entropy-production d_pS trace back to the dynamics/evolution of G_{eff}. Hence, we further regard all those quantities containing $\dot{G}_{\text{eff}}$ as nonequilibrium, such as the energy dissipation element introduced in Eq.(4.14). In the same sense, TdS itself in Eq.(4.36) is no longer a thermodynamical quasistationary expression, and we regard its $\dot{\Upsilon}_A$ bulk component as equilibrium, while its $\dot{G}_{\text{eff}}$ component as nonequilibrium. This way, the thermodynamic terminology "nonequilibrium" and "equilibrium" in our usage throughout this paper have been clarified.

Eq.(4.40) demonstrates that the entropy production effect is generally unavoidable in modified gravity unless $G_{\text{eff}} = \text{constant}$. An increasing coupling strength G_{eff} leads to an entropy increment, while more interestingly, a decreasing G_{eff} would produce negative entropy for the universe. Yet Eq.(4.40) only reflects the entropy production d_pS on the horizon, and the total entropy change of the horizon as well as the entire universe needs further clarification within the generalized second law of thermodynamics within modified gravity. This problem is not tackled in this paper as we concentrate on the (unified) first law of thermodynamics. In addition, note that the dynamics of G_{eff} is different from the idea of varying gravitational constant in Dirac's "large numbers hypothesis" [44], which means nonconstancy of Newton's constant G over the cosmic time scale within GR.

If we take advantage of the on-horizon dissipation equation (4.33) in $dM \hat{=} dE$, that is to say, with the assistance of the first method in Sec. 4.4.1, the entropy production equation (4.40) can be much simplified into

$$Td_pS \,\hat{=}\, \Upsilon_A \frac{\dot{G}_{\text{eff}}}{G^2_{\text{eff}}}\, dt \qquad \text{and} \qquad d_pS \,\hat{=}\, 2\pi \Upsilon_A^2 \frac{\dot{G}_{\text{eff}}}{G^2_{\text{eff}}}\, dt\,. \tag{4.41}$$

It can reduce the calculations in specifying the amount of entropy production, when we need not distinguish the two sources represented by the two terms in Eq.(4.40). This simplification also indicates the $dM = dE$ method nicely complements the Clausius method.

4.5 Further discussion on the unified formulation

So far a unified formulation has been developed to derive the Friedmann equations from nonequilibrium thermodynamics within generic metric gravity $R_{\mu\nu} - Rg_{\mu\nu}/2 = 8\pi G_{\text{eff}} T^{(\text{eff})}_{\mu\nu}$, and the whole operation is:

(1) Inside the apparent horizon $\Upsilon < \Upsilon_A$, the total derivative dM of the geometric mass and the unified first law of nonequilibrium thermodynamics $dE = A\boldsymbol{\psi} + WdV + \mathcal{E}$ yield Friedmann equations via $dE = dM$. This method also applies to the horizon by taking the smooth limit $\Upsilon \to \Upsilon_A$.

(2) Alternatively, consider the change of total internal energy during the time interval dt. When evaluated

on the horizon $\Upsilon = \Upsilon_A$, the extended nonequilibrium Clausius relation $TdS + Td_pS \,\hat{=}\, \delta Q$ yields the second Friedmann equation, which can reproduce the first one with the continuity equation.

(3) Derivations for the interior $\Upsilon < \Upsilon_A$ and the horizon Υ_A should be consistent, which sets up the thermodynamic sign convention $T(dS + d_pS) \,\hat{=}\, \delta Q \,\hat{=}\, -dE \,\hat{=}\, -(A_A\psi_t + \mathcal{E}_A)$.

In this section we will further investigate some problems involved in the unified formulation.

4.5.1 A viability test of the extended Hawking and Misner-Sharp masses

We have replaced G with G_{eff} to generalize the Hawking mass and the Misner-Sharp mass into Eqs.(4.15) and (4.16), respectively. Such geometric mass worked well in deriving the Friedmann equations in the unified formulation for the correctness of this extension. Here we provide another piece of evidence by demonstrating that equality between the physical effective mass $\mathcal{M} = \rho_{\text{eff}} V$ and the generalized geometric masses automatically reproduces the Friedmann equations.

The total derivative of the physically defined effective mass $\mathcal{M} = \rho_{\text{eff}} V = (\rho_m + \rho_{(\text{MG})})\, V$ reads

$$\begin{aligned} d\mathcal{M} &= d\Big(\rho_{\text{eff}} V\Big) = \rho_{\text{eff}}\, dV + V\, \dot{\rho}_{\text{eff}}\, dt \\ &= \rho_{\text{eff}} A\, d\Upsilon - V\left(3H(\rho_{\text{eff}} + P_{\text{eff}}) + \frac{\dot{G}_{\text{eff}}}{G_{\text{eff}}}\rho_{\text{eff}}\right) dt \\ &= 4\pi\Upsilon^2 \rho_{\text{eff}}\, d\Upsilon - 4\pi\Upsilon^3 H\Big(\rho_{\text{eff}} + P_{\text{eff}}\Big) - \frac{4}{3}\pi\,\Upsilon^3 \frac{\dot{G}_{\text{eff}}}{G_{\text{eff}}}\rho_{\text{eff}}\, dt\,, \end{aligned} \tag{4.42}$$

where we have used the continuity equation (4.13) to replace $\dot{\rho}_{\text{eff}}$. Compare Eq.(4.42) with Eq.(4.19),

$$dM = \frac{\Upsilon^3 H}{G_{\text{eff}}}\left(\dot{H} - \frac{k}{a^2}\right) dt + \frac{3\Upsilon^2}{2G_{\text{eff}}}\left(H^2 + \frac{k}{a^2}\right) d\Upsilon - \frac{\Upsilon^3 \dot{G}_{\text{eff}}}{2G_{\text{eff}}^2}\left(H^2 + \frac{k}{a^2}\right) dt\,,$$

and straightforwardly, by assuming the physically defined effective mass $\mathcal{M} = \rho_{\text{eff}} V$ equal to the geometric effective mass in Eq.(4.17), which comes from Eqs.(4.15) and (4.16) that are defined solely out of the spacetime metric, we will automatically recover the two Friedmann equations from $d\mathcal{M} = dM$:

$$H^2 + \frac{k}{a^2} = \frac{8\pi G_{\text{eff}}}{3}\rho_{\text{eff}} \quad , \quad \dot{H} - \frac{k}{a^2} = -4\pi G_{\text{eff}}\Big(\rho_{\text{eff}} + P_{\text{eff}}\Big)\,.$$

In this sense we argue that the generalized definitions in Eqs.(4.15) and (4.16) for the Hawking and the Misner-Sharp masses are intuitive. Also, the equality to $\mathcal{M} = \rho_{\text{eff}} V$ indicates that Eqs.(4.15) and (4.16) only refer to the effective matter content and do not include the energy of gravitational field.

Having obtained the first Friedmann equation (4.26), we can now combine Eqs.(4.17) and (4.26) to eventually see that

$$M_{\text{MS}} = \frac{\Upsilon^3}{2G_{\text{eff}}}\left(H^2 + \frac{k}{a^2}\right) = \frac{\Upsilon^3}{2G_{\text{eff}}} \cdot \frac{8\pi G_{\text{eff}}}{3}\rho_{\text{eff}} = \frac{4}{3}\pi\Upsilon^3 \rho_{\text{eff}} = V\rho_{\text{eff}} = \mathcal{M}\,, \tag{4.43}$$

so the geometric effective mass Eq.(4.17) is really equal to the physically defined mass $V\rho_{\text{eff}}$ with the effective density determined by Eqs.(4.11) and (4.12). Note that [13] has generalized the Misner-Sharp masses for the $f(R)$ gravity with $G_{\text{eff}} = G/f_R$ and the scalar-tensor gravity with $G_{\text{eff}} = G/f(\phi)$, and their results actually refer to the pure mass $V\rho_m$ of the physical matter content compared with our generalizations, as will be clearly shown in Sec. 4.6.1 and Sec. 4.6.4 later. Also, the following masslike function was assumed in [14]

$$\text{Masslike} := \frac{\Upsilon}{2G_{\text{eff}}}\left(1 + h^{\alpha\beta}\partial_\alpha\Upsilon\partial_\beta\Upsilon\right) \equiv \frac{\Upsilon}{2G_{\text{eff}}}\left(2 - \frac{\Upsilon^2}{\Upsilon_{\text{A}}^2}\right) \mathrel{\hat{=}} \frac{\Upsilon_{\text{A}}}{2G_{\text{eff}}}\,, \tag{4.44}$$

in an attempt to recover the Friedmann equations on the horizon itself from the equilibrium Clausius relation without the entropy-production correction d_pS. However, it is not suitable in our more general formulation in Sec. 4.3 and Sec. 4.4, especially in the $dM = dE$ approach for the whole region $\Upsilon \leq \Upsilon_{\text{A}}$, and it does not pass the test just above as in Eq.(4.42).

On the other hand, recall that in recent studies on the interesting idea of "chemistry" of anti-de Sitter black holes [45], the mass M has been treated as the enthalpy $\mathcal{H}$ rather than total internal energy E, i.e. $M = \mathcal{H} = E + PV$ where the pressure P is proportional to the cosmological constant Λ. Since Λ the the simplest modified-gravity term, similarly, is it possible to identify the mass M in a sphere of radius $\Upsilon \leq \Upsilon_{\text{A}}$ in the FRW universe as the enthalpy $\mathcal{H} = E + \widetilde{P}V$ for some kind of pressure $\widetilde{P}$ (it can be P_{eff}, $P_{(\text{MG})}$, etc.)? We find that the answer seems to be negative. The equality between Eqs.(4.18)(4.19) for dM and Eqs.(4.24)(4.25) for dE, as well as the consistency among Eqs.(4.19), (4.25) and (4.42) clearly shows that the mass M should be identified as the total internal energy E. Moreover, if forcing the equality $M = \mathcal{H}$, then $dM = d\mathcal{H} = d(E + \widetilde{P}V)$ implies that necessarily that $\widetilde{P} \equiv 0$ and $\dot{\widetilde{P}} \equiv 0$ and thus we still have $M \equiv E$.

4.5.2 The continuity/conservation equation

As emphasized before in Sec. 4.1, we are considering ordinary modified gravity under minimal geometry-matter coupling, $\mathscr{L}_{\text{total}} = \mathscr{L}_{\text{gravity}} + 16\pi G\mathscr{L}_m$, with an isolated matter density $\mathscr{L}_m$ in the total lagrangian density and thus no curvature-matter coupling terms like $R\mathscr{L}_m$; or equivalently, the gravity/geometry part and the matter part in the total action are fully separable, $\mathcal{I}_{\text{total}} = \mathcal{I}_{\text{gravity}} + \mathcal{I}_m$. For the matter action $\mathcal{I}_m = \int d^4x\sqrt{-g}\mathscr{L}_m$ itself, the SEM tensor $T^{(m)}_{\mu\nu}$ is defined by the following stationary variation (eg. [21]),

$$\delta\mathcal{I}_m = \delta\int d^4x\sqrt{-g}\,\mathscr{L}_m = -\frac{1}{2}\int d^4x\sqrt{-g}\,T^{(m)}_{\mu\nu}\,\delta g^{\mu\nu} \quad \text{with} \quad T^{(m)}_{\mu\nu} := \frac{-2}{\sqrt{-g}}\frac{\delta\left(\sqrt{-g}\,\mathscr{L}_m\right)}{\delta g^{\mu\nu}}\,. \tag{4.45}$$

On the other hand, since $\mathscr{L}_m$ is a scalar invariant, Noether's conservation law yields

$$\nabla^\mu\left(\frac{1}{\sqrt{-g}}\frac{\delta\left(\sqrt{-g}\,\mathscr{L}_m\right)}{\delta g^{\mu\nu}}\right) = 0\,. \tag{4.46}$$

Comparison with Eq.(4.45) yields that Eq.(4.46) can be rewritten into $-\frac{1}{2}\nabla^\mu T^{(m)}_{\mu\nu} = 0$. Hence, the definition of the SEM tensor $T^{(m)}_{\mu\nu}$ as in Eq.(4.45) is Noether-compatible, and the definition of $T^{(m)}_{\mu\nu}$ by itself automatically guarantees stress-energy-momentum conservation

$$\nabla^\mu T^{(m)}_{\mu\nu} = 0\,. \tag{4.47}$$

For a time-dependent perfect-fluid matter content $T^{\mu\,(\mathrm{m})}_{\nu} = \mathrm{diag}\left[-\rho_m(t)\,, P_m(t)\,, P_m(t)\,, P_m(t)\right]$ (say for the FRW universe), $\nabla^\mu T^{(m)}_{\mu\nu} = 0$ gives rise to the continuity equation

$$\dot{\rho}_m + 3H\left(\rho_m + P_m\right) = 0\,. \tag{4.48}$$

Hence, the total continuity equation (4.13) can be reduced into

$$\dot{\rho}_{(\mathrm{MG})} + 3H\left(\rho_{(\mathrm{MG})} + P_{(\mathrm{MG})}\right) = -\frac{\dot{G}_{\mathrm{eff}}}{G_{\mathrm{eff}}}\left(\rho_m + \rho_{(\mathrm{MG})}\right). \tag{4.49}$$

Also, note that ρ_m collects the energy density of all possible physical material content,

$$\rho_m = \sum \rho_{m(i)} = \rho_m(\text{baryon dust}) + \rho_m(\text{radiation}) + \rho_m(\text{dark energy}) + \rho_m(\text{dark matter}) + \cdots\,, \tag{4.50}$$

and for each type of component $\rho_{m(i)}$, by decomposing Eq.(4.48) we have individually

$$\dot{\rho}_{m(i)} + 3H\left(\rho_{m(i)} + P_{m(i)}\right) = Q_{m(i)} \quad \text{with} \quad \sum Q_{m(i)} = 0\,, \tag{4.51}$$

where $Q_{m(i)}$ denotes the energy exchange due to the possible self- and cross-interactions among different matter components.

These results are applicable to the situation of minimal geometry-matter couplings. The thermodynamics of nonminimally coupled theories like $\mathscr{L} = f(R\,,T^{(m)}) + 16\pi G\mathscr{L}_m$ [46] (where $T^{(m)} = g_{\mu\nu}T^{\mu\nu}_{(m)}$) and $\mathscr{L} = f(R\,,T^{(m)}\,,R_{\mu\nu}T^{\mu\nu}_{(m)}) + 16\pi G\mathscr{L}_m$ [47] have been attempted using the traditional formulation as in [9] for $f(R)$ gravity. However, more profound thermodynamic properties may hide in these theories, as there is direct energy exchange between spacetime geometry and the energy-matter content under nonminimal curvature-matter couplings [29, 30, 21]. For example, very recently Harko [48] has interpreted the generalized conservation equations in $\mathscr{L} = f(R\,,\mathscr{L}_m)$ and $\mathscr{L} = f(R\,,T^{(m)}) + 16\pi G\mathscr{L}_m$ gravity as a matter creation process with an irreversible energy flow from the gravitational field to the created matter in accordance with the second law of thermodynamics. The unusual thermodynamic effects in these theories go beyond the scope of this paper, but for the chameleon effect [27, 31] which is another type of nonminimal coupling in scalar-tensor alternative gravity, we manage to find the extra energy dissipation and entropy production caused by the chameleon field, as will be shown later in Sec. 4.6.4.

4.5.3 "Negative temperature" on the horizon could remove the entropy production d_pS

In Sec. 4.4.2, by studying the energy change during dt across the horizon we have derived the second Friedmann equation from the nonequilibrium Clausius relation $T(dS + d_pS) \hat{=} -(A_\mathrm{A}\boldsymbol{\psi}_t + \mathcal{E}_\mathrm{A})$ with a necessary entropy-production element d_pS. However, we also observe that if the geometric temperature of the horizon were to be defined by the following "negative temperature"

$$\mathcal{T} \equiv -\frac{1}{2\pi\Upsilon_\mathrm{A}} < 0\,, \tag{4.52}$$

which is the opposite to Eq.(4.35), then it is easily seen from Sec. 4.4.2 that

$$\begin{aligned}\mathcal{T}dS - A_{\mathrm{A}}\boldsymbol{\psi}_t - \mathcal{E}_{\mathrm{A}} &\,\hat{=}\, \left(\frac{\dot{\Upsilon}_{\mathrm{A}}}{G_{\mathrm{eff}}}dt - A_{\mathrm{A}}\boldsymbol{\psi}_t\right) - \left(\frac{1}{2}\Upsilon_{\mathrm{A}}\frac{\dot{G}_{\mathrm{eff}}}{G_{\mathrm{eff}}^2}dt + \mathcal{E}_{\mathrm{A}}\right)\\ \hat{=} -\left(\frac{H\Upsilon_{\mathrm{A}}^3}{G_{\mathrm{eff}}}\left(\dot{H} - \frac{k}{a^2}\right) + A_{\mathrm{A}}\left(\rho_{\mathrm{eff}} + P_{\mathrm{eff}}\right)H\Upsilon_{\mathrm{A}}\right)dt &- \left(\frac{1}{2}\Upsilon_{\mathrm{A}}\frac{\dot{G}_{\mathrm{eff}}}{G_{\mathrm{eff}}^2} - \frac{4}{3}\pi\,\Upsilon_{\mathrm{A}}^3\frac{\dot{G}_{\mathrm{eff}}}{G_{\mathrm{eff}}}\rho_{\mathrm{eff}}\right)dt\,.\end{aligned} \tag{4.53}$$

In the last row of Eq.(4.53), the vanishing of the former parentheses leads to the second Friedmann equation, while in the second parentheses, the $\dot{G}_{\mathrm{eff}}$ component of $\mathcal{T}dS$ and the overall energy dissipation term $\mathcal{E}_{\mathrm{A}}$ cancel out each other to yield the first Friedmann equation. Hence, with the negative horizon temperature Eq.(4.52), both Friedmann equations could be obtained from the standard equilibrium Clausius relation

$$\mathcal{T}dS \,\hat{=}\, dE \,\hat{=}\, A_{\mathrm{A}}\boldsymbol{\psi}_t + \mathcal{E}_{\mathrm{A}} \tag{4.54}$$

without employing an entropy-production term d_pS.

However, the negative temperature ansatz Eq.(4.52) is problematic in various aspects. For example, negative absolute temperature is forbidden by the third law of thermodynamics (as is well known, the so-called "negative temperature" state in atomic physics actually occurs at a unusual phase of very high temperature where the entropy decreases with increasing internal energy, $T^{-1} := \partial S/\partial E < 0$). Also, if tracing back to the past history of the expanding Universe, one will find the horizon carrying a more and more negative temperature $\mathcal{T}$ while enclosing a more and more (positively) hot interior. From these perspectives, the observation from Eq.(4.52) that $\mathcal{T} = -1/(2\pi\Upsilon_{\mathrm{A}})$ could provide a most economical way to recover the Friedmann equations on the apparent horizon from equilibrium thermodynamics may just be an interesting coincidence.

4.5.4 Equilibrium situations with $G_{\mathrm{eff}} = G$ = constant and thus $\mathcal{E} = 0$

When the effective gravitational coupling strength G_{eff} reduces to become Newton's constant G, the field equation (4.11) reduces to

$$R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} \;=\; 8\pi G\, T_{\mu\nu}^{(\mathrm{eff})} \;=\; 8\pi G\left(T_{\mu\nu}^{(m)} + T_{\mu\nu}^{(\mathrm{MG})}\right). \tag{4.55}$$

For theories in this situation, the Lagrangian density generally takes the form

$$\mathscr{L} \;=\; R + f(R_{\mu\nu}R^{\mu\nu}, R_{\mu\alpha\nu\beta}R^{\mu\alpha\nu\beta}, \mathcal{R}_i \cdots) + \omega\left(\phi, \nabla_\mu\phi\nabla^\mu\phi\right) + 16\pi G\mathscr{L}_m\,, \tag{4.56}$$

where $\mathcal{R}_i$ denotes an arbitrary algebraic or differential Riemannian invariant $\mathcal{R}_i = \mathcal{R}_i\,(g_{\alpha\beta}, R_{\mu\alpha\nu\beta}, \nabla_\gamma R_{\mu\alpha\nu\beta}, \ldots, \nabla_{\gamma_1}\nabla_{\gamma_2}\ldots\nabla_{\gamma_q}R_{\mu\alpha\nu\beta})$ which is beyond the Ricci scalar R and makes no contribution to the coefficient of $R_{\mu\nu}$ in the field equation. ω is a generic function of the scalar field $\phi = \phi(x^\mu)$ and its kinetic term $\nabla_\mu\phi\nabla^\mu\phi$. For example, the $\mathscr{L} = R + f(R_{\mu\nu}R^{\mu\nu}, R_{\mu\alpha\nu\beta}R^{\mu\alpha\nu\beta}) + 16\pi G\mathscr{L}_m$ fourth-order gravity and typical scalarial dark-energy models [28] (like quintessence, phantom, k-essence) all belong to this class.

To apply the unified formulation developed in Sec. 4.3 and Sec. 4.4 for this situation, we just need to replace G_{eff} by G, set $\dot{G}_{\mathrm{eff}} = 0$, and remove the energy dissipation term $\mathcal{E}$. Hence, the Hawking or Misner-Sharp mass enclosed by a sphere of radius Υ is $M = (\Upsilon^3/2G)(H^2 + k/a^2)$. Compare the transverse gradient

dM of the mass with the change of internal energy $dE = A\psi + WdV$, and by matching the coefficients of

$$\begin{aligned} dM &= \frac{\Upsilon^3 H}{2G}\left(2\dot{H} + 3H^2 + \frac{k}{a^2}\right)dt + \frac{3\Upsilon^2}{2G}\left(H^2 + \frac{k}{a^2}\right)adr \\ dE &= -4\pi\Upsilon^3\, H\, P_{\text{eff}}\, dt + 4\pi\Upsilon^2\,\rho_{\text{eff}}\, adr \end{aligned} \tag{4.57}$$

in the comoving coordinates $(t\,,r)$, or

$$\begin{aligned} dM &= \frac{\Upsilon^3 H}{G}\left(\dot{H} - \frac{k}{a^2}\right)dt + \frac{3\Upsilon^2}{2G}\left(H^2 + \frac{k}{a^2}\right)d\Upsilon \\ dE &= -4\pi\Upsilon^3\, H\left(\rho_{\text{eff}} + P_{\text{eff}}\right)dt + 4\pi\Upsilon^2\,\rho_{\text{eff}}\, d\Upsilon\ , \end{aligned} \tag{4.58}$$

in the astrophysical areal coordinates $(t\,,\Upsilon)$, one obtains the Friedmann equations with $G_{\text{eff}} = G$:

$$H^2 + \frac{k}{a^2} = \frac{8\pi G}{3}\rho_{\text{eff}} \quad \text{and} \quad \dot{H} - \frac{k}{a^2} = -4\pi G\left(\rho_{\text{eff}} + P_{\text{eff}}\right) \quad \text{or} \quad 2\dot{H} + 3H^2 + \frac{k}{a^2} = -8\pi G P_{\text{eff}}\ . \tag{4.59}$$

Moreover, in the smooth limit $\Upsilon \to \Upsilon_{\text{A}}$ Eqs. (4.57) and (4.58) recover the complete set of Friedmann equations on the apparent horizon $\Upsilon = \Upsilon_{\text{A}}$ by $dM \,\hat{=}\, dE$. Alternatively, with the absolute temperature T and the entropy S of the horizon being

$$T \,\hat{=}\, \frac{1}{2\pi\Upsilon_{\text{A}}} \qquad \text{and} \qquad S \,\hat{=}\, \frac{A_{\text{A}}}{4G} \,\hat{=}\, \frac{\pi\Upsilon_{\text{A}}}{G}\ , \tag{4.60}$$

we have

$$T dS = \frac{\dot{\Upsilon}_{\text{A}}}{G}\,dt \quad \text{and} \quad A_{\text{A}}\psi_t \,\hat{=}\, -A_{\text{A}}\left(\rho_{\text{eff}} + P_{\text{eff}}\right)H\Upsilon_{\text{A}}\, dt\ . \tag{4.61}$$

Thus, the equilibrium Clausius relation $TdS \,\hat{=}\, \delta Q \,\hat{=}\, -A_{\text{A}}\psi_t$ with Eq.(4.61) for an isochoric process leads to the second Friedmann equation $\dot{H} - k/a^2 \,\hat{=}\, -4\pi G(\rho_{\text{eff}} + P_{\text{eff}})$. Taking into account the continuity equation with vanishing dissipation $\mathcal{E} = 0$:

$$\dot{\rho}_{\text{eff}} + 3H\left(\rho_{\text{eff}} + P_{\text{eff}}\right) = 0\ , \tag{4.62}$$

integration of the second Friedmann equation leads to the first equation $H^2 + k/a^2 = 8\pi G\,\rho_{\text{eff}}/3$, where the integration constant has been neglected or absorbed into ρ_{eff}. Moreover, the continuity/conservation equation (4.62) together with conservation of $T^{(m)}_{\mu\nu}$ in Eq.(4.48) lead to

$$\dot{\rho}_{(\text{MG})} + 3H\left(\rho_{(\text{MG})} + P_{(\text{MG})}\right) = 0\ . \tag{4.63}$$

For the componential convariant Lagrangian density $\sqrt{-g}\, f(R_{\mu\nu}R^{\mu\nu}\,, R_{\mu\alpha\nu\beta}R^{\mu\alpha\nu\beta}\,, \mathcal{R}_i \cdots)$ in Eq.(4.56), this is actually the "generalized contracted Bianchi identities" [21] in perfect-fluid form under the FRW background.

4.6 Examples

In this section, we will apply the unified formulation in Sec. 4.3 and Sec. 4.4 to some concrete theories of modified gravity. Compatible with the FRW metric Eq.(4.1) in the signature $(-,+++)$, we will adopt the geometric sign convention $\Gamma^\alpha_{\delta\beta} = \Gamma^\alpha{}_{\delta\beta}\,, R^\alpha{}_{\beta\gamma\delta} = \partial_\gamma\Gamma^\alpha_{\delta\beta} - \partial_\delta\Gamma^\alpha_{\gamma\beta}\cdots$ and $R_{\mu\nu} = R^\alpha{}_{\mu\alpha\nu}$.

4.6.1 $f(R)$ gravity

The $f(R)$ gravity [22] is the simplest class of fourth-order gravity, which straightforwardly generalizes the Hilbert-Einstein Lagrangian density $\mathscr{L}_{\text{HE}} = R + 16\pi G\mathscr{L}_m$ into $\mathscr{L} = f(R) + 16\pi G\mathscr{L}_m$ by replacing the Ricci scalar R with its arbitrary function $f(R)$. The field equation in the form of Eq.(4.11) is

$$R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} = 8\pi\frac{G}{f_R}T^{(m)}_{\mu\nu} + \frac{1}{f_R}\left(\frac{1}{2}(f - f_R R)\,g_{\mu\nu} + (\nabla_\mu\nabla_\nu - g_{\mu\nu}\Box)\,f_R\right), \tag{4.64}$$

where $f_R \coloneqq \partial f(R)/\partial R$ and $\Box \equiv \nabla^\alpha\nabla_\alpha$ denotes the covariant d'Alembertian. From the coefficient of $T^{(m)}_{\mu\nu}$ we learn that the effective gravitational coupling strength for $f(R)$ gravity is

$$G_{\text{eff}} = \frac{G}{f_R}\,, \tag{4.65}$$

and thus the modified-gravity SEM tensor is

$$T^{(\text{MG})}_{\mu\nu} = \frac{1}{8\pi G}\left(\frac{1}{2}(f - f_R R)g_{\mu\nu} + (\nabla_\mu\nabla_\nu - g_{\mu\nu}\Box)f_R\right), \tag{4.66}$$

which has collected the contributions from nonlinear and fourth-order curvature terms. Substituting the FRW metric Eq.(4.26) into this $T^{(\text{MG})}_{\mu\nu}$ and keeping in mind $T^{\mu\,(\text{MG})}_{\ \nu} = \text{diag}[-\rho_{(\text{MG})}, P_{(\text{MG})}, P_{(\text{MG})}, P_{(\text{MG})}]$, the energy density and pressure from the $f(R)$ modified-gravity effect are found to be

$$\rho_{(\text{MG})} = \frac{1}{8\pi G}\left(\frac{1}{2}f_R R - \frac{1}{2}f - 3H\dot{f}_R\right) \qquad \text{and} \qquad P_{(\text{MG})} = \frac{1}{8\pi G}\left(\frac{1}{2}f - \frac{1}{2}f_R R + \ddot{f}_R + 2H\dot{f}_R\right). \tag{4.67}$$

Given $G_{\text{eff}} = G/f_R$, the Hawking or Misner-Sharp mass in a sphere of radius Υ in the universe is

$$M = \frac{f_R\Upsilon^3}{2G}\left(H^2 + \frac{k}{a^2}\right) \qquad \text{with} \qquad M_{\text{A}} \mathrel{\hat{=}} \frac{f_R\Upsilon_{\text{A}}}{2G}\,. \tag{4.68}$$

Also, the geometric nonequilibrium energy dissipation term associated with G_{eff} and the geometric Wald-Kodama entropy of the horizon Υ_{A}

$$\mathcal{E} = \frac{4}{3}\pi\Upsilon^3\frac{\dot{f}_R}{f_R}\rho_{\text{eff}}\,dt \qquad \text{and} \qquad S = \frac{A_{\text{A}} f_R}{4G}\,. \tag{4.69}$$

Note that in $\mathcal{E}$ the term $\frac{4}{3}\pi\Upsilon^3\rho_{\text{eff}}$ should not be combined into the mass $V\rho_{\text{eff}} = \mathcal{M}$ at this stage for the reason stressed after Eq.(4.14). Applying the unified formulation developed in Sec. 4.3 and Sec. 4.4 to the FRW universe governed by $f(R)$ gravity, for the interior and the horizon $\Upsilon \leq \Upsilon_{\text{A}}$, the unified first law $dE = A\boldsymbol{\psi} + WdV + \mathcal{E} = dM$ of nonequilibrium thermodynamics and the nonequilibrium Clausius relation $T(dS + d_P S) \mathrel{\hat{=}} \delta Q \mathrel{\hat{=}} -(A_{\text{A}}\boldsymbol{\psi} + \mathcal{E}_{\text{A}})$ give rise to

$$H^2 + \frac{k}{a^2} = \frac{8\pi}{3}\frac{G}{f_R}\rho_m + \frac{1}{3f_R}\left(\frac{1}{2}f_R R - \frac{1}{2}f - 3H\dot{f}_R\right), \tag{4.70}$$

$$\dot{H} - \frac{k}{a^2} = -4\pi\frac{G}{f_R}\left(\rho_m + P_m\right) - \frac{1}{2f_R}\left(\ddot{f}_R - H\dot{f}_R\right). \tag{4.71}$$

In the meantime, the nonequilibrium entropy production d_pS on the horizon turns out to be

$$d_pS \;\hat{=}\; -2\pi\Upsilon_{\rm A}^2\frac{\dot{f}_R}{G}\,dt\;\;. \tag{4.72}$$

Substituting the FRW metric Eq.(4.1) into Eq.(4.64), we have verified that, Eqs.(4.70) and (4.71) are exactly the Friedmann equations of the FRW universe in $f(R)$ gravity. Such thermodynamics-gravity correspondence within $f(R)$ gravity has been investigated before in [9, 10] with different setups for the quantities $\{M\,,\rho_{(\rm MG)}\,,P_{(\rm MG)}\cdots\}$ and thus $\{\boldsymbol{\psi}\,,W\cdots\}$; compared with these earlier works, we have revised the thermodynamic setups and improved the result of entropy production.

Also note that, compact notations have been used in Eqs.(4.70) and (4.71), and f_R itself is treated as a function of the comoving time t. Otherwise, one can further write $\dot{f}_R$ into $f_{RR}\,\dot{R}$ and $\ddot{f}_R$ into $f_{RR}\,\dot{R}+f_{RRR}\,\dot{R}^2$ as in [9, 15], and for the FRW spacetime with metric Eq.(4.1), we have already known the Ricci scalar that

$$R \;=\; R(t) \;=\; 6\left(\dot{H}+2H^2+\frac{k}{a^2}\right)\,, \tag{4.73}$$

which in turn indicates the third-derivative $\ddot{H}$ and thus fourth-derivative $\ddot{\ddot{a}}$ get involved in Eqs.(4.70) and (4.71), and these terms are gone once we return to GR with $f_R=1$.

In [13], Cai et al. have generalized the Misner-Sharp energy/(mass) to $f(R)$ gravity by the integration and the conserved-charge methods. Specifically for the FRW universe, they found that the energy/mass within a sphere of radius Υ is

$$\begin{aligned} E_{\rm eff} \;&=\; \frac{\Upsilon}{2G}\left((1-h^{\alpha\beta}\partial_\alpha\Upsilon\partial_\beta\Upsilon)+\frac{1}{6}\,\Upsilon^2\,(f-f_RR)-\Upsilon\,h^{\alpha\beta}\,\partial_\alpha f_R\,\partial_\beta\Upsilon\right)\\ &=\; \frac{\Upsilon^3}{2G}\left(\frac{1}{\Upsilon_{\rm A}^2}\,f_R+\frac{1}{6}\,(f-f_RR)+H\,\dot{f}_R\right), \end{aligned} \tag{4.74}$$

with $\Upsilon_{\rm A}=1/\sqrt{H^2+k/a^2}$. What are the differences between this $E_{\rm eff}$ and our extended Misner-Sharp mass in Eqs.(4.16) and (4.17) in this paper? In the first and second row of Eq.(4.74), the first terms therein are respectively the definition Eq.(4.16) and the concrete mass Eq.(4.17) in our usage. To further understand the remaining terms in Eq.(4.74), one can manipulate it into

$$\begin{aligned} E_{\rm eff} \;&=\; \frac{f_R\Upsilon^3}{2G}\left(H^2+\frac{k}{a^2}\right)-\frac{\Upsilon^3}{2G}\left(\frac{1}{6}(f_RR-f)-H\dot{f}_R\right)\\ &=\; \frac{f_R\Upsilon^3}{2G}\left(H^2+\frac{k}{a^2}\right)-\frac{4}{3}\pi\Upsilon^3\cdot\frac{1}{8\pi G}\left(\frac{1}{2}f_RR-\frac{1}{2}f-3H\,\dot{f}_R\right). \end{aligned} \tag{4.75}$$

Recall that in Eq.(4.43), we have already proved the geometric mass Eq.(4.17) with which we start our formulation is equal to the physically defined mass $\rho_{\rm eff}\,V=\left(\rho_m+\rho_{(\rm MG)}\right)V$. Then from the density $\rho_{(\rm MG)}$ in Eq.(4.67) and the mass M in Eq.(4.68) for $f(R)$ gravity in our unified formulation, it turns out that the $E_{\rm eff}$ in Eq.(4.75) is actually

$$E_{\rm eff} \;=\; M-\rho_{(\rm MG)}V \;=\; \left(\rho_m+\rho_{(\rm MG)}\right)V-\rho_{(\rm MG)}V \;=\; \rho_mV\;. \tag{4.76}$$

Hence, the "generalized Misner-Sharp energy $E_{\rm eff}$" in [13] for the FRW universe within $f(R)$ gravity exactly match the pure mass of the physical matter content in our formulation of $f(R)$ cosmology.

4.6.2 Generalized Brans-Dicke gravity with self-interaction potential

Now, consider a generalized Brans-Dicke gravity with self-interaction potential in the Jordan frame given by the following Lagrangian density,

$$\mathscr{L}_{\text{GBD}} = \phi R - \frac{\omega(\phi)}{\phi} \nabla_\alpha\phi\nabla^\alpha\phi - V(\phi) + 16\pi G\mathscr{L}_m \,, \tag{4.77}$$

where, to facilitate the comparison with the proceeding case of $f(R)$ gravity, we have adopted the convention with an explicit G in $16\pi G\mathscr{L}_m$, rather than just $16\pi\mathscr{L}_m$ which encodes G into ϕ^{-1} [26]. The gravitational field equation $\delta(\sqrt{-g}\,\mathscr{L}_{\text{GBD}})/\delta g^{\mu\nu} = 0$ is

$$R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} = 8\pi\frac{G}{\phi}T^{(m)}_{\mu\nu} + \frac{1}{\phi}\left(\nabla_\mu\nabla_\nu - g_{\mu\nu}\Box\right)\phi + \frac{\omega(\phi)}{\phi^2}\Big(\nabla_\mu\phi\nabla_\nu\phi - \frac{1}{2}g_{\mu\nu}\nabla_\alpha\phi\nabla^\alpha\phi\Big) - \frac{1}{2\phi}V g_{\mu\nu} \,, \tag{4.78}$$

from which we directly read that the effective coupling strength and the modified-gravity SEM tensor are

$$G_{\text{eff}} = \frac{G}{\phi} \qquad \text{and} \tag{4.79}$$

$$T^{(\text{MG})}_{\mu\nu} = \frac{1}{8\pi G}\bigg(\left(\nabla_\mu\nabla_\nu - g_{\mu\nu}\Box\right)\phi + \frac{\omega(\phi)}{\phi}\Big(\nabla_\mu\phi\nabla_\nu\phi - \frac{1}{2}g_{\mu\nu}\nabla_\alpha\phi\nabla^\alpha\phi\Big) - \frac{1}{2}V g_{\mu\nu}\bigg) \,, \tag{4.80}$$

where $T^{(\text{MG})}_{\mu\nu}$ encodes the gravitational effects of the scalar field ϕ. Put the FRW metric Eq.(4.26) back to $T^{(\text{MG})}_{\mu\nu}$ with $T^{\mu\,(\text{MG})}_{\ \nu} = \text{diag}[-\rho_{(\text{MG})}, P_{(\text{MG})}, P_{(\text{MG})}, P_{(\text{MG})}]$, and the energy density and pressure from ϕ are found to be

$$\rho_{(\text{MG})} = \frac{1}{8\pi G}\Big(-3H\dot\phi + \frac{\omega}{2\phi}\dot\phi^2 + \frac{1}{2}V\Big) \quad \text{with} \quad P_{(\text{MG})} = \frac{1}{8\pi G}\Big(\ddot\phi + 2H\dot\phi + \frac{\omega}{2\phi}\dot\phi^2 - \frac{1}{2}V\Big) \,. \tag{4.81}$$

since $G_{\text{eff}} = G/\phi$, the geometric mass enveloped in a sphere of radius Υ is

$$M = \frac{\phi\Upsilon^3}{2G}\left(H^2 + \frac{k}{a^2}\right) \qquad \text{with} \qquad M_{\text{A}} \mathrel{\hat=} \frac{\phi\Upsilon_{\text{A}}}{2G} \,, \tag{4.82}$$

which in fact matches the Misner-Sharp mass of black holes in standard Brans-Dicke gravity in [36]. Also the nonequilibrium energy dissipation term $\mathcal{E}$ associated with the evolution of G_{eff} and the Wald-Kodama entropy S of the horizon are

$$\mathcal{E} = \frac{4}{3}\pi\Upsilon^3\frac{\dot\phi}{\phi}\rho_{\text{eff}}\,dt \qquad \text{and} \qquad S \mathrel{\hat=} \frac{A_{\text{A}}\phi}{4G} \,. \tag{4.83}$$

Following the unified formulation developed in Sec. 4.3 and Sec. 4.4 to study $dM = dE = A\boldsymbol{\psi} + WdV + \mathcal{E}$ for the region $\Upsilon \leq \Upsilon_{\text{A}}$ and $T(dS + d_P S) \mathrel{\hat=} \delta Q \mathrel{\hat=} -(A_{\text{A}}\boldsymbol{\psi} + \mathcal{E}_{\text{A}})$ for the horizon itself, we find

$$H^2 + \frac{k}{a^2} = \frac{8\pi}{3}\frac{G}{\phi}\rho_m + \frac{1}{3\phi}\Big(-3H\dot\phi + \frac{\omega}{2\phi}\dot\phi^2 + \frac{1}{2}V\Big) \,, \tag{4.84}$$

$$\dot{H} - \frac{k}{a^2} = -4\pi\frac{G}{\phi}\Big(\rho_m + P_m\Big) - \frac{1}{2\phi}\Big(\ddot{\phi} - H\dot{\phi} + \frac{\omega}{\phi}\dot{\phi}^2\Big)\,, \tag{4.85}$$

where as we can see, the scalar kinetics $\frac{\omega(\phi)}{\phi}\nabla_\alpha\phi\nabla^\alpha\phi$ and the potential $V(\phi)$ does not influence the evolution of the Hubble parameter H, and meanwhile the dynamics of ϕ and its nonminimal coupling to R in Eq.(4.149) leads to the entropy production

$$d_pS \mathrel{\hat{=}} -2\pi\Upsilon_{\rm A}^2\frac{\dot{\phi}}{G}\,dt \tag{4.86}$$

for the horizon. We have already verified that Eqs.(4.84) and (4.85) are just the Friedmann equations of the FRW universe in the generalized Brans-Dicke gravity by directly applying the FRW metric Eq.(4.1) to the gravitational field equation (4.78). Specifically when $\omega(\phi) \equiv \omega_{\rm BD}$=constant and $V(\phi) = 0$ (and erase G as $G \mapsto 1/\phi$ in standard Brans-Dicke), the thermodynamics-gravity correspondence just above reduces to the situation for the standard Brans-Dicke gravity [26] and its FRW cosmology. Moreover, our results improves the setups of $\{\rho_{\rm (MG)}\,, P_{\rm (MG)}\,, \boldsymbol{\psi}\,, W\cdots\}$ and the entropy production in [9] and [11] for a similar scalar-tensor theory with $\mathscr{L} = f(\phi)R/(16\pi G) - \frac{1}{2}\nabla_\alpha\phi\nabla^\alpha\phi - V(\phi) + \mathscr{L}_m$.

4.6.3 Equivalence between $f(R)$ and modified Brans-Dicke without kinetic term

The two models analyzed just above have exhibited pretty similar behaviors. Next we consider a modified Brans-Dicke gravity $\mathscr{L} = \phi R - V(\phi) + 16\pi G\,\mathscr{L}_m$, which is just the Lagrangian density Eq.(4.149) in Sec. 4.6.2 without the kinetic term $-\frac{\omega(\phi)}{\phi}\nabla_\alpha\phi\nabla^\alpha$. Compare its field equation with that of the $\mathscr{L} = f(R) + 16\pi G\,\mathscr{L}_m$ gravity in Sec. 4.6.1:

$$\begin{aligned} \phi\, R_{\mu\nu} - \frac{1}{2}\Big(\phi R - V(\phi)\Big)\, g_{\mu\nu} + \Big(g_{\mu\nu}\,\Box - \nabla_\mu\nabla_\nu\Big)\,\phi &= 8\pi G\, T_{\mu\nu}^{(m)}\,, \\ f_R\, R_{\mu\nu} - \frac{1}{2} f(R)\, g_{\mu\nu} + \Big(g_{\mu\nu}\,\Box - \nabla_\mu\nabla_\nu\Big) f_R &= 8\pi G\, T_{\mu\nu}^{(m)}\,. \end{aligned} \tag{4.87}$$

Clearly, these two field equations become identical with the following relations:

$$f_R = \phi \qquad \text{and} \qquad f(R) = \phi R - V(\phi) \qquad \Rightarrow \qquad f_R\, R - f(R) = V(\phi)\,. \tag{4.88}$$

That is to say, the $f(R)$ fourth-order modified gravity in Sec. 4.6.1 and the generalized Brans-Dicke alternative gravity in Sec. 4.6.2 are not totally independent. Instead, the former can be regarded as a subclass of the latter with vanishing coefficient $\omega(\phi) \equiv 0$ for the kinematic term $\nabla_\alpha\phi\nabla^\alpha$, and the equivalence is built upon Eq.(4.88). Applying the replacements $f_R \mapsto \phi$ and $f_R\, R - f(R) \mapsto V(\phi)$ to Sec. 4.6.1, we obtain the modified-gravity SEM tensor as

$$T_{\mu\nu}^{\rm (MG)} = \frac{1}{8\pi G}\bigg((\nabla_\mu\nabla_\nu - g_{\mu\nu}\Box)\,\phi - \frac{1}{2}V\, g_{\mu\nu}\bigg)\,, \tag{4.89}$$

the energy density and pressure in $T^{\mu\,\rm (MG)}_{\ \nu} = {\rm diag}[-\rho_{\rm (MG)}, P_{\rm (MG)}, P_{\rm (MG)}, P_{\rm (MG)}]$ as

$$\rho_{\rm (MG)} = \frac{1}{8\pi G}\Big(-3H\dot{\phi} + \frac{1}{2}V\Big) \quad \text{and} \quad P_{\rm (MG)} = \frac{1}{8\pi G}\Big(\ddot{\phi} + 2H\dot{\phi} - \frac{1}{2}V\Big)\,, \tag{4.90}$$

as well as the geometric mass M, nonequilibrium energy dissipation term $\mathcal{E}$, horizon entropy S and the nonequilibrium entropy production d_pS to be

$$M = \frac{\phi\Upsilon^3}{2G}\left(H^2 + \frac{k}{a^2}\right) \quad , \quad \mathcal{E} = \frac{4}{3}\pi\Upsilon^3\frac{\dot{\phi}}{\phi}\rho_{\text{eff}}\, dt \quad , \quad S \mathrel{\hat{=}} \frac{A_{\text{A}}\phi}{4G} \quad \text{and} \quad d_pS \mathrel{\hat{=}} -2\pi\Upsilon_{\text{A}}^2\frac{\dot{\phi}}{G}\, dt\,. \tag{4.91}$$

Finally the following equations are obtained from thermodynamics-gravity correspondence

$$H^2 + \frac{k}{a^2} = \frac{8\pi}{3}\frac{G}{\phi}\rho_m + \frac{1}{3\phi}\left(-3H\dot{\phi} + \frac{1}{2}V\right) \qquad \text{and} \qquad \dot{H} - \frac{k}{a^2} = -4\pi\frac{G}{\phi}\left(\rho_m + P_m\right) - \frac{1}{2\phi}\left(\ddot{\phi} - H\dot{\phi}\right). \tag{4.92}$$

It is easy to verify that, these thermodynamics quantities and equations precisely match the generalized Brans-Dicke in Sec. 4.6.2 with $\omega(\phi) \equiv 0$.

Conversely, if start from these setups just above or those in Sec. 4.6.2 with $\omega(\phi) \equiv 0$, the formulation in Sec. 4.6.1 can be recovered by applying the replacements $\phi \mapsto f_R$ and $V(\phi) \mapsto f_R R - f(R)$.

4.6.4 Scalar-tensor-chameleon gravity

Consider the following Lagrangian density for the generic scalar-tensor-chameleon gravity [27] in the Jordan frame ,

$$\mathscr{L}_{\text{STC}} = F(\phi)R - Z(\phi)\nabla_\alpha\phi\nabla^\alpha\phi - 2U(\phi) + 16\pi G E(\phi)\mathscr{L}_m\,, \tag{4.93}$$

where $\{F(\phi)\,, Z(\phi)\,, E(\phi)\}$ are arbitrary functions of the scalar field ϕ, and $E(\phi)$ is the chameleon function describing the coupling between ϕ and the matter Lagrangian density $\mathscr{L}_m$. The name "chameleon" comes from the fact that in the presence of $E(\phi)$, the wave equation $\delta(\sqrt{-g}\,\mathscr{L}_{\text{STC}})/\delta\phi = 0$ of ϕ becomes explicitly dependent on the matter content of the universe (eg. $\mathscr{L}_m$ or $T^{(m)} = g^{\mu\nu}T^{(m)}_{\mu\nu}$), which makes the wave equation change among different cosmic epoches as the dominant matter content varies [31]. The gravitational field equation $\delta(\sqrt{-g}\,\mathscr{L}_{\text{STC}})/\delta g^{\mu\nu} = 0$ is

$$R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} = 8\pi G\frac{E(\phi)}{F(\phi)}T^{(m)}_{\mu\nu} + \frac{1}{F(\phi)}\left(\nabla_\mu\nabla_\nu - g_{\mu\nu}\Box\right)F(\phi) + \frac{Z(\phi)}{F(\phi)}\left(\nabla_\mu\phi\nabla_\nu\phi - \frac{1}{2}g_{\mu\nu}\nabla_\alpha\phi\nabla^\alpha\right) - \frac{U(\phi)}{F(\phi)}g_{\mu\nu}\,, \tag{4.94}$$

so from the coefficient of $T^{(m)}_{\mu\nu}$ we recognize

$$G_{\text{eff}} = \frac{E(\phi)}{F(\phi)}G \qquad \text{and} \tag{4.95}$$

$$T^{(\text{MG})}_{\mu\nu} = \frac{1}{8\pi G E(\phi)}\left(\left(\nabla_\mu\nabla_\nu - g_{\mu\nu}\Box\right)F(\phi) + Z(\phi)\left(\nabla_\mu\phi\nabla_\nu\phi - \frac{1}{2}g_{\mu\nu}\nabla_\alpha\phi\nabla^\alpha\phi\right) - U(\phi)g_{\mu\nu}\right). \tag{4.96}$$

Note that [27] however adopted $G_{\text{eff}} = G/F(\phi)$ to study the second law of thermodynamics for the flat FRW universe, the chameleon function $E(\phi)$ excluded from G_{eff}. Substituting the FRW metric Eq.(4.26) into $T^{(\text{MG})}_{\mu\nu}$, the energy density and pressure for $T^{\mu\,(\text{MG})}_{\ \nu} = \text{diag}[-\rho_{(\text{MG})}, P_{(\text{MG})}, P_{(\text{MG})}, P_{(\text{MG})}]$ are found to be

$$\rho_{(\text{MG})} = \frac{1}{8\pi G\, E(\phi)}\left(-3H\dot{F} + \frac{1}{2}Z(\phi)\,\dot{\phi}^2 + U\right) \quad \text{and} \quad P_{(\text{MG})} = \frac{1}{8\pi G\, E(\phi)}\left(\ddot{F} + 2H\dot{F} + \frac{1}{2}Z(\phi)\,\dot{\phi}^2 - U\right), \tag{4.97}$$

where the compact notations $\dot{F}$ and $\ddot{F}$ can be replaced by $F_\phi\,\dot{\phi}$ and $F_\phi\,\ddot{\phi} + F_{\phi\phi}\,\dot{\phi}^2$, respectively. As $G_{\text{eff}} = GE(\phi)/F(\phi)$, the Hawking or Misner-Sharp geometric mass becomes

$$M \;=\; \frac{F(\phi)\Upsilon^3}{2GE(\phi)}\left(H^2+\frac{k}{a^2}\right) \qquad \text{with} \qquad M_{\text{A}} \,\hat{=}\, \frac{F(\phi)\Upsilon_{\text{A}}}{2GE(\phi)}\,, \tag{4.98}$$

while the nonequilibrium energy dissipation $\mathcal{E}$ in the conservation equation and the Wald-Kodama entropy of the horizon S are respectively

$$\mathcal{E} \;=\; \frac{4}{3}\pi\,\Upsilon^3\frac{G}{F(\phi)^2}\Big(E(\phi)\dot{F}-F(\phi)\dot{E}\Big)\rho_{\text{eff}}\,dt \qquad \text{and} \qquad S \;=\; \frac{A_{\text{A}}F(\phi)}{4GE(\phi)}\,, \tag{4.99}$$

where in $\mathcal{E}$ the compact notation $E(\phi)\dot{F} - F(\phi)\dot{E}$ can be expanded into $(EF_\phi - FE_\phi)\,\dot{\phi}$. Moreover, using the unified formulation developed in Sec. 4.3 and Sec. 4.4, for the interior and the horizon we obtain

$$H^2+\frac{k}{a^2} \;=\; \frac{8\pi}{3}\frac{GE(\phi)}{F(\phi)}\,\rho_m+\frac{1}{3F(\phi)}\Big(-3H\dot{F}+\frac{1}{2}\,Z(\phi)\,\dot{\phi}^2+U\Big)\,, \tag{4.100}$$

$$\dot{H}-\frac{k}{a^2} \;=-4\pi\frac{GE(\phi)}{F(\phi)}\Big(\rho_m+P_m\Big)-\frac{1}{2F(\phi)}\Big(\ddot{F}-H\dot{F}+Z(\phi)\,\dot{\phi}^2\Big)\,. \tag{4.101}$$

With $\dot{F} = F_\phi\dot{\phi}$ and $\ddot{F} = F_\phi\ddot{\phi} + F_{\phi\phi}\,\dot{\phi}^2$, they can be recast into

$$H^2+\frac{k}{a^2} \;=\; \frac{8\pi}{3}\frac{GE(\phi)}{F(\phi)}\,\rho_m+\frac{1}{3F(\phi)}\Big(-3HF_\phi\,\dot{\phi}+\frac{1}{2}Z(\phi)\,\dot{\phi}^2+U\Big)\,, \tag{4.102}$$

$$\dot{H}-\frac{k}{a^2} = -4\pi\frac{GE(\phi)}{F(\phi)}\Big(\rho_m+P_m\Big)-\frac{1}{2F(\phi)}\Big(F_\phi\ddot{\phi}+F_{\phi\phi}\dot{\phi}^2-HF_\phi\dot{\phi}+Z(\phi)\dot{\phi}^2\Big). \tag{4.103}$$

At the same time, the nonequilibrium entropy production turns out to be

$$d_pS \;=\; 2\pi\Upsilon_{\text{A}}^2\,\frac{1}{GE(\phi)^2}\Big(FE_\phi-EF_\phi\Big)\,\dot{\phi}\,dt\,. \tag{4.104}$$

We have verified by direct substitution of the FRW metric Eq.(4.1) into Eq.(4.94) that Eqs.(4.102) and (4.102) are indeed the Friedmann equations of the FRW universe in the scalar-tensor-chameleon gravity.

Compare the scalar-tensor-chameleon theory with the generalized Brans-Dicke gravity in Sec. 4.6.2, and we find that besides the nonminimal coupling $F(\phi)R$ in the Lagrangian density, the chameleon field $E(\phi)$ coupled to $\mathscr{L}_m$ causes extra nonequilibrium energy dissipation and entropy production, as shown by Eqs.(4.99) and (4.104). On the other hand, in the absence of the chameleon function, $E(\phi) \equiv 1$, $E_\phi = 0$, and with $F(\phi) \mapsto \phi$, $F_\phi \mapsto 1$, $F_{\phi\phi} \mapsto 0$, $Z(\phi) \mapsto \omega(\phi)/\phi$, $U \mapsto \frac{1}{2}V$, we recover the generalized Brans-Dicke in Sec. 4.6.2.

In [13], for the scalar-tensor gravity $\mathscr{L} = F(\phi)R/(16\pi G) - \frac{1}{2}\nabla_\alpha\phi\nabla^\alpha\phi - V(\phi) + \mathscr{L}_m$, the generalized Misner-Sharp mass/energy in the FRW universe is found to be

$$E_{\text{eff}} \;=\; \frac{\Upsilon^3}{2G}\left(F(\phi)\Big(H^2+\frac{k}{a^2}\Big)+H\dot{F}-\frac{4\pi}{3}\Big(\frac{1}{2}\,\dot{\phi}^2+V\Big)\right). \tag{4.105}$$

(Note: A typo in Eq.(A8) of [13] is corrected here by either checking the derivation of Eq.(A8), or by referring to Eq.(4.74) with the correspondence $f_R = \phi$ and $f_R R - f(R) = V$ as in Eq.(4.88), despite the nonzero kinetic term $-\frac{1}{2}\nabla_\alpha\phi\nabla^\alpha\phi$.) Compared with Eq.(4.93), [13] actually adopts a different scaling convention for the Lagrangian density; in accordance with Eq.(4.93), we rescale [13] by

$$\mathscr{L} = F(\phi)R - \frac{1}{2}\nabla_\alpha\phi\nabla^\alpha\phi - V(\phi) + 16\pi G\mathscr{L}_m\,, \tag{4.106}$$

and consequently

$$E_{\text{eff}} \;=\; \frac{\Upsilon^3}{2G}\Big(F(\phi)\Big(H^2+\frac{k}{a^2}\Big)+H\dot{F}-\frac{1}{6}\Big(\frac{1}{2}\,\dot{\phi}^2+V\Big)\Big)\,, \tag{4.107}$$

which can be expanded into

$$E_{\text{eff}} \;=\; \frac{F(\phi)\Upsilon^3}{2G}\Big(H^2+\frac{k}{a^2}\Big)-\frac{4}{3}\pi\Upsilon^3\cdot\frac{1}{8\pi G}\Big(-3H\dot{F}+\frac{1}{4}\,\dot{\phi}^2+\frac{1}{2}\,V\Big)\,. \tag{4.108}$$

As a subclass of the generic scalar-tensor-chameleon gravity Eq.(4.93) with $E(\phi)\mapsto 1$, $Z(\phi)\mapsto\frac{1}{2}$ and $U\mapsto\frac{1}{2}V$ for the Lagrangian density Eq.(4.106), the energy density $\rho_{(\text{MG})}$ in Eq.(4.97) and the mass M in Eq.(4.98) reduce to become

$$\rho_{(\text{MG})} \;=\; \frac{1}{8\pi G}\Big(-3H\dot{F}+\frac{1}{4}\,\dot{\phi}^2+\frac{1}{2}V\Big)\quad\text{and}\quad M \;=\; \frac{F(\phi)\Upsilon^3}{2G}\Big(H^2+\frac{k}{a^2}\Big)\,, \tag{4.109}$$

which finally recast Eq.(4.110) into

$$E_{\text{eff}} \;=\; M-\rho_{(\text{MG})}V \;=\; \Big(\rho_m+\rho_{(\text{MG})}\Big)V-\rho_{(\text{MG})}V \;=\; \rho_m V\,. \tag{4.110}$$

Hence, the "generalized Misner-Sharp energy E_{eff}" for the FRW universe within the scalar-tensor gravity in [13] is in fact the pure Misner-Sharp mass of physical matter for the same gravity in our work, just like the case of $f(R)$ gravity in Sec. 4.6.1.

4.6.5 Reconstruction of the physical mass $\rho_m V$ in generic modified gravity

Before proceeding to analyze more examples, we would like to give some remarks on the problem of reconstructing physical mass. Recall that in GR the mass $\rho_m V$ of the physical matter (like baryon dust, radiation) can be geometrically recovered by the Hawking mass for twist-free spacetimes [39] and the Misner-Sharp mass for spherically symmetric spacetimes [12]. In modified gravity, the physical matter content determines the FRW spacetime geometry Eq.(4.1) through more generic field equations which usually contain nonlinear and higher-order curvature terms beyond GR. Thus, how to reconstruct the mass of the physical matter from the spacetime geometry?

In [13], Cai el al. generalized the Misner-Sharp mass of GR into higher-dimensional Gauss-Bonnet gravity and the $f(R)$ (plus the scalar-tensor FRW) gravity in four dimensions. As just shown in Sec.4.6.1 and Sec. 4.6.4, for the FRW universe the results in [13] do match the physical material mass $\rho_m V$ in our unified formulation. In fact, for the FRW universe governed by generic modified gravity with the field equation $R_{\mu\nu} - Rg_{\mu\nu}/2 = 8\pi G_{\text{eff}} T^{(\text{eff})}_{\mu\nu}$, the mass $\mathcal{M}^{(m)} = \rho_m V$ of the physical matter content can be reconstructed from an geometric approach by

$$\mathcal{M}^{(m)} = \frac{\Upsilon^3}{2G_{\text{eff}}}\left(H^2+\frac{k}{a^2}\right)-\frac{4\pi\Upsilon^3}{3}\rho_{(\text{MG})}\,, \tag{4.111}$$

where $\rho_{(\text{MG})}$ is the density of modified-gravity effects collecting the nonlinear and higher-order geometric terms and joining $T^{\mu\,(\text{MG})}_{\ \nu} = \text{diag}[-\rho_{(\text{MG})}, P_{(\text{MG})}, P_{(\text{MG})}, P_{(\text{MG})}]$, as concretely shown just before for $f(R)$, generalized Brans-Dicke and scalar-tensor-chameleon gravity. When going beyond the FRW geometry in modified gravity, however, the validity of

$$\begin{aligned}\mathcal{M}^{(m)}_{\text{Hk}} &= \frac{1}{4\pi G_{\text{eff}}}\left(\int\frac{dA}{4\pi}\right)^{\frac{1}{2}}\int\Big(-\Psi_2-\sigma_{\text{NP}}\lambda_{\text{NP}}+\Phi_{11}+\Lambda_{\text{NP}}\Big)dA-\frac{4\pi\Upsilon^3}{3}\rho_{(\text{MG})}\\ &= \frac{1}{4\pi G_{\text{eff}}}\left(\int\frac{dA}{4\pi}\right)^{\frac{1}{2}}\left(2\pi-\int\rho_{\text{NP}}\,\mu_{\text{NP}}\,dA\right)-\frac{4\pi\Upsilon^3}{3}\rho_{(\text{MG})}\end{aligned} \tag{4.112}$$

to recover the physical mass $\rho_m V$ for an arbitrary twist-free spacetime based on the effective Hawking mass Eq.(4.15) in our unified formulation, and the feasibility of

$$\mathcal{M}^{(m)}_{\text{MS}} = \frac{\Upsilon}{2G_{\text{eff}}}\Big(1-h^{\alpha\beta}\partial_\alpha\Upsilon\partial_\beta\Upsilon\Big)-\frac{4\pi\Upsilon^3}{3}\rho_{(\text{MG})}\,, \tag{4.113}$$

for generic spherically symmetric spacetimes based on the effective Misner-Sharp mass Eq.(4.16), remain to be examined.

4.6.6 Quadratic gravity

For quadratic gravity [25], the Lagrangian density is constructed by combining the Hilbert-Einstein density of GR with the linear superposition of some well-known quadratic (as opposed to cubic and quartic) algebraic curvature invariants such as R^2, $R_{\mu\nu}R^{\mu\nu}$, $S_{\mu\nu}S^{\mu\nu}$ (with $S_{\mu\nu} := R_{\mu\nu} - \frac{1}{4}R\,g_{\mu\nu}$), $R_{\mu\alpha\nu\beta}R^{\mu\alpha\nu\beta}$, $C_{\mu\alpha\nu\beta}C^{\mu\alpha\nu\beta}$ (Weyl tensor square), say $\mathscr{L} = R + a\,R^2 + b\,R_{\mu\nu}R^{\mu\nu} + c\,S_{\mu\nu}S^{\mu\nu} + d\,R_{\mu\alpha\nu\beta}R^{\mu\alpha\nu\beta} + e\,C_{\mu\alpha\nu\beta}C^{\mu\alpha\nu\beta} + 16\pi G\mathscr{L}_m$ where $\{a,b,c,d,e\}$ are real-valued constants. However, these quadratic invariants are not totally independent of each other, as $S_{\mu\nu}S^{\mu\nu} = R_{\mu\nu}R^{\mu\nu} - \frac{1}{4}R^2$, $C_{\mu\alpha\nu\beta}C^{\mu\alpha\nu\beta} = R_{\mu\alpha\nu\beta}R^{\mu\alpha\nu\beta} - 2R_{\mu\nu}R^{\mu\nu} + R^2/3$, and moreover $R_{\mu\alpha\nu\beta}R^{\mu\alpha\nu\beta}$ can be absorbed into the Gauss-Bonnet invariant $\mathcal{G} := R^2 - 4R_{\mu\nu}R^{\mu\nu} + R_{\mu\alpha\nu\beta}R^{\mu\alpha\nu\beta}$ which does not contribute to the field equation since $\delta\int d^4x\sqrt{-g}\,\mathcal{G}/\delta g^{\mu\nu} \equiv 0$ (eg. [21]). Hence, it is sufficient to consider the following Lagrangian density for quadratic gravity

$$\mathscr{L}_{\text{QG}} = R + a\,R^2 + b\,R_{\mu\nu}R^{\mu\nu} + 16\pi G\mathscr{L}_m\,, \tag{4.114}$$

and the field equation is [21]

$$-\frac{1}{2}(R + a\cdot R^2 + b\cdot R_c^2)\,g_{\mu\nu} + (1+2aR)\,R_{\mu\nu} + 2a\,(g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu)\,R + b\cdot H^{(\text{QG})}_{\mu\nu} = 8\pi G\,T^{(m)}_{\mu\nu}\,, \tag{4.115}$$

where R_c^2 is the straightforward abbreviation for the Ricci tensor square $R_{\mu\nu}R^{\mu\nu}$ to shorten some upcoming expressions below, and

$$H^{(\text{QG})}_{\mu\nu} = 2R_{\mu\alpha\nu\beta}R^{\alpha\beta} + (\frac{1}{2}\,g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu)\,R + \Box R_{\mu\nu}\,. \tag{4.116}$$

It can be rewritten into

$$R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} = 8\pi\frac{G}{1+2aR}\left(T^{(m)}_{\mu\nu} + T^{(\mathrm{MG})}_{\mu\nu}\right) \tag{4.117}$$

where

$$G_{\mathrm{eff}} = \frac{G}{1+2aR} \qquad \text{and} \tag{4.118}$$

$$T^{(\mathrm{MG})}_{\mu\nu} = \frac{1}{8\pi G}\left(\frac{1}{2}\left(b\cdot R_c^2 - aR^2\right)g_{\mu\nu} + (2a+b)\,\nabla_\mu\nabla_\nu R - (2a+\frac{b}{2})\,g_{\mu\nu}\Box R - 2b\left(2R_{\mu\alpha\nu\beta}R^{\alpha\beta} + \Box R_{\mu\nu}\right)\right). \tag{4.119}$$

Substitute the FRW metric Eq.(4.1) into $T^{(\mathrm{MG})}_{\mu\nu}$, and with $T^{\mu}{}_{\nu}^{(\mathrm{MG})} = \mathrm{diag}[-\rho_{(\mathrm{MG})}, P_{(\mathrm{MG})}, P_{(\mathrm{MG})}, P_{(\mathrm{MG})}]$ we get

$$\rho_{(\mathrm{MG})} = \frac{1}{8\pi G}\left(\frac{a}{2}R^2 - \frac{b}{2}R_c^2 + \frac{b}{2}\,\ddot{R} - (4a+b)\,H\dot{R} + 4b\,R^{t}{}_{\alpha t\beta} + 2b\,\Box R_{t}{}^{t}\right), \tag{4.120}$$

$$P_{(\mathrm{MG})} = \frac{1}{8\pi G}\left(\frac{b}{2}R_c^2 - \frac{a}{2}R^2 + (2a+\frac{b}{2})\,\ddot{R} + (4a+\frac{b}{2})\,H\dot{R} - 4b\,R^{r}{}_{\alpha r\beta}R^{\alpha\beta} - 2b\,\Box R_{r}{}^{r}\right). \tag{4.121}$$

where we have used $R^{t}{}_{\alpha t\beta} = -R_{t\alpha t\beta}$ and $\Box R_{t}{}^{t} = -\Box R_{tt}$ in $\rho_{(\mathrm{MG})}$ under the FRW metric Eq.(4.1). Also, since $G_{\mathrm{eff}} = G/\phi$, the geometric mass enclosed in a sphere of radius Υ is

$$M = \frac{(1+2aR)\,\Upsilon^3}{2G}\left(H^2 + \frac{k}{a^2}\right) \qquad \text{with} \qquad M_{\mathrm{A}} \mathrel{\hat{=}} \frac{(1+2aR)\,\Upsilon_{\mathrm{A}}}{2G}\,, \tag{4.122}$$

while the nonequilibrium energy dissipation $\mathcal{E}$ associated with the evolution of G_{eff} and the Wald-Kodama entropy E of the horizon are respectively

$$\mathcal{E} = \frac{4}{3}\pi\,\Upsilon^3\frac{2a\dot{R}}{1+2aR}\,\rho_{\mathrm{eff}}\,dt \qquad \text{and} \qquad S = \frac{A_{\mathrm{A}}\,(1+2aR)}{4G}\,. \tag{4.123}$$

Following the unified formulation developed in Sec. 4.3 and Sec. 4.4 to study $dM = dE = A\boldsymbol{\psi} + WdV + \mathcal{E}$ for the region $\Upsilon \le \Upsilon_{\mathrm{A}}$ and $T(dS + d_P S) \mathrel{\hat{=}} \delta Q \mathrel{\hat{=}} -(A_{\mathrm{A}}\boldsymbol{\psi} + \mathcal{E}_{\mathrm{A}})$ for the horizon itself, we find

$$H^2 + \frac{k}{a^2} = \frac{8\pi}{3}\frac{G}{1+2aR}\,\rho_m + \frac{1}{3(1+2aR)}\left(\frac{a}{2}R^2 - \frac{b}{2}R_c^2 + \frac{b}{2}\,\ddot{R} - (4a+b)\,H\dot{R} + 4b\,R^{t}{}_{\alpha t\beta} + 2b\,\Box R_{t}{}^{t}\right) \tag{4.124}$$

$$\dot{H} - \frac{k}{a^2} = -4\pi\frac{G}{1+2aR}\left(\rho_m + P_m\right) - \frac{1}{2(1+2aR)}\left((2a+b)\,\ddot{R} - \frac{b}{2}\,H\dot{R} + 4b\,(R^{t}{}_{\alpha t\beta} - R^{r}{}_{\alpha r\beta})R^{\alpha\beta} + 2b\,\Box(R_{t}{}^{t} - R_{r}{}^{r})\right), \tag{4.125}$$

while the nonequilibrium entropy production on the horizon is

$$d_p S \mathrel{\hat{=}} -4\pi\Upsilon_{\mathrm{A}}^2\,\frac{a\dot{R}}{G}\,dt\,. \tag{4.126}$$

We have verified that the thermodynamic relations Eqs.(4.124) and (4.125) are equivalent to the gravitational Friedmann equations by substituting the FRW metric Eq.(4.1) into the quadratic field equations (4.117) and (4.119).

Just like the treatment of $f(R)$ gravity in Sec. 4.6.1, to keep the expressions of $\rho_{(\text{MG})}$, $P_{(\text{MG})}$ and the Friedmann equations (4.124) and (4.125) clear and readable, we continue using compact notations for R, R_c^2, $\dot{R}$, $\ddot{R}$, $R^t{}_{\alpha t\beta}R^{\alpha\beta}$, $R^r{}_{\alpha r\beta}R^{\alpha\beta}$, $\Box R_t{}^t$ and $\Box R_r{}^r$, and one should keep in mind that for the FRW metric Eq.(4.1), these quantities are already known and can be fully expanded into higher-derivative and nonlinear terms of H or a.

4.6.7 $f(R,\mathcal{G})$ generalized Gauss-Bonnet gravity

The generalized Gauss-Bonnet gravity under discussion is given by the Lagrangian density $\mathscr{L}_{\text{GB}} = f(R,\mathcal{G}) + 16\pi G\mathscr{L}_m$ [23] where $\mathcal{G} = R^2 - 4R_{\mu\nu}R^{\mu\nu} + R_{\mu\alpha\nu\beta}R^{\mu\alpha\nu\beta}$ is the Gauss-Bonnet invariant. This is in fact a subclass of the $\mathscr{L} = f(R\,, R_{\mu\nu}R^{\mu\nu}\,, R_{\mu\alpha\nu\beta}R^{\mu\alpha\nu\beta}) + 16\pi G\mathscr{L}_m$ gravity [24] with explicit dependence on R^2 and satisfying the "coherence condition" $f_{R^2} = f_{R_m^2} = -f_{R_c^2}/4$ [21] (R_m^2 and R_c^2 are the intuitive abbreviations for the Riemann tensor square $R_{\mu\alpha\nu\beta}R^{\mu\alpha\nu\beta}$ and the Ricci tensor square $R_{\mu\nu}R^{\mu\nu}$, respectively). The field equation for $f(R,\mathcal{G})$ gravity reads

$$\begin{aligned} R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} \;=\; & 8\pi\frac{G}{f_R + 2Rf_{\mathcal{G}}}T^{(m)}_{\mu\nu} + (f_R + 2Rf_{\mathcal{G}})^{-1}\bigg(\frac{1}{2}\Big(f - (f_R + 2Rf_{\mathcal{G}})\,R\Big)\,g_{\mu\nu} \\ & +(\nabla_\mu\nabla_\nu - g_{\mu\nu}\Box)\,f_R + 2R\,(\nabla_\mu\nabla_\nu - g_{\mu\nu}\Box)\,f_{\mathcal{G}} + 4R_{\mu\nu}\Box f_{\mathcal{G}} + H^{(\text{GB})}_{\mu\nu}\bigg)\,, \end{aligned} \tag{4.127}$$

where

$$\begin{aligned} H^{(\text{GB})}_{\mu\nu} \;:=\; & 4f_{\mathcal{G}}\cdot R_\mu{}^\alpha R_{\alpha\nu} + 4f_{\mathcal{G}}\cdot R_{\mu\alpha\nu\beta}R^{\alpha\beta} - 2f_{\mathcal{G}}\cdot R_{\mu\alpha\beta\gamma}R_\nu{}^{\alpha\beta\gamma} - 4R_\mu{}^\alpha\nabla_\alpha\nabla_\nu f_{\mathcal{G}} \\ & -4R_\nu{}^\alpha\nabla_\alpha\nabla_\mu f_{\mathcal{G}} + 4g_{\mu\nu}\cdot R^{\alpha\beta}\nabla_\alpha\nabla_\beta f_{\mathcal{G}} - 4\,R_{\alpha\mu\beta\nu}\nabla^\beta\nabla^\alpha f_{\mathcal{G}}\,, \end{aligned} \tag{4.128}$$

and $\{f, f_R, f_{\mathcal{G}} = \partial f/\partial\mathcal{G}\}$ are all functions of $(R,\mathcal{G})$. Note that in $H^{(\text{GB})}_{\mu\nu}$ the second-order-derivative operators $\{\Box, \nabla_\alpha\nabla_\nu, \text{etc}\}$ only act on the scalar functions $f_{\mathcal{G}}$. Hence,

$$G_{\text{eff}} \;=\; \frac{G}{f_R + 2Rf_{\mathcal{G}}} \qquad \text{and} \tag{4.129}$$

$$T^{(\text{MG})}_{\mu\nu} \;=\; \frac{1}{8\pi G}\bigg(\frac{1}{2}\Big(f - (f_R + 2Rf_{\mathcal{G}})\,R\Big)\,g_{\mu\nu} + (\nabla_\mu\nabla_\nu - g_{\mu\nu}\Box)\,f_R + 2R\,(\nabla_\mu\nabla_\nu - g_{\mu\nu}\Box)\,f_{\mathcal{G}} + 4R_{\mu\nu}\Box f_{\mathcal{G}} + H^{(\text{GB})}_{\mu\nu}\bigg)\,. \tag{4.130}$$

Substitute the FRW metric Eq.(4.1) into $T^{(\text{MG})}_{\mu\nu}$ with $T^{\mu\,(\text{MG})}_{\;\nu} = \text{diag}[-\rho_{(\text{MG})}, P_{(\text{MG})}, P_{(\text{MG})}, P_{(\text{MG})}]$, and in compact notations we obtain

$$\rho_{(\text{MG})} \;=\; \frac{1}{8\pi G}\bigg(\frac{1}{2}\,(f_R + 2Rf_{\mathcal{G}})\,R - \frac{1}{2}\,f - 3H\dot{f}_R - 6RH\dot{f}_{\mathcal{G}} + 4R_t{}^t(\ddot{f}_{\mathcal{G}} + 3H\dot{f}_{\mathcal{G}}) - H_t{}^t{}_{(\text{GB})}\bigg)\,, \tag{4.131}$$

$$P_{(\mathrm{MG})} = \frac{1}{8\pi G}\left(\frac{1}{2}f - \frac{1}{2}(f_R + 2Rf_{\mathcal{G}})R + \ddot{f}_R + 2H\dot{f}_R + 2R(\ddot{f}_{\mathcal{G}} + 2H\dot{f}_{\mathcal{G}}) - 4R_r{}^r(\ddot{f}_{\mathcal{G}} + 3H\dot{f}_{\mathcal{G}}) + H_r{}^r_{(\mathrm{GB})}\right), \tag{4.132}$$

where we have used the properties $R_t{}^t = -R_{tt}$ and $H_t{}^t_{(\mathrm{GB})} = -H_{tt}^{(\mathrm{GB})}$ in $\rho_{(\mathrm{MG})}$ under the FRW metric Eq.(4.1). Since $G_{\mathrm{eff}} = G/(f_R + 2Rf_{\mathcal{G}})$, the geometric mass within a sphere of radius Υ is

$$M = \frac{(f_R + 2Rf_{\mathcal{G}})\Upsilon^3}{2G}\left(H^2 + \frac{k}{a^2}\right) \qquad \text{with} \qquad M_{\mathrm{A}} \triangleq \frac{(f_R + 2Rf_{\mathcal{G}})\Upsilon_{\mathrm{A}}}{2G}, \tag{4.133}$$

while the nonequilibrium energy dissipation $\mathcal{E}$ associated with the evolution of G_{eff} and the Wald-Kodama entropy S of the horizon are respectively

$$\mathcal{E} = \frac{4}{3}\pi\Upsilon^3\frac{\dot{f}_R + 2\dot{R}f_{\mathcal{G}} + 2R\dot{f}_{\mathcal{G}}}{f_R + 2Rf_{\mathcal{G}}}\rho_{\mathrm{eff}}\,dt \qquad \text{and} \qquad S = \frac{A_{\mathrm{A}}(f_R + 2Rf_{\mathcal{G}})}{4G}. \tag{4.134}$$

Following the unified formulation developed in Sec. 4.3 and Sec. 4.4 to study $dM = dE = A\boldsymbol{\psi} + WdV + \mathcal{E}$ for the region $\Upsilon \leq \Upsilon_{\mathrm{A}}$ and $T(dS + d_pS) \triangleq \delta Q \triangleq -(A_{\mathrm{A}}\boldsymbol{\psi} + \mathcal{E}_{\mathrm{A}})$ for the horizon itself, we find

$$\begin{aligned} H^2 + \frac{k}{a^2} = \frac{8\pi}{3}\frac{G}{f_R + 2Rf_{\mathcal{G}}}\rho_m + \frac{1}{3(f_R + 2Rf_{\mathcal{G}})}\bigg(&\frac{1}{2}(f_R + 2Rf_{\mathcal{G}})R - \frac{1}{2}f - 3H(\dot{f}_R + 2R\dot{f}_{\mathcal{G}}) \\ &+4R_t{}^t(\ddot{f}_{\mathcal{G}} + 3H\dot{f}_{\mathcal{G}}) - H_t{}^t_{(\mathrm{GB})}\bigg), \end{aligned} \tag{4.135}$$

$$\begin{aligned} \dot{H} - \frac{k}{a^2} = -4\pi\frac{G}{f_R + 2Rf_{\mathcal{G}}}\left(\rho_m + P_m\right) - \frac{1}{2(f_R + 2Rf_{\mathcal{G}})}\bigg(&\ddot{f}_R - H\dot{f}_R + 2R\ddot{f}_{\mathcal{G}} - 2RH\dot{f}_{\mathcal{G}} \\ &+4(R_t{}^t - R_r{}^r)(\ddot{f}_{\mathcal{G}} + 3H\dot{f}_{\mathcal{G}}) - H_t{}^t_{(\mathrm{GB})} + H_r{}^r_{(\mathrm{GB})}\bigg), \end{aligned} \tag{4.136}$$

while the nonequilibrium entropy production on the horizon is

$$d_pS \triangleq -2\pi\Upsilon_{\mathrm{A}}^2\frac{\dot{f}_R + 2\dot{R}f_{\mathcal{G}} + 2R\dot{f}_{\mathcal{G}}}{G}dt. \tag{4.137}$$

We have verified that the thermodynamic relations Eqs.(4.135) and (4.136) are really the gravitational Friedmann equations by substituting the FRW metric Eq.(4.1) into the generalized Gauss-Bonnet field equations (4.127) and (4.128). Moreover, by setting $f_{\mathcal{G}} = 0$ and thus $\dot{f}_{\mathcal{G}} = \ddot{f}_{\mathcal{G}} = 0$, the situation of the $f(R,\mathcal{G})$ generalized Gauss-Bonnet gravity reduces to become the case of $f(R)$ gravity in Sec. 4.6.1.

4.6.8 Self-inconsistency of $f(R,\mathcal{G})$ gravity

The $f(R,\mathcal{G})$ example just above is based on Eqs.(4.127) and (4.128), which together with their contravariant forms constitute the standard field equations of the $f(R,\mathcal{G})$ gravity that are proposed in [23] and adopted in existing papers related to generic dependence on $\mathcal{G}$. On the other hand, recall that in *four* dimensions the

Gauss-Bonnet invariant $\mathcal{G}$ is proportional to the Euler-Poincaré topological density as

$$\mathcal{G} = \left(\frac{1}{2}\epsilon_{\alpha\beta\gamma\zeta}R^{\gamma\zeta\eta\xi}\right)\cdot\left(\frac{1}{2}\epsilon_{\eta\xi\rho\sigma}R^{\rho\sigma\alpha\beta}\right) = {}^{*}R_{\alpha\beta}{}^{\eta\xi}\,{}^{*}R_{\eta\xi}{}^{\alpha\beta}\,, \tag{4.138}$$

where $\epsilon_{\alpha\beta\gamma\zeta}$ refers to the totally antisymmetric Levi-Civita (pseudo)tensor with $\epsilon_{0123} = \sqrt{-g}$. The integral $\int dx^4\sqrt{-g}\,\mathcal{G}$ is equal to the Euler characteristic number χ (just a constant) of the spacetime, and thus

$$\frac{\delta}{\delta g^{\mu\nu}}\int dx^4\sqrt{-g}\,\mathcal{G} \equiv 0\,. \tag{4.139}$$

By explicitly carrying out this variational derivative, one could find the following Bach-Lanczos identity [49]:

$$2RR_{\mu\nu} - 4R_{\mu}{}^{\alpha}R_{\alpha\nu} - 4R_{\alpha\mu\beta\nu}R^{\alpha\beta} + 2R_{\mu\alpha\beta\gamma}R_{\nu}{}^{\alpha\beta\gamma} \equiv \frac{1}{2}\mathcal{G}\,g_{\mu\nu}, \tag{4.140}$$

with which the standard field equations (4.127) and (4.128) of the $f(R,\mathcal{G})$ gravity can be simplified into

$$\begin{aligned} R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} \;&= 8\pi\frac{G}{f_R}\,T^{(m)}_{\mu\nu} + \frac{1}{f_R}\bigg(\frac{1}{2}(f - f_{\mathcal{G}}\mathcal{G} - f_R R)g_{\mu\nu} + (\nabla_\mu\nabla_\nu - g_{\mu\nu}\Box)f_R \\ &\quad + 2R\,(\nabla_\mu\nabla_\nu - g_{\mu\nu}\Box)f_{\mathcal{G}} + 4R_{\mu\nu}\Box f_{\mathcal{G}} + \mathcal{H}^{(\mathrm{GB})}_{\mu\nu}\bigg), \end{aligned} \tag{4.141}$$

where

$$\mathcal{H}^{(\mathrm{GB})}_{\mu\nu} \;\coloneqq\; -4R_{\mu}{}^{\alpha}\nabla_\alpha\nabla_\nu f_{\mathcal{G}} - 4R_{\nu}{}^{\alpha}\nabla_\alpha\nabla_\mu f_{\mathcal{G}} + 4g_{\mu\nu}\cdot R^{\alpha\beta}\nabla_\alpha\nabla_\beta f_{\mathcal{G}} - 4\,R_{\alpha\mu\beta\nu}\nabla^\beta\nabla^\alpha f_{\mathcal{G}}\,. \tag{4.142}$$

This way, the effective gravitational coupling strength is recognized to be

$$G_{\mathrm{eff}} \;=\; \frac{G}{f_R}\,, \tag{4.143}$$

as opposed to the $G_{\mathrm{eff}} = G/(f_R + 2Rf_{\mathcal{G}})$ in Eq.(4.129); this is because the $2f_{\mathcal{G}}RR_{\mu\nu}$ term directly joining Eq.(4.127) is now absorbed by the $\frac{1}{2}f_{\mathcal{G}}\mathcal{G}\,g_{\mu\nu}$ term in Eq.(4.141) due to the Bach-Lanczos identity and thus no longer shows up in Eq.(4.141). The SEM tensor from modified-gravity effects becomes

$$T^{(\mathrm{MG})}_{\mu\nu} = \frac{1}{8\pi G}\left(\frac{1}{2}(f - f_{\mathcal{G}}\mathcal{G} - f_R R)g_{\mu\nu} + (\nabla_\mu\nabla_\nu - g_{\mu\nu}\Box)f_R + 2R\,(\nabla_\mu\nabla_\nu - g_{\mu\nu}\Box)f_{\mathcal{G}} + 4R_{\mu\nu}\Box f_{\mathcal{G}} + \mathcal{H}^{(\mathrm{GB})}_{\mu\nu}\right), \tag{4.144}$$

which with the FRW metric Eq.(4.1) gives rise to

$$\rho_{(\mathrm{MG})} \;=\; \frac{1}{8\pi G}\left(\frac{1}{2}\,(f_R R + f_{\mathcal{G}}\mathcal{G}) - \frac{1}{2}\,f - 3H\dot{f}_R - 6RH\dot{f}_{\mathcal{G}} + 4R_t{}^t(\ddot{f}_{\mathcal{G}} + 3H\dot{f}_{\mathcal{G}}) - \mathcal{H}_t{}^t{}_{(\mathrm{GB})}\right) \tag{4.145}$$

and

$$P_{(\mathrm{MG})} \;=\; \frac{1}{8\pi G}\left(\frac{1}{2}\,f - \frac{1}{2}\,(f_R R + f_{\mathcal{G}}\mathcal{G}) + \ddot{f}_R + 2H\dot{f}_R + 2R(\ddot{f}_{\mathcal{G}} + 2H\dot{f}_{\mathcal{G}}) - 4R_r{}^r(\ddot{f}_{\mathcal{G}} + 3H\dot{f}_{\mathcal{G}}) + \mathcal{H}_r{}^r{}_{(\mathrm{GB})}\right). \tag{4.146}$$

Since the $G_{\mathrm{eff}} = G/f_R$ coincides with that of $f(R)$ gravity, the Hawking or Misner-Sharp geometric mass M, the nonequilibrium energy dissipation $\mathcal{E}$, the horizon entropy S and the entropy production element d_pS

are all the same with those of $f(R)$ gravity, as derived before in Eqs.(4.68), (4.69) and (4.72) in Sec. 4.6.1, respectively. Then the thermodynamical approach of Sec. 4.3 and Sec. 4.4 yields

$$H^2+\frac{k}{a^2}=\frac{8\pi}{3}\frac{G}{f_R}\rho_m+\frac{1}{3f_R}\Big(\frac{1}{2}(f_R R+f_{\mathcal{G}}\mathcal{G})-\frac{1}{2}f-3H\,(\dot{f}_R+2R\dot{f}_{\mathcal{G}})+4R_t^{\ t}\,(\ddot{f}_{\mathcal{G}}+3H\dot{f}_{\mathcal{G}})-\mathcal{H}_{t\,(\text{GB})}^{\ t}\Big) \quad (4.147)$$

and

$$\dot{H}-\frac{k}{a^2}=-4\pi\frac{G}{f_R}(\rho_m+P_m)-\frac{1}{2f_R}\Big(\ddot{f}_R-H\dot{f}_R+2R\ddot{f}_{\mathcal{G}}-2RH\dot{f}_{\mathcal{G}}+4(R_t^{\ t}-R_r^{\ r})(\ddot{f}_{\mathcal{G}}+3\mathcal{H}\dot{f}_{\mathcal{G}})-\mathcal{H}_{t\,(\text{GB})}^{\ t}+\mathcal{H}_{r\,(\text{GB})}^{\ r}\Big), \quad (4.148)$$

which match the Friedmann equations obtained from substituting the FRW metric Eq.(4.1) into the simplified $f(R,\mathcal{G})$ field equation (4.141).

However, these thermodynamical quantities and relations of $f(R,\mathcal{G})$ gravity differ dramatically with those in the previous Sec. 4.6.7. The contrast may be seen even more evidently in the $\mathscr{L}=R+f(\mathcal{G})+16\pi G\mathscr{L}_m$ modified Gauss-Bonnet gravity [50] which is a special subclass of the $f(R,\mathcal{G})$ theory. It follows from Sec. 4.6.7 that $G_{\text{eff}}=G/(1+2Rf_{\mathcal{G}})$ for $f(R,\mathcal{G})=R+f(\mathcal{G})$, and it is a nonequilibrium scenario with nonvanishing energy dissipation $\mathcal{E}$ and entropy production d_pS on the apparent horizon. On the contrary, we have $G_{\text{eff}}=G$ in accordance with Eq.(4.141) as $f_R=1$, which corresponds to an equilibrium gravitational thermodynamics with $\mathcal{E}=0=d_pS$.

Note that the existence of the two distinct formulations for the thermodynamics of $f(R,\mathcal{G})$ gravity does not indicate a failure of our unified formulation. Instead, it reveals a *self-inconsistency* feature of the $f(R,\mathcal{G})$ theory itself. Although the simplified field equations (4.141) and (4.142) are equivalent to Eqs.(4.127) and (4.128) in Sec. 4.6.7 via the identity Eq.(4.140), practically they will behave differently with each other in any problems relying on the input of the effective coupling strength G_{eff}. Moreover, we also expect this self-inconsistency of $f(R,\mathcal{G})$ gravity to arise in other problems such as the black-hole thermodynamics.

4.6.9 Dynamical Chern-Simons gravity

So far we have applied our unified formulation to the $f(R)$, generalized Brans-Dicke, scalar-tensor-chameleon, quadratic and $f(R,\mathcal{G})$ gravity; they are all nonequilibrium theories with nontrivial G_{eff} in the coefficient of $T_{\mu\nu}^{(\text{m})}$. As a final example we will continue to consider the (dynamical) Chern-Simons modification of GR [51], which is a thermodynamically equilibrium theory with $G_{\text{eff}}=G$. Its Lagrangian density reads

$$\mathscr{L}_{\text{CS}}=R+\frac{a\,\vartheta}{2\sqrt{-g}}{}^*\widehat{RR}-b\,\nabla_\mu\vartheta\nabla^\mu\vartheta-V(\vartheta)+16\pi G\mathscr{L}_m, \quad (4.149)$$

where $\vartheta=\vartheta(x^\mu)$ is a scalar field, $\{a,b\}$ are constants, and ${}^*\widehat{RR}$ denotes the parity-violating Pontryagin invariant

$${}^*\widehat{RR}={}^*R_{\alpha\beta\gamma\delta}\,R^{\alpha\beta\gamma\delta}=\Big(\frac{1}{2}\epsilon_{\alpha\beta\mu\nu}R^{\mu\nu}{}_{\gamma\delta}\Big)R^{\alpha\beta\gamma\delta}\,. \quad (4.150)$$

${}^*\widehat{RR}$ is proportional to the divergence of the Chern-Simons topological current K^μ [51]:

$${}^*\widehat{RR}=-2\,\partial_\mu K^\mu \qquad \text{and} \qquad K^\mu=2\epsilon^{\mu\alpha\beta\gamma}\Big(\frac{1}{2}\Gamma^\xi_{\alpha\tau}\partial_\beta\Gamma^\tau_{\gamma\xi}+\frac{1}{3}\Gamma^\xi_{\alpha\tau}\Gamma^\tau_{\beta\eta}\Gamma^\eta_{\gamma\xi}\Big), \quad (4.151)$$

with $\epsilon^{0123} = 1/\sqrt{-g}$, hence the name Chern-Simons gravity. Variational derivative of $\sqrt{-g}\mathscr{L}_{\text{CS}}$ with respect to the inverse metric $g^{\mu\nu}$ yields the field equation

$$R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} = 8\pi G T^{(m)}_{\mu\nu} - \frac{a}{\sqrt{-g}}\,C_{\mu\nu} + b\left(\nabla_\mu\vartheta\nabla_\nu\vartheta - \frac{1}{2}g_{\mu\nu}\nabla_\alpha\vartheta\nabla^\alpha\vartheta\right) - \frac{1}{2}V(\vartheta)g_{\mu\nu}\,, \tag{4.152}$$

where

$$C_{\mu\nu} \;=\; \nabla^\alpha\vartheta\cdot\left(\epsilon_{\alpha\beta\gamma\mu}\nabla^\gamma R_\nu{}^\beta + \epsilon_{\alpha\beta\gamma\nu}\nabla^\gamma R_\mu{}^\beta\right) + \nabla^\alpha\nabla^\beta\vartheta\cdot\left({}^*R_{\beta\mu\nu\alpha} + {}^*R_{\beta\nu\mu\alpha}\right). \tag{4.153}$$

Eq.(4.152) directly shows that the Chern-Simons gravitational coupling strength is just Newton's constant, $G_{\text{eff}} = G$, and

$$T^{(\text{MG})}_{\mu\nu} = -a\,C_{\mu\nu} + b\left(\nabla_\mu\vartheta\nabla_\nu\vartheta - \frac{1}{2}g_{\mu\nu}\nabla_\alpha\vartheta\nabla^\alpha\vartheta\right) - \frac{1}{2}V(\vartheta)g_{\mu\nu}. \tag{4.154}$$

With the FRW metric Eq.(4.26), this $T^{(\text{MG})}_{\mu\nu}$ leads to

$$\rho_{(\text{MG})} \;=\; \frac{1}{16\pi G}\left(b\,\dot\vartheta^2 + V(\vartheta)\right) \quad\text{and}\quad P_{(\text{MG})} \;=\; \frac{1}{16\pi G}\left(b\,\dot\vartheta^2 - V(\vartheta)\right). \tag{4.155}$$

Since $G_{\text{eff}} = G = $ constant, we can make use of the reduced formulation in Sec.4.5.4 for equilibrium situations. The geometric mass and the horizon entropy are respectively

$$M \;=\; \frac{\Upsilon^3}{2G}\left(H^2 + \frac{k}{a^2}\right) \quad\text{with}\quad M_{\text{A}} \;\hat{=}\; \frac{\Upsilon_{\text{A}}}{2G} \tag{4.156}$$

and

$$S \;=\; \frac{A_{\text{A}}}{4G} \;=\; \frac{\pi\Upsilon_{\text{A}}^2}{G}\,, \tag{4.157}$$

which are the same with those of GR [8]. Also, there are no energy dissipation $\mathcal{E}$ and the on-horizon entropy production d_pS,

$$\mathcal{E} = 0 \quad\text{and}\quad d_pS = 0\,. \tag{4.158}$$

Following the procedures in Sec.4.5.4, for the interior and the horizon we obtain from the thermodynamical approach that

$$H^2 + \frac{k}{a^2} \;=\; \frac{8\pi G}{3}\rho_m + \frac{1}{6}\left(b\,\dot\vartheta^2 + V(\vartheta)\right) \tag{4.159}$$

and

$$\dot H - \frac{k}{a^2} \;=\; -4\pi G\left(\rho_m + P_m\right) - \frac{b}{2}\,\dot\vartheta^2\,. \tag{4.160}$$

By substituting the FRW metric Eq.(4.1) into the field equation (4.152), we have confirmed that Eqs.(4.159) and (4.160) are really the Friedmann equations of the FRW universe governed by the Chern-Simons gravity.

4.7 Conclusions

In this paper, we have developed a unified formulation to derive the Friedmann equations from (non)equilibrium thermodynamics within modified gravity with field equations of the form $R_{\mu\nu} - Rg_{\mu\nu}/2 = 8\pi G_{\text{eff}}T^{(\text{eff})}_{\mu\nu}$. We firstly made the necessary preparations by locating the marginally inner trapped horizon Υ_{A} of the expanding FRW universe as the apparent horizon of relative causality, and then rewrote the continuity equation from

$\nabla^{\mu}(G_{\text{eff}}T^{(\text{eff})}_{\mu\nu}) = 0$ to introduce the energy dissipation element $\mathcal{E}$ which is related with the evolution of G_{eff}.

With these preparations, we began to study the thermodynamics of the FRW universe. We have generalized the Hawking and Misner-Sharp geometric definitions of mass by replacing Newton's constant G with G_{eff}, and calculated the total derivative of M in the comoving (t, r) and the areal (t, Υ) transverse coordinates. Also, we have supplemented Hayward's unified first law of thermodynamics into $dE = A\boldsymbol{\psi} + WdV + \mathcal{E}$ with the dissipation term $\mathcal{E}$, where the work density W and the heat flux covector $\boldsymbol{\psi}$ are computed using the effective matter content $T^{(\text{eff})}_{\mu\nu}$. By identifying the geometric mass M enveloped by a sphere of radius $\Upsilon < \Upsilon_{\text{A}}$ as the total internal energy E, the Friedmann equations have been derived from the thermodynamic equality $dM = dE$.

On the horizon $\Upsilon = \Upsilon_{\text{A}}$, besides the smooth limit $\Upsilon \to \Upsilon_{\text{A}}$ of $dM = dE$ from the untrapped interior $\Upsilon < \Upsilon_{\text{A}}$ to the horizon, we have employed an alternative Clausius method. By considering the heat flow during the infinitesimal time interval dt for an isochoric process using the unified first law $dE \,\hat{=}\, A_{\text{A}}\boldsymbol{\psi}_t + \mathcal{E}_{\text{A}}$ and the generic nonequilibrium Clausius relation $T(dS + d_pS) \,\hat{=}\, \delta Q$ respectively, we have obtained the second Friedmann equation $\dot{H} - k/a^2 \,\hat{=}\, -4\pi G_{\text{eff}}(\rho_{\text{eff}} + P_{\text{eff}})$ from the thermodynamics equality $T(dS + d_pS) \,\hat{=}\, \delta Q \,\hat{=}\, -dE \,\hat{=}\, -(A_{\text{A}}\boldsymbol{\psi}_t + \mathcal{E}_{\text{A}})$, while the first Friedmann equation $H^2 + k/a^2 \,\hat{=}\, 8\pi G_{\text{eff}}\rho_{\text{eff}}/3$ can be recovered using the generalized continuity equation $\dot{G}_{\text{eff}}\rho_{\text{eff}} + G_{\text{eff}}\dot{\rho}_{\text{eff}} + 3G_{\text{eff}}H(\rho_{\text{eff}} + P_{\text{eff}}) = 0$. Here we have taken the temperature ansatz $T = 1/(2\pi\Upsilon_{\text{A}})$ in [8] and the Wald-Kodama dynamical entropy $S \,\hat{=}\, A_{\text{A}}/(4G_{\text{eff}})$ for the horizon, and the equality $T(dS + d_pS) \,\hat{=}\, -(A_{\text{A}}\boldsymbol{\psi}_t + \mathcal{E}_{\text{A}})$ has also determined the entropy production d_pS which is generally nonzero unless $G_{\text{eff}} = \text{constant}$. In the meantime, we have adjusted the thermodynamic sign convention by the consistency between the thermodynamics of the horizon and the interior.

After developing the unified formulation for generic relativistic gravity, we have extensively discussed some important problems related to the formulation. A viability test of the generalized effective mass has been proposed, which shows that the equality between the physically defined effective mass $\mathcal{M} = \rho_{\text{eff}}V = (\rho_m + \rho_{(\text{MG})})V$ and the geometric effective mass automatically yields the Friedmann equations. Also, we have argued that for the modified-gravity theories under discussion with minimal geometry-matter coupling, the continuity equation can be further simplified due to the Noether-compatible definition of $T^{(m)}_{\mu\nu}$. Furthermore, we have discussed the reduced situation of the unified formulation for $G_{\text{eff}} = G = \text{constant}$ with vanishing dissipation $\mathcal{E} = 0$ and entropy production $d_pS = 0$, which is of particular importance for typical scalarial dark-energy models and some fourth-order gravity.

Finally, we have applied our unified formulation to the $f(R)$, generalized Brans-Dicke, scalar-tensor-chameleon, quadratic, $f(R, \mathcal{G})$ generalized Gauss-Bonnet and dynamical Chern-Simons gravity, to derive the Friedmann equations from thermodynamics-gravity correspondence, where compact notations have been employed to simplify the thermodynamic quantities $\{\rho_{(\text{MG})}, P_{(\text{MG})}\}$. In addition, we have verified that, the "generalized Misner-Sharp energy" for $f(R)$ and scalar-tensor gravity FRW cosmology in [13] matches the pure mass ρ_mV of the physical matter content in our formulation, and then continued to reconstruct the physical mass ρ_mV from the spacetime geometry for generic modified gravity. We also found the self-inconsistency of $f(R, \mathcal{G})$ gravity in such problems which require to specify the G_{eff}.

In our prospective studies, we will apply the unified formulation developed in this paper to the generalized second law of thermodynamics for the FRW universe, and extend our formulation to more generic theories of modified gravity which allow for nonminimal curvature-matter couplings. Moreover, we will try to loosen the restriction of spherical symmetry and look into the problem of thermodynamics-gravity correspondence in the Bianchi classes of cosmological solutions.

Acknowledgement

The authors are grateful to Prof. Rong-Gen Cai (Beijing) for helpful discussion. This work was financially supported by the Natural Sciences and Engineering Research Council of Canada.

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Chapter 5. Apparent horizon and gravitational thermodynamics of the Universe: Solutions to the temperature and entropy confusions, and extensions to modified gravity [*Phys. Rev. D* **92** (2015), 024001]

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Abstract

The thermodynamics of the Universe is restudied by requiring its compatibility with the holographic-style gravitational equations which govern the dynamics of both the cosmological apparent horizon and the entire Universe, and possible solutions are proposed to the existent confusions regarding the apparent-horizon temperature and the cosmic entropy evolution. We start from the generic Lambda Cold Dark Matter (ΛCDM) cosmology of general relativity (GR) to establish a framework for the gravitational thermodynamics. The Cai–Kim Clausius equation $\delta Q = T_{\text{A}} dS_{\text{A}} = -dE_{\text{A}} = -A_{\text{A}}\psi_t$ for the isochoric process of an instantaneous apparent horizon indicates that, the Universe and its horizon entropies encode the *positive heat out* thermodynamic sign convention, which encourages us to adjust the traditional positive-heat-in Gibbs equation into the positive-heat-out version $dE_m = -T_m dS_m - P_m dV$. It turns out that the standard and the generalized second laws (GSLs) of nondecreasing entropies are always respected by the event-horizon system as long as the expanding Universe is dominated by nonexotic matter $-1 \leq w_m \leq 1$, while for the apparent-horizon simple open system the two second laws hold if $-1 \leq w_m < -1/3$; also, the artificial local equilibrium assumption is abandoned in the GSL. All constraints regarding entropy evolution are expressed by the equation of state parameter, which show that from a thermodynamic perspective the phantom dark energy is less favored than the cosmological constant and the quintessence. Finally, the whole framework is extended from GR and ΛCDM to modified gravities with field equations $R_{\mu\nu} - Rg_{\mu\nu}/2 = 8\pi G_{\text{eff}} T^{(\text{eff})}_{\mu\nu}$. Furthermore, this paper argues that the Cai–Kim temperature is more suitable than Hayward, both temperatures are independent of the inner or outer trappedness of the apparent horizon, and the Bekenstein–Hawking and Wald entropies cannot unconditionally apply to the event and particle horizons.

PACS numbers: 04.20.Cv , 04.50.Kd , 98.80.Jk

5.1 Introduction

The thermodynamics of the Universe is quite an interesting problem and has attracted a lot of discussion. Pioneering work dates back to the investigations of cosmic entropy evolutions for the spatially flat de Sitter Universe [1] dominated by a positive cosmological constant, while recent studies have covered both the first

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and second laws of thermodynamics for the Friedmann-Robertson-Walker (FRW) Universe with a generic spatial curvature.

Recent interest on the first law of thermodynamics for the Universe was initiated by Cai and Kim's derivation of the Friedmann equations from a thermodynamic approach [2]: this is actually a continuation of Jacobson's work to recover Einstein's equation from the equilibrium Clausius relation on local Rindler horizons [3], and also a part of the effort to seek the connections between thermodynamics and gravity [4] following the discovery of black hole thermodynamics [5]. For general relativity (GR), Gauss-Bonnet and Lovelock gravities, Akbar and Cai reversed the formulation in [2] by rewriting the Friedmann equations into the heat balance equation and the unified first law of thermodynamics at the cosmological apparent horizon [6]. The method of [6] was soon generalized to other theories of gravity to construct the effective total energy differentials by the corresponding modified Friedmann equations, such as the scalar-tensor gravity in [7], $f(R)$ gravity in [8], braneworld scenarios in [9, 10], generic $f(R, \phi, \nabla_\alpha\phi\nabla^\alpha\phi)$ gravity in [11], and Horava-Lifshitz gravity in [12]. Also, at a more fundamental level, the generic field equations of $F(R, \phi, -\frac{1}{2}\nabla_\alpha\phi\nabla^\alpha\phi, \mathcal{G})$ gravity are recast into the form of Clausius relation in [13].

Besides the first laws on the construction of various energy-conservation and heat-transfer equations, the entropy evolution of the Universe has also drawn plenty of attention. However, the cosmic entropies are almost exclusively studied in the generalized rather than the standard second laws [14–25]. In fact, investigations via the traditional Gibbs equation $dE_m = T_m d\tilde{S}_m - P_m dV$ show that in GR and modified gravities, the evolution of the physical entropy $\tilde{S}_m$ for the matter inside the apparent and the event horizons departs dramatically from the desired nondecreasing behaviors; especially that $\tilde{S}_m$ inside the future-pointed event horizon always decreases under the dominance of nonexotic matter above the phantom divide. Thus the generalized second law (GSL) has been employed, which adds up $\tilde{S}_m$ with the geometrically defined entropy of the cosmological causal boundaries and anticipates the total entropy to be nondecreasing so that the standard second law could be rescued. For example, GSL has been studied in [14] for a flat Universe with multiple entropy sources (thermal, geometric, quantum etc.) by the entropy ansatz $S = |H|^\alpha$ $(\alpha > -3)$, in [15] for the event-horizon system of a quintom-dominated flat Universe, and [16] for various interacting dark energy models.

Moreover, the GSL has also been used as a validity constraint on modified and alternative theories of gravity. For instance, the GSL has been imposed on the event-horizon system of the flat Universe of $f(R)$ gravity in [17], tentatively to the flat apparent-horizon system of generic modified gravities in [18], to the higher-dimensional Gauss-Bonnet and Lovelock gravities in [19], to the Gauss-Bonnet, Randall-Sundrum and Dvali-Gabadadze-Porrati braneworlds in [20], the Horava-Lifshitz gravity in [21], $F(R, \mathcal{G})$ generalized Gauss-Bonnet gravity in [22], $f(T)$ generalized teleparallel gravity in [23], scalar-tensor-chameleon gravity in [24], and the self-interacting $f(R)$ gravity in [25]. Note that in the studies of GSLs, the debatable "local equilibrium assumption" has been widely adopted which supposes that the matter content and the causal boundary in use (mainly the apparent or the event horizon) would have the same temperature [16, 19–22, 24, 25].

Unlike *laboratory* thermodynamics which is a well-developed self-consistent framework, the thermodynamics of the Universe is practically a mixture of ordinary thermodynamics with analogous gravitational quantities, for which the consistency between the first and second laws and among the setups of thermodynamic functions are not yet verified. For example, the Hayward temperature $\kappa/2\pi$ [7, 9] or $|\kappa|/2\pi$ [8, 10] which formally resembles the Hawking temperature of (quasi)stationary black holes [5] has been adopted in the first laws, while in GSLs both $|\kappa|/2\pi$ [18–20, 24, 25] and the Cai–Kim temperature [16, 21, 22] are used. Moreover, in existent literature we have noticed six questions regarding the gravitational thermodynamics of the Universe:

(1) For the Cai–Kim and the Hayward temperatures, which one is more appropriate for the cosmological boundaries? By solving this *temperature confusion*, the equations of total energy differential at the horizons could also be determined;

(2) For the Bekenstein–Hawking entropy in GR and the Wald entropy in modified gravities, are they unconditionally applicable to both the cosmological apparent and the event horizons?

(3) Is the standard second law for the physical matter really ill-behaved and thus needs to be saved by the GSL? This constitutes the cosmological *entropy confusion*;

(4) Is the artificial local equilibrium assumption really necessary for the GSL?

(5) The region enveloped by the apparent horizon is actually a thermodynamically open system with the absolute cosmic Hubble flow crossing the horizon; how will this fact influence the entropy evolution?

(6) Are the thermodynamic quantities fully consistent with each other when the cosmic gravitational thermodynamics is systemized?

In this paper, we will try to answer these questions.

This paper is organized as follows. Starting with GR and the ΛCDM Universe (where Λ denotes generic dark energy), in Sec. 5.2 we derive the holographic-style dynamical equations governing the apparent-horizon dynamics and the cosmic spatial expansion, which yield the constraints from the EoS parameter w_m on the evolution and metric signature of the apparent horizon. Section 5.3 demonstrates how these holographic-style gravitational equations imply the unified first law of thermodynamics and the Clausius equation, and shows the latter encodes the positive-heat-out sign convention for the horizon entropy. In Sec. 5.4 the Cai–Kim temperature is extensively compared with Hayward, with the former chosen for further usage in Sec. 5.5, where we adjust the traditional Gibbs equation into the Positive Out convention to investigate the entropy evolution for the simple open systems enveloped by the apparent and event horizons. Finally the whole framework of gravitational thermodynamics is extended from ΛCDM model and GR to generic modified gravity in Sec. 5.6. Throughout this paper, we adopt the sign convention $\Gamma^{\alpha}_{\beta\gamma} = \Gamma^{\alpha}{}_{\beta\gamma}$, $R^{\alpha}{}_{\beta\gamma\delta} = \partial_\gamma \Gamma^{\alpha}_{\delta\beta} - \partial_\delta \Gamma^{\alpha}_{\gamma\beta} \cdots$ and $R_{\mu\nu} = R^{\alpha}{}_{\mu\alpha\nu}$ with the metric signature $(-, +++)$.

5.2 Dynamics of the cosmological apparent horizon

5.2.1 Apparent horizon and observable Universe

The FRW metric provides the most general description for the spatially homogeneous and isotropic Universe. In the (t, r, θ, φ) coordinates for an observer comoving with the cosmic Hubble flow, it has the line element (e.g. [2, 26])

$$\begin{aligned} ds^2 &= -dt^2 + \frac{a(t)^2}{1-kr^2}dr^2 + a(t)^2 r^2 (d\theta^2 + \sin^2\theta d\varphi^2) \\ &= h_{\alpha\beta} dx^\alpha dx^\beta + \Upsilon^2 (d\theta^2 + \sin^2\theta d\varphi^2), \end{aligned} \tag{5.1}$$

where $a(t)$ refers to the scale factor to be specified by the gravitational field equations, and the index k denotes the normalized spatial curvature, with $k = \{+1\,,0\,,-1\}$ corresponding to closed, flat and open Universes, respectively. $h_{\alpha\beta} := \mathrm{diag}[-1\,, \frac{a(t)^2}{1-kr^2}]$ represents the transverse two-metric spanned by $x^\alpha = (t, r)$, and $\Upsilon := a(t)\, r$ stands for the astronomical circumference/areal radius. Based on Eq.(5.1), one can establish the following null tetrad adapted to the spherical symmetry and the null radial flow,

$$\ell^\mu = \left(1\,, \frac{\sqrt{1-kr^2}}{a}\,, 0\,, 0\right), \quad n^\mu = \frac{1}{2}\left(-1\,, \frac{\sqrt{1-kr^2}}{a}\,, 0\,, 0\right), \quad m^\mu = \frac{1}{\sqrt{2}\,\Upsilon}\left(0, 0, 1, \frac{i}{\sin\theta}\right), \tag{5.2}$$

which has been adjusted to be compatible with the metric signature $(-, +++)$ (e.g. Appendix B in [27]). By calculating the Newman-Penrose spin coefficients $\rho_{\rm NP} := -m^\mu \bar{m}^\nu \nabla_\nu \ell_\mu$ and $\mu_{\rm NP} := \bar{m}^\mu m^\nu \nabla_\nu n_\mu$, the outward expansion rate $\theta_{(\ell)} = -(\rho_{\rm NP} + \bar{\rho}_{\rm NP})$ and the inward expansion $\theta_{(n)} = \mu_{\rm NP} + \bar{\mu}_{\rm NP}$ are respectively found to be

$$\theta_{(\ell)} = 2H + 2\Upsilon^{-1}\sqrt{1-\frac{k\Upsilon^2}{a^2}}\,, \quad \theta_{(n)} = -H + \Upsilon^{-1}\sqrt{1-\frac{k\Upsilon^2}{a^2}}\,, \tag{5.3}$$

where H refers to the time-dependent Hubble parameter of cosmic spatial expansion, and $H := \dfrac{\dot{a}}{a}$ with the overdot denoting the derivative with respect to the comoving time t. For the expanding $(H > 0)$ Universe, $\theta_{(\ell)}$ and $\theta_{(n)}$ locate the apparent horizon $\Upsilon = \Upsilon_{\rm A}$ by the unique marginally inner trapped horizon [28] at

$$\Upsilon_{\rm A} = \frac{1}{\sqrt{H^2 + \dfrac{k}{a^2}}}\,, \tag{5.4}$$

with $\theta_{(\ell)} = 4H > 0$, $\theta_{(n)} = 0$, and also $\partial_\mu \Upsilon$ becomes a null vector with $g^{\mu\nu}\partial_\mu \Upsilon \partial_\nu \Upsilon = 0$ at $\Upsilon_{\rm A}$. Immediately the temporal derivative of Eq.(5.4) yields the kinematic equation

$$\dot{\Upsilon}_{\rm A} = -H\Upsilon_{\rm A}^3 \left(\dot{H} - \frac{k}{a^2}\right). \tag{5.5}$$

Just like $\Upsilon_{\rm A}$ and $\dot{\Upsilon}_{\rm A}$, hereafter quantities evaluated on or related to the apparent horizon will be highlighted by the subscript A.

$\{\ell^\mu, n^\mu\}$ in Eq.(5.2) coincide with the outgoing and ingoing tangent vector fields of the null radial congruence that is sent towards infinity by the comoving observer at $r = 0$, and ingoing signals from the antitrapped region $\Upsilon > \Upsilon_{\rm A}$ (where $\theta_{(\ell)} > 0$, $\theta_{(n)} > 0$) can no longer cross the marginally inner trapped $\Upsilon_{\rm A}$ and return to the observer. However, the region $\Upsilon \leq \Upsilon_{\rm A}$ is not necessarily the standard *observable Universe* in astronomy where ultrahigh redshift and visually superluminal recession can be detected [29, 30]: $\Upsilon_{\rm A}$ is a future-pointed horizon determined in active measurement by the observer, while the observable Universe is the past-pointed region measured by passive reception of distant signals and thus more related to the past particle horizon.

Note that we are working with the generic FRW metric Eq.(5.1) which allows for a nontrivial spatial curvature. This is not just for theoretical generality: in fact, astronomical observations indicate that the Universe may not be perfectly flat. For example, in the $o\Lambda$CDM sub-model with a strict vacuum-energy condition $w_\Lambda = -1$, the nine-years data from the Wilkinson Microwave Anisotropy Probe (WMAP) and other sources like the Baryon Acoustic Oscillations (BAO) yield the fractional energy density $\Omega_k = -0.0027^{+0.0039}_{-0.0038}$ [31] for the spatial curvature, independently the time-delay measurements of two strong gravitational lensing systems along with the seven-years WMAP data find $\Omega_k = 0.003^{+0.005}_{-0.006}$ [32], while most recently analyses based on BAO data give $\Omega_k = -0.003 \pm 0.003$ [33].

5.2.2 Holographic-style dynamical equations

The matter content of the Universe is usually portrayed by a perfect-fluid type stress-energy-momentum tensor, and in the metric-independent form it reads

$$T^{\mu\,(m)}_{\ \nu} = \text{diag}[\,-\rho_m, P_m, P_m, P_m] \quad \text{with} \quad P_m/\rho_m =: w_m\,, \tag{5.6}$$

where w_m refers to the equation of state (EoS) parameter. Substituting this $T^{(m)}_{\mu\nu}$ and the metric Eq.(5.1) into Einstein's equation $R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} = 8\pi G T^{(m)}_{\mu\nu}$, one obtains the first and the second Friedmann equations

$$\begin{aligned} H^2 + \frac{k}{a^2} &= \frac{8\pi G}{3}\rho_m \quad \text{and} \\ \dot{H} - \frac{k}{a^2} &= -4\pi G\,(1+w_m)\,\rho_m = -4\pi G h_m \\ \text{or} \quad 2\dot{H} + 3H^2 + \frac{k}{a^2} &= -8\pi G P_m\,, \end{aligned} \tag{5.7}$$

where $h_m = \rho_m + P_m = (1+w_m)\rho_m$ refers to the enthalpy density.

Primarily, the first and second Friedmann equations are respectively the first and second order differential equations of the scale factor $a(t)$, which is the only unspecified function in the metric Eq.(5.1). On the other hand, recall the location and the time-derivative of the cosmological apparent horizon in Eqs. (5.4) and (5.5), and thus Eq.(5.7) can be rewritten into

$$\Upsilon_\text{A}^{-2} \;=\; \frac{8\pi G}{3}\,\rho_m\,, \tag{5.8}$$

$$\dot{\Upsilon}_\text{A} \;=\; 4\pi G H \Upsilon_\text{A}^3 (1+w_m)\,\rho_m \;=\; 4\pi G H \Upsilon_\text{A}^3 h_m\,, \tag{5.9}$$

which manifest themselves as the dynamical equations of the apparent horizon. However, they also describe the dynamics of spatial expansion for the entire Universe, so for this usage we will dub Eqs.(5.8) and (5.9) the "holographic-style" dynamical equations since they reflect the spirit of holography [we are using the word "holographic" in a generic sense as opposed to the standard terminology *holographic principle* in quantum gravity and string theory [34] or the holographic gravity method [35]].

Eq.(5.8) immediately implies that, for the late-time Universe dominated by dark energy $\rho_m = \rho_\Lambda$, the apparent horizon serves as the natural infrared cutoff for the holographic dark energy model [36], in which the dark-energy density $\rho_\Lambda^{(\text{HG})}$ relies on the scale of the infrared cutoff Υ_IR by $\rho_\Lambda^{(\text{HG})} = 3\Upsilon_\text{IR}^{-2}/(8\pi G)$.

Moreover, with the apparent-horizon area $A_\text{A} = 4\pi\Upsilon_\text{A}^2$, it follows from Eq.(5.8) that

$$\rho_m A_\text{A} \;=\; \frac{3}{2G}\,, \tag{5.10}$$

so Eq.(5.9) can be further simplified into

$$\dot{\Upsilon}_\text{A} \;=\; \frac{3}{2} H \Upsilon_\text{A}\,(1+w_m)\,. \tag{5.11}$$

With the help of Eqs.(5.8) and (5.11), for completeness the third member (the P_m one) in Eq.(5.7) can be directly translated into

$$\Upsilon_{\rm A}^{-3}\left(\dot{\Upsilon}_{\rm A}-\frac{3}{2}H\Upsilon_{\rm A}\right) = 4\pi GHP_m\,, \tag{5.12}$$

and we keep it in this form without further manipulations for later use in Sec. 5.3.1.

From a mathematical point of view, it might seem trivial to rewrite the Friedmann equations (5.7) into the holographic-style gravitational equations (5.8)-(5.12). However, considering that existent studies on the gravitational thermodynamics of the cosmological apparent horizon always start from the relevant Friedmann equations [6–12, 14–25], we wish that the manipulations of Eq.(7) into Eqs.(8)-(12) could make the formulations physically more meaningful and more concentrative on the horizon $\Upsilon_{\rm A}$ itself. Also, we will proceed to investigate some useful properties of the apparent horizon as necessary preparations for the horizon thermodynamics.

Eq.(5.11) clearly shows that, for an expanding Universe ($H > 0$) the apparent-horizon radius $\Upsilon_{\rm A}$ can be either expanding, contracting or even static, depending on the domain of the EoS parameter w_m or equivalently the sign of the enthalpy density h_m. In the ΛCDM cosmology, ρ_m could be decomposed into all possible components, $\rho_m = \sum\rho_m^{(i)} = \rho_m(\text{baryon}) + \rho_m(\text{radiation}) + \rho_m(\text{neutrino}) + \rho_m(\text{dark matter}) + \rho_m(\text{dark energy}) + \cdots$, and the same for P_m. In principle there should be an EoS parameter $w_m^{(i)} = P_m^{(i)}/\rho_m^{(i)}$ associated to each energy component. However, practically we can regard w_m either as that of the absolutely dominating matter, or the weighted average for all relatively dominating components

$$w_m = \frac{\sum P_m^{(i)}}{\rho_m} = \frac{\sum w_m^{(i)}\rho_m^{(i)}}{\rho_m} = \sum\alpha_i\, w_m^{(i)}\,, \tag{5.13}$$

with the weight coefficient given by $\alpha_i = \rho_m^{(i)}/\rho_m$, and thus w_m varies over cosmic time scale. Then it follows from Eq.(5.11) that:

w_m	dominating matter	enthalpy density	$\dot{\Upsilon}_{\rm A}$
$-1/3 \leq w_m\,(\leq 1)$ and $-1 < w_m < -1/3$	ordinary matter, and quintessence [37]	$h_m > 0$	$\dot{\Upsilon}_{\rm A} > 0$, expanding
$w_m = -1$	cosmological constant or vacuum energy [38]	$h_m = 0$	$\dot{\Upsilon}_{\rm A} = 0$, static
$w_m < -1$	phantom [39]	$h_m < 0$	$\dot{\Upsilon}_{\rm A} < 0$, contracting

The dominant energy condition [40] $\rho_m \geq |P_m|$ imposes the constraint $-1 \leq w_m \leq 1$ for *nonexotic* matter. Here we retain the upper limit $w_m \leq 1$ but loosen the lower limit, allowing w_m to cross the barrier $w_m = -1$ into the *exotic* phantom domain $w_m < -1$. The upper limit however is bracketed as (≤ 1) to indicate that it is a physical rather than mathematical constraint.

5.2.3 Induced metric of the apparent horizon

The total derivative of $\Upsilon = \Upsilon(t, r)$ yields $adr = d\Upsilon - H\Upsilon dt$, which recasts the FRW line element Eq.(5.1) into the $(t, \Upsilon, \theta, \varphi)$ coordinates as

$$ds^2 = \left(1 - \frac{k\Upsilon^2}{a^2}\right)^{-1}\left(-\left(1 - \frac{\Upsilon^2}{\Upsilon_{\rm A}^2}\right)dt^2 - 2H\Upsilon dt d\Upsilon + d\Upsilon^2\right) + \Upsilon^2\left(d\theta^2 + \sin^2\theta d\varphi^2\right). \tag{5.14}$$

Although the comoving transverse coordinates (t, r) are easier to work with, we will switch to the more physical coordinates (t, Υ) whenever necessary. The metric Eq.(5.14) reduces to become a three-dimensional hypersurface in the (t, θ, φ) coordinates at the apparent horizon $\Upsilon_{\rm A} = \Upsilon_{\rm A}(t)$, and with Eq.(5.11), the induced horizon metric turns out to be

$$\begin{aligned} ds^2 &= (H\Upsilon_{\rm A})^{-2}(\dot{\Upsilon}_{\rm A} - 2H\Upsilon_{\rm A})\dot{\Upsilon}_{\rm A} dt^2 + \Upsilon_{\rm A}^2(d\theta^2 + \sin^2\theta d\varphi^2) \\ &= \frac{9}{4}(w_m + 1)(w_m - \frac{1}{3})dt^2 + \Upsilon_{\rm A}^2(d\theta^2 + \sin^2\theta d\varphi^2). \end{aligned} \tag{5.15}$$

Here w_m shows up in the coefficients of dt^2, and indeed the spirit of geometrodynamics allows and encourages physical parameters to directly participate in the spacetime metric, just like the mass, electric charge and angular momentum parameters in the Kerr-Newmann solution. It is easily seen that the signature of the apparent horizon solely relies on the domain of w_m regardless of the Universe being expanding or contracting.

(1) For $-1 < w_m < 1/3$, the apparent horizon $\Upsilon_{\rm A}$ has the signature $(-, ++)$ and is timelike, which shares the signature of a quasilocal timelike membrane in black-hole physics [28, 41].

(2) For $w_m < -1$ or $1/3 < w_m (\leq 1)$, the signature is $(+, ++)$ and thus $\Upsilon_{\rm A}$ is spacelike. This situation has the same signature with the dynamical black-hole horizons [42].

(3) For $w_m = -1$ or $w_m = 1/3$, $\Upsilon_{\rm A}$ is a null surface with the signature $(0, ++)$, so it coincides with the cosmological event horizon $\Upsilon_{\rm E} := a\int_t^\infty a^{-1}d\hat{t}$ [26, 43] which by definition is a future-pointed null causal boundary, and it shares the signature of isolated black-hole horizons [27].

Note that these analogies between $\Upsilon_{\rm A}$ and black-hole horizons are limited to the metric signature, while the behaviors of their expansions $\{\theta_{(\ell)}, \theta_{(n)}\}$ and the horizon trappedness are entirely different. Among the two critical values, $w_m = -1$ corresponds to the de Sitter Universe dominated by a positive cosmological constant (or vacuum energy) [1], while $w_m = 1/3$ refers to the highly relativistic limit of w_m and the EoS of radiation, with the trace of the the stress-energy-momentum tensor $g^{\mu\nu}T^{(m)}_{\mu\nu} = (3w_m - 1)\rho_m$ vanishing at $w_m = 1/3$. As will be shown later in Sec. 5.4, $w_m = 1/3$ also serves as the "zero temperature divide" if the apparent-horizon temperature were measured by $\kappa/2\pi$ in terms of the Hayward surface gravity κ.

5.2.4 Relative evolution equations

The nontrivial t-component of $\nabla_\mu T^{\mu\,(m)}_{\ \nu} = 0$ with respect to the metric Eq.(5.1) leads to the continuity equation for the cosmic perfect fluid

$$\dot{\rho}_m + 3H(1 + w_m)\rho_m = 0\,. \tag{5.16}$$

Thus for the relative evolution rate of the energy density $\dot{\rho}_m/\rho_m$, its ratio over that of the cosmic scale factor $\dot{a}/a = H$ synchronizes with the instantaneous value of the EoS parameter, $\frac{\dot{\rho}_m}{\rho_m}\Big/\frac{\dot{a}}{a} = -3(1 + w_m)$.

This relation is not alone, as one could easily observe from Eq.(5.11) that the relative evolution rate of the apparent-horizon radius $\dot{\Upsilon}_{\rm A}/\Upsilon_{\rm A}$ is normalized by $\dot{a}/a$ into $\frac{\dot{\Upsilon}_{\rm A}}{\Upsilon_{\rm A}}\Big/\frac{\dot{a}}{a} = \frac{3}{2}(1+w_m)$. These two equations reveal the interesting result that throughout the history of the Universe, the relative evolution rate of the energy density is always proportional to that of the apparent-horizon radius:

$$\frac{\dot{\rho}_m}{\rho_m}\Big/\frac{\dot{\Upsilon}_{\rm A}}{\Upsilon_{\rm A}} = -2\,. \tag{5.17}$$

In fact, integration of Eq.(5.17) yields $\ln\rho_m \propto -2\ln\Upsilon_{\rm A}$ and thus $\rho_m \propto \Upsilon_{\rm A}^{-2}$, which matches the holographic-style dynamical equation (5.8) with the proportionality constant identified as $\frac{3}{8\pi G}$.

5.3 Thermodynamic implications of the holographic-style dynamical equations

In Sec. 5.2, based on Eqs.(5.8)-(5.12) we have analyzed some properties of the cosmological apparent horizon $\Upsilon_{\rm A}$ to facilitate the subsequent discussion; one can refer to [43] for more discussion of the horizon $\Upsilon_{\rm A}$. From this section on, we will continue to investigate the thermodynamic implications of the holographic-style gravitational equations (5.8)-(5.12).

5.3.1 Unified first law of thermodynamics

The mass $M = \rho_m V$ of cosmic fluid within a sphere of radius Υ, surface area $A = 4\pi\Upsilon^2$ and volume $V = \frac{4}{3}\pi\Upsilon^3$, can be geometrically recovered from the spacetime metric and we will identify it as the total internal energy E. With the Misner-Sharp mass/energy [44] $E_{\rm MS} := \frac{\Upsilon}{2G}(1-h^{\alpha\beta}\partial_\alpha\Upsilon\partial_\beta\Upsilon)$ for spherically symmetric spacetimes, Eq.(5.1) with $h^{\alpha\beta}=\text{diag}[-1\,,\frac{a^2}{1-kr^2}]$ for the Universe yields

$$E = \frac{\Upsilon^3}{2G\Upsilon_{\rm A}^2}\,, \tag{5.18}$$

and its equivalence with the physically defined mass $E = M = \rho_m V$ is guaranteed by Eq.(5.8). Equation (5.18) can also be reconstructed in the tetrad Eq.(5.2) from the Hawking energy [45] $E_{\rm Hk} := \frac{1}{4\pi G}\left(\int\frac{dA}{4\pi}\right)^{1/2}\int(-\Psi_2-\sigma_{\rm NP}\lambda_{\rm NP}+\Phi_{11}+\Lambda_{\rm NP})dA \equiv \frac{1}{4\pi G}\left(\int\frac{dA}{4\pi}\right)^{1/2}\left(2\pi-\int\rho_{\rm NP}\mu_{\rm NP}dA\right)$ for twist-free spacetimes. Immediately, the total derivative or transverse gradient of $E=E(t,r)$ is

$$dE = -\frac{1}{G}\frac{\Upsilon^3}{\Upsilon_{\rm A}^3}\left(\dot{\Upsilon}_{\rm A}-\frac{3}{2}H\Upsilon_{\rm A}\right)dt+\frac{3}{2G}\frac{\Upsilon^2}{\Upsilon_{\rm A}^2}\,adr \tag{5.19}$$

$$= -\frac{\dot{\Upsilon}_{\rm A}}{G}\frac{\Upsilon^3}{\Upsilon_{\rm A}^3}\,dt+\frac{3}{2G}\frac{\Upsilon^2}{\Upsilon_{\rm A}^2}\,d\Upsilon\,, \tag{5.20}$$

where the relation $adr = d\Upsilon - H\Upsilon dt$ has been employed to rewrite Eq.(5.19) into Eq.(5.20), with the transverse coordinates from (t,r) to $(t\,,\Upsilon)$. According to the holographic-style dynamical equations (5.8), (5.9) and (5.12), the energy differentials Eqs.(5.19) and (5.20) can be rewritten into

$$dE = -A\Upsilon H P_m\, dt + A\,\rho_m\, a dr \tag{5.21}$$

$$= -A\,(1+w_m)\rho_m\, H\Upsilon\, dt + A\,\rho_m\, d\Upsilon\,. \tag{5.22}$$

Eqs.(5.21) and (5.22) can be formally compactified into

$$dE = A\boldsymbol{\psi} + WdV\,, \tag{5.23}$$

where $\boldsymbol{\psi}$ and W are respectively the energy supply covector

$$\boldsymbol{\psi} = -\frac{1}{2}\,\rho_m(1+w_m)\,H\Upsilon\,dt + \frac{1}{2}\,\rho_m(1+w_m)\,adr \tag{5.24}$$

$$= -\,\rho_m(1+w_m)\,H\Upsilon\,dt + \frac{1}{2}\,\rho_m(1+w_m)\,d\Upsilon\,, \tag{5.25}$$

and the work density

$$W = \frac{1}{2}(1-w_m)\,\rho_m\,. \tag{5.26}$$

Eq.(5.23) is exactly the unified first law of (equilibrium) thermodynamics proposed by Hayward [46], and one can see from the derivation process that it applies to a volume of arbitrary areal radius Υ, no matter $\Upsilon < \Upsilon_A$, $\Upsilon = \Upsilon_A$ or $\Upsilon > \Upsilon_A$. Moreover, W and $\boldsymbol{\psi}$ can respectively be traced back to the scalar invariant $W := -\frac{1}{2}T^{\alpha\beta}_{(m)}h_{\alpha\beta}$ and the covector invariant $\boldsymbol{\psi}_\alpha := T_{\alpha\,(m)}^{\;\;\beta}\partial_\beta\Upsilon + W\partial_\alpha\Upsilon$ [46], which are valid for all spherically symmetric spacetimes besides FRW, and have Eqs.(5.24), (5.25) and (5.26) as their concrete components with respect to the metric Eq.(5.1).

Note that the "unified" first law Eq.(5.23) for the gravitational thermodynamics of the Universe is totally different from the first laws in black-hole thermodynamics which balance the energy differential with the first-order variations of the Arnowitt-Deser-Misner type quantities (such as mass, electric charge, and angular momentum). Instead, Eq.(5.23) is more related to the geometrical aspects of the thermodynamics-gravity correspondence.

5.3.2 Clausius equation on the apparent horizon for an isochoric process

Having seen that the full set of holographic-style dynamical equations (5.8), (5.9) and (5.12) yield the unified first law $dE = A\boldsymbol{\psi} + WdV$ for an arbitrary region in the FRW Universe, we will focus on the volume enclosed by the apparent horizon Υ_A. Firstly, Eq.(5.9) leads to

$$\frac{\dot{\Upsilon}_A}{G}dt = A_A\,(1+w_m)\,\rho_m\,H\Upsilon_A\,dt\,, \tag{5.27}$$

and the left hand side can be manipulated into

$$\frac{\dot{\Upsilon}_A}{G}dt = \frac{1}{2\pi\Upsilon_A}\left(\frac{2\pi\Upsilon_A\dot{\Upsilon}_A}{G}dt\right) = \frac{1}{2\pi\Upsilon_A}\frac{d}{dt}\left(\frac{\pi\Upsilon_A^2}{G}\right). \tag{5.28}$$

Applying the geometrically defined Hawking-Bekenstein entropy [5] (in the units $\hbar = c = k$ [Boltzmann] $=$ 1) to the apparent horizon

$$S_{\rm A} = \frac{\pi \Upsilon_{\rm A}^2}{G} = \frac{A_{\rm A}}{4G}\,, \tag{5.29}$$

then employing the Cai–Kim temperature [2, 47]

$$T_{\rm A} \equiv \frac{1}{2\pi\Upsilon_{\rm A}}\,, \tag{5.30}$$

thus $T_{\rm A} dS_{\rm A} = \dot{\Upsilon}_{\rm A}/Gdt$ and Eq.(5.28) can be rewritten into

$$T_{\rm A} dS_{\rm A} = \delta Q_{\rm A} = -A_{\rm A} \boldsymbol{\psi}_t = -dE_{\rm A}\Big|_{d\Upsilon=0}\,, \tag{5.31}$$

where $\boldsymbol{\psi}_t$ is the t-component of the energy supply covector $\boldsymbol{\psi} = \boldsymbol{\psi}_t + \boldsymbol{\psi}_\Upsilon = \psi_\alpha dx^\alpha$ in Eq.(5.25). This basically reverses Cai and Kim's formulation in [2], and differs from [6] by the setup of the horizon temperature. Eq.(5.31) is actually the Clausius equation for equilibrium and reversible thermodynamic processes, and the meaning of reversibility compatible with the cosmic dynamics is clarified in Appendix 5.7. Comparing Eq.(5.31) with the unified first law Eq.(5.23), one could find that Eq.(5.31) is just Eq.(5.23) with the two $d\Upsilon$ components removed and then evaluated at $\Upsilon_{\rm A}$. Assuming that the apparent horizon locates at $\Upsilon_{\rm A0} \equiv \Upsilon_{\rm A}(t = t_0)$ at an arbitrary moment t_0, then during the infinitesimal time interval dt the horizon will move to $\Upsilon_{\rm A0} + \dot{\Upsilon}_{\rm A0} dt$; meanwhile, for the isochoric process of the volume $V(\Upsilon_{\rm A0})$ (i.e. a "controlled volume"), the amount of energy across the horizon $\Upsilon_{\rm A0}$ is just $dE_{\rm A} = A_{\rm A0} \boldsymbol{\psi}_t$ evaluated at t_0, and for brevity we will drop the subscript "0" whenever possible as t_0 is arbitrary.

The energy-balance equation (5.31) implies that the region $\Upsilon \leq \Upsilon_{\rm A}$ enveloped by the cosmological apparent horizon is thermodynamically an *open* system which exchanges both heat and matter (condensed components in the Hubble flow) with its surroundings/reservoir $\Upsilon \geq \Upsilon_{\rm A}$. Here we emphasize again that $\Upsilon_{\rm A}$ is simply a visual boundary preventing ingoing null radial signals from reaching the comoving observer, and the absolute cosmic Hubble flow can still cross $\Upsilon_{\rm A}$. Also, unlike nonrelativistic thermodynamics in which δQ exclusively refers to the heat transfer (i.e. electromagnetic flow), the $\delta Q_{\rm A}$ in Eq.(5.31) is used in a mass-energy-equivalence sense and denotes the Hubble energy flow which generally contains different matter components.

Finally, for the open system enveloped by $\Upsilon_{\rm A}$, we combine the Clausius equation (5.31) and the unified first law Eq.(5.23) into the total energy differential

$$\begin{aligned} dE_{\rm A} &= A_{\rm A} \psi_t\, dt + A_{\rm A}(\psi_\Upsilon + W)\, d\Upsilon_{\rm A} \\ &= -T_{\rm A} dS_{\rm A} + \rho_m A_{\rm A} d\Upsilon_{\rm A} \\ &= -T_{\rm A} dS_{\rm A} + \rho_m\, dV_{\rm A}\,. \end{aligned} \tag{5.32}$$

In fact, by the continuity equation (5.16) one can verify $-T_{\rm A} dS_{\rm A} = V_{\rm A} d\rho_m$, which agrees with the thermodynamic connotation that the heat $-T_{\rm A} dS_{\rm A} = \delta Q_{\rm A}$ measures the loss of internal energy that can no longer be used to do work. In this sense, one may further regard $dE_{\rm A} + T_{\rm A} dS_{\rm A}$ to play the role of the relativistic differential Helmholtz free energy $d\mathbb{F}_{\rm A}$ for the instantaneous $\Upsilon_{\rm A0}$ of temperature $T_{\rm A0}$,

$$d\mathbb{F}_{\rm A} := dE_{\rm A} + T_{\rm A} dS_{\rm A} = \rho_m\, dV_{\rm A} = (\psi_\Upsilon + W)\, dV_{\rm A}\,, \tag{5.33}$$

which represents the maximal work element that can be extracted from the interior of Υ_{A0}; one could also identify the relativistic differential Gibbs free energy $d\mathbb{G}_A$, which means the "useful" work element, as

$$d\mathbb{G}_A := dE_A + T_A dS_A + P_m dV_A = \rho_m (1 + w_m) dV_A . \tag{5.34}$$

Note that $d\mathbb{F}_A$ and $d\mathbb{G}_A$ contain $+T_A dS_A$ with a plus instead of a minus sign, because the Cai–Kim Clausius relation $dE_A = -T_A dS_A$ encodes that the horizon entropy S_A is defined in a "positive heat out" rather than the traditional positive-heat-in thermodynamic sign convention, as will be extensively discussed in Sec. 5.5.1.

5.4 Solution to the horizon-temperature confusion

5.4.1 The horizon-temperature confusion

In the thermodynamics of (quasi)stationary black holes [5], the Hawking temperature satisfies $T = \tilde{\kappa}/(2\pi)$ based on the traditional Killing surface gravity $\tilde{\kappa}$ and the Killing generators of the horizon. For the FRW Universe, one has the Hayward inaffinity parameter κ [46] in place of the Killing inaffinity, which yields the Hayward surface gravity on the apparent horizon,

$$\begin{aligned} \kappa &:= \frac{1}{2} h^{\alpha\beta} \nabla_\alpha \nabla_\beta \Upsilon = \frac{1}{2\sqrt{-h}} \partial_\alpha \Big(\sqrt{-h}\, h^{\alpha\beta} \partial_\beta \Upsilon \Big) \\ &\equiv -\frac{\Upsilon}{\Upsilon_A^2} \left(1 - \frac{\dot{\Upsilon}_A}{2H\Upsilon_A} \right) = -\frac{1}{\Upsilon_A} \left(1 - \frac{\dot{\Upsilon}_A}{2H\Upsilon_A} \right) \Big|_{\Upsilon_A} , \end{aligned} \tag{5.35}$$

where $h_{\alpha\beta} = \text{diag}[-1\,, \frac{a^2}{1-kr^2}]$ refers to the transverse two-metric in Eq.(5.1). Then formally following the Hawking temperature, the Hayward temperature of the apparent horizon Υ_A is defined either by [7, 9]

$$\mathcal{T}_A := \frac{\kappa}{2\pi} = -\frac{1}{2\pi\Upsilon_A} \left(1 - \frac{\dot{\Upsilon}_A}{2H\Upsilon_A} \right) \tag{5.36}$$

or [8, 10, 18–20, 24, 25]

$$\mathcal{T}_A^{(+)} := \frac{(\kappa|}{2\pi} = \frac{1}{2\pi\Upsilon_A} \left(1 - \frac{\dot{\Upsilon}_A}{2H\Upsilon_A} \right) , \tag{5.37}$$

where we use the symbol $(\kappa|$ to denote the *partial* absolute value of κ, because existing papers have *a priori* abandoned the possibility of $\dot{\Upsilon}_A/(2H\Upsilon_A) \geq 1$ for $\mathcal{T}_A^{(+)}$. Equation (5.37) is always supplemented by the assumption [8, 10, 18–20, 24, 25]

$$\frac{\dot{\Upsilon}_A}{2H\Upsilon_A} < 1 \tag{5.38}$$

to guarantee a positive $\mathcal{T}_A^{(+)}$ which is required by the third law of thermodynamics, and even the condition [18]

$$\frac{\dot{\Upsilon}_A}{2H\Upsilon_A} << 1 \tag{5.39}$$

so that $\mathcal{T}_A^{(+)}$ can be approximated into the Cai–Kim temperature [2, 47]

$$\mathcal{T}_A^{(+)} \approx \frac{1}{2\pi\Upsilon_A} = T_A . \tag{5.40}$$

Historically the inverse problem "from thermodynamics to gravitational equations for the Universe" [2] was formulated earlier, in which the Cai–Kim temperature works perfectly for all theories of gravity. Later on, the problem "from FRW gravitational equations to thermodynamics" [6–8] (as the logic in this paper) came into attention in which the Hayward temperature seems to become effective. Considering that two different temperatures make the two mutually inverse problems asymmetric, attempts have been made to reduce the differences between them, mainly the assumptions Eqs.(5.38) and (5.39).

Note that when the conditions Eqs.(5.39) and (5.40) are applied to Eq.(5.36), $\mathcal{T}_\text{A}$ would become a negative temperature. [7] has suggested that it might be possible to understand this phenomenon as a consequence of the cosmological apparent horizon being inner trapped $[\theta_{(\ell)} > 0,\ \theta_{(n)} = 0]$, as opposed to the positive temperatures of black-hole apparent horizons which are always marginally outer trapped $[\theta_{(\ell)} = 0,\ \theta_{(n)} < 0]$. However, this proposal turns out to be inappropriate; as will be shown at the end of Sec. 5.4.3, the signs of $\mathcal{T}_\text{A}$ actually keep pace with the metric signatures rather than the inner/outer trappedness of the horizon Υ_A.

5.4.2 Effects of $\mathcal{T}_\text{A} dS_\text{A}$ and $\mathcal{T}^{(+)}_\text{A} dS_\text{A}$

In Sec. 5.3.2, we have seen $T_\text{A} dS_\text{A} = A_\text{A}\boldsymbol{\psi}_t$ for the Cai–Kim $T_\text{A} = 1/(2\pi\Upsilon_\text{A})$, and now let's examine the effects of $\mathcal{T}_\text{A}$ and $\mathcal{T}^{(+)}_\text{A}$. Given the Bekenstein–Hawking entropy $S_\text{A} = A_\text{A}/4G$, the dynamical equation $\dot{\Upsilon}_\text{A} = A_\text{A} H\Upsilon_\text{A} G(1+w_m)\rho_m$ and the energy supply covector $\boldsymbol{\psi} = \boldsymbol{\psi}_t + \boldsymbol{\psi}_\Upsilon = -(1+w_m)\rho_m H\Upsilon_\text{A} dt + \frac{1}{2}(1+w_m)\rho_m\, d\Upsilon_\text{A}$, one has

$$\begin{aligned}
\mathcal{T}_\text{A} dS_\text{A} &= -\frac{\dot{\Upsilon}_\text{A}}{G} + \frac{\dot{\Upsilon}_\text{A}}{2GH\Upsilon_\text{A}}\dot{\Upsilon}_\text{A} dt \\
&= -A_\text{A} H\Upsilon_\text{A}(1+w_m)\rho_m dt + \frac{1}{2}A_\text{A}(1+w_m)\rho_m d\Upsilon_\text{A} \\
&= A_\text{A}\boldsymbol{\psi}_t + A_\text{A}\boldsymbol{\psi}_\Upsilon = A_\text{A}\boldsymbol{\psi}\,.
\end{aligned} \tag{5.41}$$

Similarly, for the $\mathcal{T}^{(+)}_\text{A}$ defined in Eq.(5.37),

$$\mathcal{T}^{(+)}_\text{A} dS_\text{A} = -\Big(A_\text{A}\boldsymbol{\psi}_t + A_\text{A}\boldsymbol{\psi}_\Upsilon\Big) = -A_\text{A}\boldsymbol{\psi}\,. \tag{5.42}$$

Hence, for the two terms comprising $\mathcal{T}_\text{A}$ and $\mathcal{T}^{(+)}_\text{A}$, the $\pm\frac{1}{2\pi\Upsilon_\text{A}} dS_\text{A}$ is balanced by $\mp A_\text{A}\boldsymbol{\psi}_t$, while the $\pm\frac{\dot{\Upsilon}_\text{A}}{2H\Upsilon_\text{A}} dS_\text{A}$ is equal to $\pm A_\text{A}\boldsymbol{\psi}_\Upsilon$. As obtained in e.g. [6]-[12], for the open system enveloped by the cosmological apparent horizon, combining Eqs.(5.41) and (5.42) with the unified first law Eq.(5.23) leads to the total energy differential

$$\begin{aligned}
dE_\text{A} &= \mathcal{T}_\text{A} dS_\text{A} + W dV_\text{A} \\
&= -\mathcal{T}^{(+)}_\text{A} dS_\text{A} + W dV_\text{A}\,,
\end{aligned} \tag{5.43}$$

as opposed to $dE_\text{A} = -T_\text{A} dS_\text{A} + \rho_m dV_\text{A}$ for the Cai–Kim T_A.

5.4.3 "Zero temperature divide" $w_m = 1/3$ and preference of Cai–Kim temperature

Now apply the dynamical equation (5.11) to $\{\mathcal{T}_\text{A}, \mathcal{T}_\text{A}^{(+)}\}$ and the assumptions in Eqs.(5.38) and (5.39). With $\dot{\Upsilon}_\text{A} = \frac{3}{2}H\Upsilon_\text{A}(1+w_m)$, the Hayward surface gravity becomes

$$\kappa \;=\; -\frac{1}{\Upsilon_\text{A}}\left(1-\frac{\dot{\Upsilon}_\text{A}}{2H\Upsilon_\text{A}}\right) \;=\; -\frac{3}{4\Upsilon_\text{A}}\left(\frac{1}{3}-w_m\right), \tag{5.44}$$

so it follows that

$$\begin{cases} w_m > \dfrac{1}{3}: & \kappa > 0\,, \quad |\kappa| = \dfrac{3}{4\Upsilon_\text{A}}\left(w_m - \dfrac{1}{3}\right) \\ w_m = \dfrac{1}{3}: & \kappa = |\kappa| = 0 \\ w_m < \dfrac{1}{3}: & \kappa < 0\,, \quad |\kappa| = \dfrac{3}{4\Upsilon_\text{A}}\left(\dfrac{1}{3} - w_m\right) \end{cases}. \tag{5.45}$$

The Hayward temperature $\mathcal{T}_\text{A}$ in Eq.(5.36) and its partially absolute value $\mathcal{T}_\text{A}^{(+)}$ in Eq.(5.37) become

$$\begin{aligned} \mathcal{T}_\text{A} &= -\frac{3}{8\pi\Upsilon_\text{A}}\left(\frac{1}{3}-w_m\right) = -\frac{1}{4}T_\text{A}(1-3w_m) \\ \mathcal{T}_\text{A}^{(+)} &= \frac{3}{8\pi\Upsilon_\text{A}}\left(\frac{1}{3}-w_m\right) = \frac{1}{4}T_\text{A}(1-3w_m)\,. \end{aligned} \tag{5.46}$$

Fortunately $\mathcal{T}_\text{A}$ and $\mathcal{T}_\text{A}^{(+)}$ remain as state functions, although Eqs.(5.36) and (5.37) carry $\{\dot{\Upsilon}_\text{A}, H\}$ and look like process quantities (see Appendix 5.7 for more discussion). Moreover, the supplementary assumption Eq.(5.38) for $\mathcal{T}_\text{A}^{(+)} > 0$ turns out to be

$$\frac{\dot{\Upsilon}_\text{A}}{2H\Upsilon_\text{A}} \;=\; \frac{3}{4}(1+w_m) < 1 \quad \Rightarrow \quad w_m < 1/3\,. \tag{5.47}$$

Thus the condition $\frac{\dot{\Upsilon}_\text{A}}{2H\Upsilon_\text{A}} \ll 1$ in Eq.(5.39) could be directly translated into $w_m \ll 1/3$, which is however inaccurate: in fact, if directly starting from Eq.(5.46), the approximation $\mathcal{T}_\text{A}^{(+)} \approx T_\text{A} = 1/(2\pi\Upsilon_\text{A})$ will require

$$w_m \;\to\; -1\,. \tag{5.48}$$

It is neither mathematically nor physically identical with $w_m \ll 1/3$ which could only be perfectly satisfied for $w_m \to -\infty$ in the extreme phantom domain.

Eqs.(5.44) – (5.48) have rewritten and simplified the original expressions of the Hayward temperatures $\{\mathcal{T}_\text{A}\,, \mathcal{T}_\text{A}^{(+)}\}$ in Eqs.(5.36, 5.37) and their supplementary conditions Eqs.(5.38, 5.39). Based on these results we realize that it becomes possible to make an extensive comparison between $\{\mathcal{T}_\text{A}\,, \mathcal{T}_\text{A}^{(+)}\}$ and the Cai–Kim $T_\text{A} = 1/(2\pi\Upsilon_\text{A})$, which reveals the following facts.

(1) $\mathcal{T}_\text{A}$ is negative definite for $1/3 < w_m$ (≤ 1), positive definite for $w_m < 1/3$, and $\mathcal{T}_\text{A} \equiv 0$ for $w_m = 1/3$. We will dub the special value $w_m = 1/3$ as the Hayward "zero temperature divide", which is inspired by the terminology "phantom divide" for $w_m = -1$ in dark-energy physics [38]. Hence, $\mathcal{T}_\text{A}$ does not respect the third law of thermodynamics. Moreover, one has $\mathcal{T}_\text{A} = 0$ at $w_m = 1/3$ and thus $\mathcal{T}_\text{A} dS_\text{A} = 0$;

following Eq.(5.41), this can be verified by

$$\begin{aligned} A_{\rm A}\boldsymbol{\psi} &= -A_{\rm A}H\Upsilon_{\rm A}(1+w_m)\rho_m dt + \frac{1}{2}A_{\rm A}(1+w_m)\rho_m d\Upsilon_{\rm A} \\ &= A_{\rm A}\rho_m(1+w_m)(\frac{1}{2}\dot{\Upsilon}_{\rm A} - H\Upsilon_{\rm A})dt \\ &= \frac{9}{8G}H\Upsilon_{\rm A}(1+w_m)(w_m - \frac{1}{3})dt. \end{aligned} \quad (5.49)$$

(2) The condition $w_m < 1/3$ for the validity of $\mathcal{T}_{\rm A}^{(+)}$ is too restrictive and unnatural, because $w_m = 1/3$ serves as the EoS of radiation and $(1 \geq)\, w_m > 1/3$ represents all highly relativistic energy components. For example, it is well known that a canonical and homogeneous scalar field $\phi(t)$ in the FRW Universe has the EoS (e.g. [2])

$$w_m^{(\phi)} = \frac{P_\phi}{\rho_\phi} = \frac{\frac{1}{2}\dot{\phi}^2 - V(\phi)}{\frac{1}{2}\dot{\phi}^2 + V(\phi)}. \quad (5.50)$$

$w_m^{(\phi)}$ can fall into the domain $1/3 \leq w_m^{(\phi)} \leq 1$ when the dynamical term $\frac{1}{2}\dot{\phi}^2$ dominates over the potential $V(\phi)$, and we donot see any physical reason to *a priori* rule out this kind of fast-rolling scalar field.

(3) The equality $\mathcal{T}_{\rm A} dS_{\rm A} = A_{\rm A}(\boldsymbol{\psi}_t + \boldsymbol{\psi}_\Upsilon) = -\mathcal{T}_{\rm A}^{(+)} dS_{\rm A}$ implies that $\mathcal{T}_{\rm A} dS_{\rm A}$ and $\mathcal{T}_{\rm A}^{(+)} dS_{\rm A}$ need to be balanced by dt and also the $d\Upsilon_{\rm A}$ component of $\boldsymbol{\psi}$, and thus the other $d\Upsilon_{\rm A}$ component from $WdV_{\rm A} = WA_{\rm A}d\Upsilon_{\rm A}$ should be nonvanishing as well. Hence, $\mathcal{T}_{\rm A} dS_{\rm A}$ and $\mathcal{T}_{\rm A}^{(+)} dS_{\rm A}$ always live together with $WdV_{\rm A}$ to form the total energy differential Eq.(5.43) rather than some Clausius-type equation $\delta\widetilde{Q} = \mathcal{T}_{\rm A}^{(+)} dS_{\rm A} = -\mathcal{T}_{\rm A} dS_{\rm A} = -A_{\rm A}\boldsymbol{\psi}$, and there exists no isochoric process ($d\Upsilon = 0$) for $\{\mathcal{T}_{\rm A}\,, \mathcal{T}_{\rm A}^{(+)}\}$.

(4) The "highly relativistic limit" $w_m = 1/3$ is more than the divide for negative, zero or positive Hayward temperature $\mathcal{T}_{\rm A}$; it is also the exact divide for the induced metric of the apparent horizon to be spacelike, null or timelike, as discussed before in Sec. 5.2.3. That is to say, the sign of the temperature synchronizes with the signature of the horizon metric. However, there are no such behaviors for analogies in black-hole physics: for example, a slowly-evolving quasilocal black-hole horizon [41, 50] can be either spacelike, null or timelike, but the horizon temperature is always positive definite regardless of the horizon signature.

(5) Unlike the Cai–Kim temperature $T_{\rm A}$, the Hayward $\{\mathcal{T}_{\rm A}, \mathcal{T}_{\rm A}^{(+)}\}$ used for the problem "from gravitational equations to thermodynamic relations for the Universe" do not work for the problem "from thermodynamic relations to gravitational equations". That is to say, $\{\mathcal{T}_{\rm A}\,, \mathcal{T}_{\rm A}^{(+)}\}$ break the symmetry between the formulations of these two mutually inverse problems.

On the other hand, the Cai–Kim temperature $T_{\rm A} = 1/(2\pi\Upsilon_{\rm A})$ is positive definite throughout the history of the Universe, it provides symmetric formulations of the conjugate problems "gravity to thermodynamics" and "thermodynamics to gravity", and it is the Hawking-like temperature measured by a Kodama observer for the matter tunneling into the untrapped interior $\Upsilon < \Upsilon_{\rm A}$ from the antitrapped exterior $\Upsilon > \Upsilon_{\rm A}$ [47]. In fact, besides the assumption Eq.(5.39) for the approximation $\mathcal{T}_{\rm A}^{(+)} \approx T_{\rm A}$ in Eq.(5.40), there have been efforts to redefine the *dynamical* surface gravity in place of Eq.(5.35) for the dynamical apparent horizon $\Upsilon_{\rm A}$; for example, inspired by the thermodynamics of dynamical black-hole horizons [42], the inaffinity $\kappa := -\frac{1}{2}\partial_\Upsilon\Xi$

with $\Xi := h^{\alpha\beta}\partial_\alpha\Upsilon\partial_\beta\Upsilon \equiv 1 - \Upsilon^2/\Upsilon_A^2$ has been employed for the FRW Universe in [48], with which the Cai–Kim temperature satisfies $T_A = \dfrac{\kappa}{2\pi}$ at the horizon $\Upsilon = \Upsilon_A$ and thus absorbs the Hayward temperature $\mathcal{T}_A = \kappa/(2\pi)$.

With these considerations, we adopt the Cai–Kim T_A for the absolute temperature of the cosmological apparent horizon. This way, we believe that the temperature confusion is solved as the Cai–Kim T_A is favored.

Furthermore, imagine a contracting Universe with $\dot{a} < 0$ and $H < 0$, and one would have a marginally *outer* trapped apparent horizon with $\theta_{(\ell)} = 0$ and $\theta_{(n)} = 2H < 0$ at $\Upsilon = \Upsilon_A$. Hence, whether $\Upsilon = \Upsilon_A$ is outer or inner trapped only relies on the Hubble parameter to be negative or positive. In Sec. 5.2.3 we have seen that the induced-metric signature of Υ_A is independent of H, and neither will the Hayward $\{\mathcal{T}_A\,, \mathcal{T}_A^{(+)}\}$. Also, Eqs.(5.52) and (5.53) clearly show that, the equality $-T_A dS_A = A_A \boldsymbol{\psi}_t = dE_A$ of the Cai–Kim T_A validates for either $H > 0$ or $H < 0$. Hence, we further conclude that:

Corollary 1 *Neither the sign of the Hayward nor the Cai–Kim temperature is related to the inner or outer trappedness of the cosmological apparent horizon.*

5.4.4 A quick note on the QCD ghost dark energy

Among the various types of quantum chromodynamics (QCD) ghost dark energy in existent literature, the following version was introduced in [51] and further discussed in [52],

$$\rho_\Lambda^{(\mathrm{QCD})} = \alpha\Upsilon_A^{-1}\left(1 - \frac{\dot{\Upsilon}_A}{2H\Upsilon_A}\right), \tag{5.51}$$

where α is a positive constant with the dimension of $[energy]^3$. It is based on the idea that the vacuum energy density is proportional to the temperature of the apparent horizon Υ_A, which was chosen as the Hayward $\{\mathcal{T}_A\,, \mathcal{T}_A^{(+)}\}$ in [51]. Following the discussion just above, we can see that Eq.(5.51) turns out to be problematic because $\rho_\Lambda^{(\mathrm{QCD})}$ is not positive definite, with $\rho_\Lambda^{(\mathrm{QCD})} \le 0$ when the Universe is dominated by superrelativistic matter $1/3 \le w_m$ (≤ 1). In fact, more viable forms of the QCD ghost dark energy can be found in e.g. [53].

5.5 The (generalized) second laws of thermodynamics

Having studied the differential forms of the energy conservation and heat transfer and distinguished the temperature of of the apparent horizon, we will proceed to investigate the entropy evolution for the Universe.

5.5.1 Positive heat out thermodynamic sign convention

As a corner stone for our formulation of the second laws and solution to the entropy confusion, we will match the thermodynamic sign convention encoded in the Cai–Kim Clausius equation $T_A dS_A = \delta Q_A = -A_A\boldsymbol{\psi}_t$. Following Secs. 5.3.1 and 5.3.2, we first check whether the heat flow element δQ_A and the isochoric energy differential $dE_{A0} = d(\rho_m V_{A0})$ take positive or negative values. δQ_A will be calculated by $T_A dS_A$, while dE_A is to be evaluated independently via $A_A\boldsymbol{\psi}_t = -A_A(1 + w_m)\rho_m H\Upsilon_A dt$. Hence, in the isochoric process for an instantaneous apparent horizon Υ_{A0},

$$T_A dS_A = \frac{\dot{\Upsilon}_A}{G} dt = \frac{3}{2G} H\Upsilon_A (1 + w_m) dt \,, \tag{5.52}$$

$$dE\big|_{\Upsilon_{A0}} = -A_A \rho_m (1 + w_m) H\Upsilon_A dt = -\frac{3}{2G} H\Upsilon_A (1 + w_m) dt, \tag{5.53}$$

where Eqs. (5.10) and (5.11) have been used to replace $A_A\rho_m$ and $\dot{\Upsilon}_A$, respectively. For an expanding Universe ($H > 0$), this clearly shows that:

(1) If the Universe is dominated by ordinary matter or quintessence, $-1 < w_m (\leq 1)$, the internal energy is decreasing $dE_A = A_A \boldsymbol{\psi}_t < 0$, with a positive Hubble energy flow $\delta Q_A = T_A dS_A > 0$ going outside to the surroundings;

(2) Under the dominance of the cosmological constant, $w_m = -1$ and $\{\rho_m, \Upsilon_A, T_A, S_A\}$ = constant; the internal energy is unchanging, $dE_A = A_A \boldsymbol{\psi}_t = 0$ and $\delta Q_A = T_A dS_A = 0$;

(3) When the Universe enters the phantom-dominated state, $w_m < -1$, the internal energy increases $dE_A = A_A \boldsymbol{\psi}_t > 0$ while $\delta Q_A = T_A dS_A < 0$.

Hence, based on the intuitive behaviors at the domain $-1 < w_m (\leq 1)$ for nonexotic matter, we set up the *positive heat out* thermodynamic sign convention for the right hand side of $dE_A = -\delta Q_A$. That is to say, heat emitted by the system takes positive values ($\delta Q_A = \delta Q_A^{\text{out}} > 0$), while heat absorbed by the system takes negative values. Obviously, this setup is totally consistent with the situations of $w_m \leq -1$. Also, because of the counterintuitive behaviors under phantom dominance, one should not take it for granted that, for a spatially expanding Universe the cosmic fluid would always flow out of the isochoric volume $V(\Upsilon = \Upsilon_0)$ with $dE = V_{A0} d\rho_m < 0$.

5.5.2 Positive heat out Gibbs equation

In existent papers, the cosmic entropy is generally studied independently of the first laws, and the entropy $\widehat{S}_m$ of the cosmic energy-matter content (with temperature T_m) is always determined by the traditional Gibbs equation $dE = T_m d\widehat{S}_m - P_m dV$ (e.g. [14]-[24]). This way, $\dot{\widehat{S}}_m$ departs dramatically from the expected non-decreasing behaviors, so people turn to the generalized version of the second law for help, which works with the sum of $\widehat{S}_m$ and the geometric entropy of the cosmological apparent or event horizons.

This popular treatment is very problematic. In fact, the equation $dE_m = T_m d\widehat{S}_m - P_m dV$ encodes the "positive heat in, positive work out" convention for the physical entropy $\widehat{S}_m$ and the heat transfer $T_m d\widehat{S}_m$. However, as extensively discussed just above, the geometric Bekenstein–Hawking entropy $S_A = A_A/4G$ for the cosmological apparent horizon is compatible with the positive-heat-out convention. *One cannot add the traditional positive-heat-in $\widehat{S}_m$ with the positive-heat-out S_A*, and this conflict[1] leads us to adjust the Gibbs equation into

$$dE_m = -T_m \, dS_m - P_m dV \,, \tag{5.54}$$

[1]Note that there is no such conflict for black holes, because both the black-hole horizon entropy and the matter entropy are defined in the positive-heat-in convention.

where S_m is defined in the positive-heat-out convention favored by the Universe for consistency with the holographic-style gravitational equations (5.8), (5.9) and (5.12). This way, one can feel free and safe to superpose or compare the matter entropy S_m and the horizon entropy $\{S_\text{A}, \text{etc.}\}$, and even more pleasantly, it turns out that this S_m is very well behaved.

Moreover, note that although the Gibbs equation is usually derived from a reversible process in a closed system ("controlled mass"), Eq.(5.54) actually applies to either reversible or irreversible processes, and either closed or open systems, because it only contains state quantities which are independent of thermodynamic processes.

For the energy $E = M = \rho_m V$ in an arbitrary volume $V = \frac{4}{3}\pi\Upsilon^3 = \frac{1}{3}A\Upsilon$, Eq.(5.54) yields $T_m dS_m = -d(\rho_m V) - P_m dV = -V d\rho_m - (\rho_m + P_m)dV$, and thus

$$\begin{aligned} T_m dS_m &= 3H(\rho_m + P_m)V dt - (\rho_m + P_m)A d\Upsilon \\ &= \rho_m A(1 + w_m)(H\Upsilon dt - d\Upsilon)\,, \end{aligned} \tag{5.55}$$

where the continuity equation (5.16) has been used. Based on Eq.(5.55), we can analyze the entropy evolution $\dot{S}_m$ for the matter inside some special radii such as the apparent and event horizons. Note that these regions are generally open thermodynamic systems with the Hubble energy flow crossing the apparent and possibly the event horizons, so one should not *a priori* anticipate $\dot{S}_m \geq 0$; instead, we will look for the circumstances where $\dot{S}_m \geq 0$ conditionally holds.

5.5.3 The second law for the interior of the apparent horizon

For the matter inside the apparent horizon $\Upsilon = \Upsilon_\text{A}(t)$, Eq.(5.55) along with the holographic-style dynamical equations (5.10) and (5.11) yield

$$\begin{aligned} T_m dS_m^{(\text{A})} &= \rho_m A_\text{A}(1 + w_m)(H\Upsilon_\text{A} - \dot{\Upsilon}_\text{A})dt \\ &= \frac{3}{2G}(1 + w_m)H\Upsilon_\text{A}\Big(1 - \frac{3}{2}(1 + w_m)\Big)dt \\ &= -\frac{9}{4G}H\Upsilon_\text{A}(w_m + 1)(w_m + \frac{1}{3})dt\,. \end{aligned} \tag{5.56}$$

Obviously the second law of thermodynamics $\dot{S}_m^{(\text{A})} \geq 0$ holds for $-1 \leq w_m \leq -1/3$. Moreover, recall that the spatial expansion of the generic FRW Unverse satisfies

$$\frac{\ddot{a}}{a} = -\frac{4\pi G}{3}(1 + 3w_m)\rho_m\,, \tag{5.57}$$

with $\ddot{a} > 0$ for $w_m < -1/3$. Hence, within GR and the ΛCDM model, we have:

Theorem 1 *The physical entropy $S_m^{(A)}$ inside the cosmological apparent horizon satisfies $\dot{S}_m^{(A)} \equiv 0$ when $w_m = -1/3$ or under the dominance of the cosmological constant $w_m = -1$, while $\dot{S}_m^{(A)} > 0$ for the stage of accelerated expansion ($\ddot{a} > 0$) dominated by quintessence $-1 < w_m < -1/3$.*

5.5.4 The second law for the interior of the event and particle horizons

Consider the future-pointed cosmological event horizon $\Upsilon_{\rm E} := a\int_t^\infty a^{-1}d\hat{t}$ which measures the distance that light signals will travel over the entire future history from $\hat{t}_0 = t$. $\Upsilon_{\rm E}$ satisfies

$$\dot{\Upsilon}_{\rm E} = H\Upsilon_{\rm E} - 1\,, \tag{5.58}$$

so for the cosmic fluid inside $\Upsilon_{\rm E}$, Eq.(5.55) leads to

$$\begin{aligned} T_m dS_m^{(\rm E)} &= \rho_m A_{\rm E}(1+w_m)(H\Upsilon_{\rm E} - \dot{\Upsilon}_{\rm E})dt \\ &= \rho_m A_{\rm E}(1+w_m)dt\,. \end{aligned} \tag{5.59}$$

Hence, we are very happy to see that:

Theorem 2 *The physical entropy $S_m^{(E)}$ inside the cosmological event horizon satisfies $\dot{S}_m^{(E)} \equiv 0$ if the Universe is dominated by the cosmological constant $w_m = -1$, while $\dot{S}_m^{(E)} > 0$ for all nonexotic matter $-1 < w_m\,(\leq 1)$ above the phantom divide.*

The importance of this result can be best seen for a closed ($k = 1$) Universe, when the event horizon $\Upsilon_{\rm E}$ has a finite radius and bounds the entire spacetime. Then the physical entropy of the whole Universe is nondecreasing as long as the dominant energy condition holds $-1 \leq w_m\,(\leq 1)$.

Similarly for the past particle horizon $\Upsilon_{\rm P} := a\int_0^t a^{-1}d\hat{t}$ (e.g. [26, 43, 54]), which supplements the event horizon $\Upsilon_{\rm E}$ and measures the distance that light has already traveled from the beginning of time (or equivalently the most distant objects one could currently observe), it satisfies $\dot{\Upsilon}_{\rm P} = H\Upsilon_{\rm P} + 1$ and thus Eq.(5.55) yields

$$\begin{aligned} T_m dS_m^{(\rm P)} &= \rho_m A_{\rm P}(1+w_m)(H\Upsilon_{\rm P} - \dot{\Upsilon}_{\rm P})dt \\ &= -\rho_m A_{\rm P}(1+w_m)dt\,. \end{aligned} \tag{5.60}$$

Besides $\dot{S}_m^{(\rm P)} \equiv 0$ for $w_m = -1$, $\dot{S}_m^{(\rm P)} < 0$ always holds at the domain $-1 < w_m\,(\leq 1)$, which means that the physical entropy is always decreasing when we trace back to the earlier age for the younger Universe that has a larger particle horizon radius $\Upsilon_{\rm P}$ or horizon area $A_{\rm P}$.

Note that with the traditional Gibbs equation $dE_m = T_m d\widehat{S}_m - P_m dV$ where $\widehat{S}_m$ is defined in the positive-heat-in convention, for the interiors of the future $\Upsilon_{\rm E}$ and the past $\Upsilon_{\rm P}$ one would always obtain

$$\begin{aligned} T_m\, d\widehat{S}_m^{(\rm E)} \;&=\; dE_m^{(\rm E)} + P_m dV_{\rm E} \;=\; -\rho_m A_{\rm E}(1+w_m)dt \\ T_m\, d\widehat{S}_m^{(\rm P)} \;&=\; dE_m^{(\rm P)} + P_m dV_{\rm P} \;=\; \rho_m A_{\rm P}(1+w_m)dt\,. \end{aligned} \tag{5.61}$$

It would imply that in the future $\dot{\widehat{S}}_m^{(\rm E)} > 0$ would never be realized and a younger Universe (larger $A_{\rm P}$) would however carry a larger internal entropy $\widehat{S}_m^{(\rm P)}$, unless the Universe were in an exotically phantom-dominated ($w_m < -1$) state in her history. We believe that Eqs.(5.59, 5.60) provide a more reasonable description for the cosmic entropy evolution than Eq.(5.61), regard this result as a support to the positive-heat-out Gibbs equation (5.54), and argue that Eqs.(5.54), (5.59) and (5.60) have solved the cosmological *entropy confusion* caused by Eq.(5.61) in traditional studies.

5.5.5 GSL for the apparent-horizon system

Historically, to rescue the disastrous result of the traditional Eq.(5.61), the *generalized* second law (GSL) for the thermodynamics of the Universe was developed, which adds up the geometrically defined entropy of the cosmological boundaries (mainly S_A, S_E) to the physical entropy of the matter-energy content S_m, aiming to make the total entropy nondecreasing under certain conditions. This idea is inspired by the GSL of black-hole thermodynamics [49], for which Bekenstein postulated that the black-hole horizon entropy plus the external matter entropy never decrease (for a thermodynamic closed system).

Eq.(5.59) clearly indicates that the second law $\dot{S}_m \geq 0$ is well respected in our formulation, but for completeness we will still re-investigate the GSLs. For the simple open system consisting of the cosmological apparent horizon Υ_A and its interior, Eqs.(5.29) and (5.56) yields

$$\begin{aligned}\dot{S}_m^{(A)} + \dot{S}_A &= -\frac{1}{T_m}\frac{9}{4G}H\Upsilon_A(w_m+1)(w_m+\frac{1}{3}) + \frac{2\pi\Upsilon_A\dot{\Upsilon}_A}{G} \\ &= -\frac{1}{T_m}\frac{9}{4G}H\Upsilon_A(w_m+1)(w_m+\frac{1}{3}) + \frac{1}{T_A}\frac{3}{2G}H\Upsilon_A(w_m+1).\end{aligned} \tag{5.62}$$

In existing papers it is generally assumed that the apparent horizon would be in thermal equilibrium with the matter content and thus $T_A = T_m$ [16, 19–22, 24, 25], or occasionally less restrictively $T_m = bT_A$ (b = constant) [17, 18]. However, such assumptions are essentially mathematical tricks to simplify Eq.(5.62), while physically they are too problematic, so we directly move ahead from Eq.(5.62) without any artificial speculations relating T_A and T_m.

The GSL $\dot{S}_m^{(A)} + \dot{S}_A \geq 0$ could hold when $\frac{1}{T_A}\frac{3}{2G}H\Upsilon_A(w_m+1) \geq \frac{1}{T_m}\frac{9}{4G}H\Upsilon_A(w_m+1)(w_m+\frac{1}{3})$, and with $\{H, \Upsilon_A, T_A, T_m\} > 0$ it leads to

$$(w_m+1)\left(\frac{T_m}{T_A} - \frac{3}{2}(w_m+\frac{1}{3})\right) \geq 0\,, \tag{5.63}$$

or equivalently $(w_m+1)(T_m - \frac{3}{2}(w_m+\frac{1}{3})T_A) \geq 0$. Hence, for the apparent-horizon system the GSL trivially validates with $\dot{S}_m + \dot{S}_A \equiv 0$ under the dominance of the cosmological constant $w_m = -1$, and:

(1) For $-1 < w_m < -1/3$ which corresponds to an accelerated Universe dominated by quintessence, $\dot{S}_m + \dot{S}_A > 0$ always holds, because $T_m/T_A > 0$ and $\frac{3}{2}(w_m+\frac{1}{3}) < 0$ [or because both $\dot{S}_m > 0$ and $\dot{S}_A > 0$];

(2) For $-1/3 \leq w_m\,(\leq 1)$ which corresponds to ordinary-matter dominance respecting the strong energy condition $\rho_m + 3P_m \geq 0$ [40], the GSL $\dot{S}_m + \dot{S}_A \geq 0$ conditionally holds when

$$\frac{T_m}{T_A} \geq \frac{3}{2}(w_m+\frac{1}{3})\,; \tag{5.64}$$

(3) For the phantom domain $w_m < -1$, the GSL never validates because it requires $T_m/T_A \leq \frac{3}{2}(w_m+\frac{1}{3}) < 0$ which violates the the third law of thermodynamics.

5.5.6 GSL for the event-horizon system

Now consider the system made up of the cosmological event horizon and its interior. Unlike the apparent horizon, the entropy $S_{\rm E}$ and temperature $T_{\rm E}$ of the event horizon $\Upsilon_{\rm E}$ are unknown yet; one should not take it for granted that $\Upsilon_{\rm E}$ would still carry the Bekenstein–Hawking entropy $S_{\rm E} = A_{\rm E}/4G$ and further assume a Cai–Kim temperature $T_{\rm E} = 1/(2\pi\Upsilon_{\rm E})$ to it.

Considering that $S_{\rm E}$ would reflect the amount of Hubble-flow energy crossing an instantaneous event horizon $\Upsilon_{\rm E} = \Upsilon_{\rm E0}$, it is still safe to make use of the unified first law Eq.(5.22) and thus

$$T_{\rm E} dS_{\rm E} \;=\; \delta Q_{\rm E} \;=\, -dE\,\Big|_{\Upsilon_{\rm E0}} \;=\; A_{\rm E}\,(1+w_m)\rho_m\, H\Upsilon_{\rm E}\, dt\,. \tag{5.65}$$

Hence for the event horizon system we have

$$\begin{aligned} \dot{S}_m^{(\rm E)} + \dot{S}_{\rm E} \;&=\; \frac{1}{T_m}(1+w_m)\rho_m A_{\rm E} + \frac{1}{T_{\rm E}} A_{\rm E}(1+w_m)\rho_m H\Upsilon_{\rm E} \\ &=\; \rho_m A_{\rm E}(1+w_m)\Big(\frac{1}{T_m} + \frac{1}{T_{\rm E}}\frac{\Upsilon_{\rm E}}{\Upsilon_{\rm H}}\Big), \end{aligned} \tag{5.66}$$

where $\Upsilon_H := 1/H$ refers to the radius of the Hubble horizon [30, 43], an auxiliary scale where the recession speed would reach that of light ($c = 1$ in our units) by Hubble's law, and it is more instructive to write H as $1/\Upsilon_{\rm H}$ when compared with $\Upsilon_{\rm E}$ and $\Upsilon_{\rm A}$. Since $\{T_{\rm A}, T_{\rm E}, H, \Upsilon_{\rm E}\} > 0$, we pleasantly conclude from Eq.(5.66) without any unnatural assumption on $\{T_m, T_{\rm E}\}$ that:

Theorem 3 *The GSL $\dot{S}_m^{(E)} + \dot{S}_E \geq 0$ for the event horizon system always holds for an expanding Universe dominated by nonexotic matter $-1 \leq w_m\ (\leq 1)$.*

Note that Mazumder and Chakraborty have discussed GSLs for the event-horizon system in various dark-energy (and modified-gravity) models in [55, 56], where $S_{\rm E}$ is calculated by the unified first law and the importance of w_m is fully realized, although it is the weak rather than the dominant energy condition that is emphasized therein and the possibility of a Bekenstein–Hawking entropy for $\Upsilon_{\rm E}$ is not analyzed.

So far we have seen that though the apparent horizon $\Upsilon_{\rm A}$ is more compatible with the unified first law and the Clausius equation, the second law is better respected by the cosmic fluid inside the event horizon $\Upsilon_{\rm E}$ – this is because $\Upsilon_{\rm E}$ better captures the philosophical concept of "the whole Universe". For both horizons $\Upsilon_{\rm A}$ and $\Upsilon_{\rm E}$, the second law is better formulated than the GSL. Moreover, from the standpoint of the second laws and the GSLs, the phantom ($w_m < -1$) dark energy is definitely less favored than the cosmological constant ($w_m = -1$) and the quintessence ($-1 < w_m < -1/3$).

5.5.7 Bekenstein–Hawking entropy and Cai–Kim temperature for the event horizon?

The entropy of the event horizon $\Upsilon_{\rm E}$ has just been calculated from the unified fist law. Now let's return to the question: Can the Bekenstein–Hawking entropy and/or the Cai–Kim temperature be applied to $\Upsilon_{\rm E}$? With the assumption $S_{\rm E} = A_{\rm E}/4G$, Eq.(5.65) yields

$$T_{\rm E}\frac{2\pi\Upsilon_{\rm E}\dot{\Upsilon}_{\rm E}}{G} = T_{\rm E}\frac{2\pi\Upsilon_{\rm E}(H\Upsilon_{\rm E}-1)}{G} = A_{\rm E}(1+w_m)\rho_m H\Upsilon_{\rm E}, \tag{5.67}$$

which further leads to

$$(\Upsilon_{\rm E} - \Upsilon_{\rm H})\, T_{\rm E} \;=\; \frac{G}{2\pi}\, \rho_m A_{\rm E}(1 + w_m)\,. \tag{5.68}$$

An expanding FRW Universe always satisfies $\Upsilon_{\rm E} \geq \Upsilon_{\rm H}$, so the third law of thermodynamics $T_{\rm E} > 0$ requires $-1 \leq w_m \,(\leq 1)$; also, $\Upsilon_{\rm E} = \Upsilon_{\rm H}$ when $w_m = -1$ and $T_{\rm E}$ becomes unspecifiable from Eq.(5.68). Moreover, if $\Upsilon_{\rm E} = \Upsilon_{\rm H}$, then $a \int_t^\infty a^{-1} d\hat{t} = \frac{a}{\dot{a}}$, thus

$$\dot{a} \int_t^\infty a^{-1} d\hat{t} = 1 \quad \Rightarrow \quad \frac{\ddot{a}}{\dot{a}} - \frac{\dot{a}}{a} = 0 \quad \Rightarrow \quad a\ddot{a} = \dot{a}^2\,, \tag{5.69}$$

where we have taken the time derivative of the left-most integral expression. In the meantime, when $w_m = -1$ we have

$$\frac{\dot{a}^2 + k}{a^2} = \frac{8}{3}\pi G\rho_m \quad , \quad \frac{\ddot{a}}{a} = \frac{8}{3}\pi G\rho_m \quad \Rightarrow \quad a\ddot{a} = \dot{a}^2 + k. \tag{5.70}$$

Comparison of Eqs.(5.69) and (5.70) shows that in addition to $w_m = -1$, $\Upsilon_{\rm E} = \Upsilon_{\rm H}$ also requires $k = 0$; note that in case of the flat Universe, the apparent and the Hubble horizons coincide, $\Upsilon_{\rm A} = \Upsilon_{\rm H}$, so $T_{\rm E}$=$T_{\rm A}$ which remedies the failure of Eq.(5.68) at $w_m = -1$. Hence,

Corollary 2 *The validation of a Bekenstein–Hawking entropy on the cosmological event horizon requires that (i) the scale factor $a(t)$ satisfies the constraint Eq.(5.68), (ii) the dominant energy condition always holds, (iii) the event and Hubble horizons would coincide and the spatial curvature vanishes under the dominance of the cosmological constant.*

If one further assumes a Cai–Kim-like $T_{\rm E} = 1/(2\pi\Upsilon_{\rm E})$ for the event horizon, Eq.(5.68) would tell us that

$$G\rho_m A_{\rm E}\,(1 + w_m) + \frac{\Upsilon_{\rm H}}{\Upsilon_{\rm E}} \;=\; 1\,. \tag{5.71}$$

Does this constraint always hold? Since $\Upsilon_{\rm E} \geq \Upsilon_{\rm A}$, thus $\rho_m A_{\rm E} \geq \rho_m A_{\rm A} = \frac{3}{2G}$, with which Eq.(5.71) yields

$$\frac{3}{2}(1 + w_m) + \frac{\Upsilon_{\rm H}}{\Upsilon_{\rm E}} \;\leq\; 1\,. \tag{5.72}$$

This result can be rearranged into

$$w_m \;\leq -\frac{1}{3} - \frac{\Upsilon_{\rm H}}{\Upsilon_{\rm E}} \;< -\frac{1}{3}\,, \tag{5.73}$$

which, together with the requirement $-1 \leq w_m \,(\leq 1)$ from Eq.(5.68) for a generic positive $T_{\rm E}$, give rise to the condition $-1 \leq w_m < -1/3$. Hence,

Corollary 3 *In addition to a Bekenstein–Hawking entropy, the validation of a Cai–Kim temperature on the cosmological event horizon further requires the scale factor to satisfy Eq.(5.71), and restricts the FRW Universe to be dominated by the cosmological constant $w_m = -1$ or quintessence $-1 < w_m < -1/3$.*

Similar conditions hold for the past particle horizon as well. [54] has derived the GSL inequalities for the Hubble-, apparent-, particle- and event-horizon systems with the logamediate and intermediate scale factors by both the first law and the Bekenstein–Hawking formula, in which one could clearly observe that these two methods yield different results in the case of the event (and particle, Hubble) horizons.

Based on these considerations we argue that for consistency with the cosmic gravitational dynamics, the geometrically defined $A/4G$ only unconditionally holds on the apparent horizon $\Upsilon_{\rm A}$, which does not support the belief that the Bekenstein–Hawking entropy could validate for all horizons in GR (e.g. [14, 43]).

5.6 Gravitational thermodynamics in ordinary modified gravities

For the ΛCDM Universe within GR, we have re-studied the first and second laws of thermodynamics by requiring the consistency with the holographic-style dynamical equations (5.8), (5.9) and (5.11), which provides possible solutions to the long-standing temperature and entropy confusions. Following the clarification of the Cai–Kim temperature and the positive-heat-out sign convention, we will take this opportunity to extend the whole framework of gravitational thermodynamics to modified and alternative theories of relativistic gravity [57, 58]; also, this is partly a continuation of our earlier work in [64] where a unified formulation has been developed to derive the cosmological dynamical equations in modified gravities from (non)equilibrium thermodynamics.

For the generic Lagrangian density $\mathscr{L}_{\rm total} = \mathscr{L}_G(R, R_{\mu\nu}R^{\mu\nu}, \mathcal{R}_i\,, \vartheta\,, \nabla_\mu\vartheta\nabla^\mu\vartheta\,, \cdots) + 16\pi G\mathscr{L}_m$, where $\mathcal{R}_i = \mathcal{R}_i\,(g_{\alpha\beta}\,, R_{\mu\alpha\nu\beta}\,, \nabla_\gamma R_{\mu\alpha\nu\beta}\,, \dots)$ refers to a generic Riemannian invariant beyond the Ricci scalar and ϑ denotes a scalarial extra degree of freedom unabsorbed by $\mathscr{L}_m$, the field equation reads

$$H_{\mu\nu} = 8\pi G T^{(m)}_{\mu\nu} \quad \text{with} \quad H_{\mu\nu} := \frac{1}{\sqrt{-g}} \frac{\delta\left(\sqrt{-g}\,\mathscr{L}_G\right)}{\delta g^{\mu\nu}}\,, \tag{5.74}$$

where total-derivative/boundary terms should be removed in the derivation of $H_{\mu\nu}$. In the spirit of reconstructing the effective dark energy [63], Eq.(5.74) can be *intrinsically* recast into a compact GR form by isolating the $R_{\mu\nu}$ in $H_{\mu\nu}$:

$$G_{\mu\nu} \equiv R_{\mu\nu} - \frac{1}{2}R g_{\mu\nu} = 8\pi G_{\rm eff} T^{(\rm eff)}_{\mu\nu} \quad \text{with} \quad H_{\mu\nu} = \frac{G}{G_{\rm eff}} G_{\mu\nu} - 8\pi G T^{(\rm MG)}_{\mu\nu}\,, \tag{5.75}$$

where $T^{(\rm eff)}_{\mu\nu} = T^{(m)}_{\mu\nu} + T^{(\rm MG)}_{\mu\nu}$, and all terms beyond GR have been packed into $T^{(\rm MG)}_{\mu\nu}$ and $G_{\rm eff}$. Here $T^{(\rm MG)}_{\mu\nu}$ collects the modified-gravity nonlinear and higher-order effects, while $G_{\rm eff}$ denotes the effective gravitational coupling strength which can be directly recognized from the coefficient of the matter tensor $T^{(m)}_{\mu\nu}$ – for example, as will be shown in Sec.5.6.8, we have $G_{\rm eff} = G/f_R$ for $f(R)$, $G_{\rm eff} = GE(\phi)/F(\phi)$ for scalar-tensor-chameleon, $G_{\rm eff} = G/\phi$ for Brans-Dicke, $G_{\rm eff} = G/(1 + 2aR)$ for quadratic, and $G_{\rm eff} = G$ for dynamical Chern-Simons gravities. Moreover, $T^{(\rm eff)}_{\mu\nu}$ is assumed to be an effective perfect-fluid content,

$$T^{\mu\,(\rm eff)}_{\ \nu} = \text{diag}\left[-\rho_{\rm eff}, P_{\rm eff}, P_{\rm eff}, P_{\rm eff}\right] \quad \text{with} \quad P_{\rm eff}/\rho_{\rm eff} =: w_{\rm eff}, \tag{5.76}$$

along with $\rho_{\rm eff} = \rho_m + \rho_{(\rm MG)}$ and $P_{\rm eff} = P_m + P_{(\rm MG)}$.

Modified gravities aim to explain the cosmic acceleration without dark-energy components, so in this section we will assume the physical matter to respect the null, weak, strong and dominant energy conditions [40], which yield $\rho_m > 0$ and $-1/3 \le w_m \le 1$. This way, the quintessence ($-1 < w_m < -1/3$), the cosmological constant ($w_m = -1$) and the most exotic phantom ($w_m < -1$) are ruled out.

5.6.1 Holographic-style dynamical equations in modified gravities

Substituting the FRW metric Eq.(5.1) and the effective cosmic fluid Eq.(5.76) into the field equation (5.75), one could obtain the modified Friedmann equations

$$
\begin{aligned}
H^2 + \frac{k}{a^2} = \frac{8\pi G_{\text{eff}}}{3}\rho_{\text{eff}} \quad \text{and} \\
\dot{H} - \frac{k}{a^2} = -4\pi G_{\text{eff}}(1 + w_{\text{eff}})\rho_{\text{eff}} = -4\pi G_{\text{eff}} h_{\text{eff}} \\
\text{or} \quad 2\dot{H} + 3H^2 + \frac{k}{a^2} = -8\pi G_{\text{eff}} P_{\text{eff}},
\end{aligned}
\tag{5.77}
$$

where $h_{\text{eff}} := (1 + w_{\text{eff}})\rho_{\text{eff}}$ denotes the effective enthalpy density. With Eqs. (5.4) and (5.5), substituting the apparent-horizon radius Υ_A and its kinematic time-derivative $\dot{\Upsilon}_A$ into Eq.(5.77), the Friedmann equations can be rewritten into

$$\Upsilon_A^{-2} = \frac{8\pi G_{\text{eff}}}{3}\rho_{\text{eff}} \tag{5.78}$$

$$\dot{\Upsilon}_A = 4\pi H \Upsilon_A^3 G_{\text{eff}}(1 + w_{\text{eff}})\rho_{\text{eff}} \tag{5.79}$$

$$= \frac{3}{2} H \Upsilon_A (1 + w_{\text{eff}}) \tag{5.80}$$

$$\Upsilon_A^{-3}\left(\dot{\Upsilon}_A - \frac{3}{2} H \Upsilon_A\right) = 4\pi G_{\text{eff}} H P_{\text{eff}}, \tag{5.81}$$

along with $A_A \rho_{\text{eff}} = \frac{3}{2G_{\text{eff}}}$. Similar to Eqs.(5.8)-(5.12) for ΛCDM of GR, Eqs.(5.78)-(5.81) constitute the full set of FRW holographic-style gravitational equations for modified gravities of the form Eq.(5.75).

5.6.2 Unified first law of nonequilibrium thermodynamics

Following our previous work [64], to geometrically reconstruct the effective total internal energy E_{eff}, one just needs to replace Newton's constant G by G_{eff} in the standard Misner-Sharp or Hawking mass used in Sec. 5.3.1, which yields

$$E_{\text{eff}} = \frac{1}{2G_{\text{eff}}} \frac{\Upsilon^3}{\Upsilon_A^2}. \tag{5.82}$$

The total derivative of $E_{\text{eff}} = E_{\text{eff}}(t, r)$ along with the holographic-style dynamical equations (5.78), (5.79) and (5.81) yield

$$dE_{\text{eff}} = -\frac{1}{G_{\text{eff}}} \frac{\Upsilon^3}{\Upsilon_A^3}\left(\dot{\Upsilon}_A - \frac{3}{2} H \Upsilon_A\right) dt + \frac{3}{2G_{\text{eff}}} \frac{\Upsilon^2}{\Upsilon_A^2} a dr - \frac{\dot{G}_{\text{eff}}}{2G_{\text{eff}}^2} \frac{\Upsilon^3}{\Upsilon_A^2} dt \tag{5.83}$$

$$= -A \Upsilon H P_{\text{eff}} dt + A \rho_{\text{eff}} a dr - V \frac{\dot{G}_{\text{eff}}}{G_{\text{eff}}} \rho_{\text{eff}} dt. \tag{5.84}$$

By the replacement $adr = d\Upsilon - H\Upsilon dt$, Eqs.(5.83) and (5.84) can be recast into the (t, Υ) transverse coordinates as

$$\begin{aligned} dE_{\text{eff}} &= -\frac{\dot{\Upsilon}_{\text{A}}}{G_{\text{eff}}}\frac{\Upsilon^3}{\Upsilon_{\text{A}}^3}dt + \frac{3}{2G_{\text{eff}}}\frac{\Upsilon^2}{\Upsilon_{\text{A}}^2}d\Upsilon - \frac{\dot{G}_{\text{eff}}}{2G_{\text{eff}}^2}\frac{\Upsilon^3}{\Upsilon_{\text{A}}^2}dt && (5.85)\\ &= -A(1+w_{\text{eff}})\rho_{\text{eff}}H\Upsilon dt + A\rho_{\text{eff}}d\Upsilon - V\frac{\dot{G}_{\text{eff}}}{G_{\text{eff}}}\rho_{\text{eff}}dt. && (5.86)\end{aligned}$$

Both Eqs.(5.84) and (5.86) can be compactified into the thermodynamic equation

$$dE_{\text{eff}} = A\Psi + \mathcal{W}dV + \mathcal{E}, \tag{5.87}$$

where $\mathcal{W}$ and Ψ respectively refer to the effective work density and the effective energy supply covector,

$$\mathcal{W} = \frac{1}{2}(1-w_{\text{eff}})\rho_{\text{eff}}, \tag{5.88}$$

$$\begin{aligned}\Psi &= -\frac{1}{2}(1+w_{\text{eff}})\rho_{\text{eff}}H\Upsilon dt + \frac{1}{2}(1+w_{\text{eff}})\rho_{\text{eff}}adr\\ &= -(1+w_{\text{eff}})\rho_{\text{eff}}H\Upsilon dt + \frac{1}{2}(1+w_{\text{eff}})\rho_{\text{eff}}d\Upsilon, && (5.89)\end{aligned}$$

and similar to Sec. 5.3.1, $\mathcal{W}$ and Ψ can trace back to the Hayward-type invariants $\mathcal{W} := -\frac{1}{2}T^{\alpha\beta}_{(\text{eff})}h_{\alpha\beta}$ and $\Psi_\alpha := T_{\alpha(\text{eff})}^{\ \ \beta}\partial_\beta\Upsilon + \mathcal{W}\partial_\alpha\Upsilon$ under spherical symmetry. The $\mathcal{E}$ in Eq.(5.87) is an extensive energy term

$$\mathcal{E} := -V\frac{\dot{G}_{\text{eff}}}{G_{\text{eff}}}\rho_{\text{eff}}\, dt. \tag{5.90}$$

As will be shown in the next subsection, $\mathcal{E}$ contributes to the irreversible extra entropy production, so we regard Eq.(5.87) as the unified first law of *nonequilibrium* thermodynamics [64], which is an extension of the equilibrium version Eq.(5.23) in GR. Moreover, it follows from the contracted Bianchi identities and Eq.(5.75) that $\nabla_\mu G^\mu{}_\nu = 0 = 8\pi\nabla_\mu(G_{\text{eff}}T^{\mu(\text{eff})}_{\nu})$, and for the FRW metric Eq.(5.1) it leads to

$$\dot{\rho}_{\text{eff}} + 3H(\rho_{\text{eff}} + P_{\text{eff}}) = \frac{\dot{\mathcal{E}}}{V} = -\frac{\dot{G}_{\text{eff}}}{G_{\text{eff}}}\rho_{\text{eff}}, \tag{5.91}$$

so $\mathcal{E}$ also shows up in the generalized continuity equation as a density dissipation effect.

5.6.3 Nonequilibrium Clausius equation on the horizon

The holographic-style dynamical equation (5.79) can be slightly rearranged into $\frac{\dot{\Upsilon}_{\text{A}}}{G_{\text{eff}}}dt = A_{\text{A}}(1+w_{\text{eff}})\rho_{\text{eff}}H\Upsilon_{\text{A}}dt$, so we have

$$\begin{aligned}&\frac{1}{2\pi\Upsilon_{\text{A}}}\cdot 2\pi\Upsilon_{\text{A}}\left(\frac{\dot{\Upsilon}_{\text{A}}}{G_{\text{eff}}}dt - \frac{1}{2}\Upsilon_{\text{A}}\frac{\dot{G}_{\text{eff}}}{G_{\text{eff}}^2}dt\right) + \frac{1}{2\pi\Upsilon_{\text{A}}}\cdot 2\pi\Upsilon_{\text{A}}\left(\frac{1}{2}\Upsilon_{\text{A}}\frac{\dot{G}_{\text{eff}}}{G_{\text{eff}}^2}dt + V_{\text{A}}\frac{\dot{G}_{\text{eff}}}{G_{\text{eff}}}\rho_{\text{eff}}dt\right)\\ &\qquad = A_{\text{A}}(1+w_{\text{eff}})\rho_{\text{eff}}H\Upsilon_{\text{A}}dt + V_{\text{A}}\frac{\dot{G}_{\text{eff}}}{G_{\text{eff}}}\rho_{\text{eff}}dt.\end{aligned} \tag{5.92}$$

It can be formally compactified into the thermodynamic relation

$$T_{\rm A}\left(dS_{\rm A}+d_pS^{\rm (A)}\right)=-(A_{\rm A}\Psi_t+\mathcal{E}_{\rm A})=-dE^{\rm A}_{\rm eff}\Big|_{d\Upsilon=0},\tag{5.93}$$

where Ψ_t is just the t-component of the covector Ψ in Eq.(5.89), $\mathcal{E}_{\rm A}$ is the energy dissipation term Eq.(5.90) evaluated at $\Upsilon_{\rm A}$, and $T_{\rm A}=\frac{1}{2\pi\Upsilon_{\rm A}}$ denotes the Cai–Kim temperature on $\Upsilon_{\rm A}$. Here $S_{\rm A}$ refers to the geometrically defined Wald entropy [65] for the dynamical apparent horizon,

$$S_{\rm A}\;=\;\frac{\pi\Upsilon_{\rm A}^2}{G_{\rm eff}}\;=\;\frac{A_{\rm A}}{4G_{\rm eff}}=\int\frac{dA_{\rm A}}{4G_{\rm eff}},\tag{5.94}$$

where $S_{\rm A}$ takes such a compact form due to $\Upsilon_{\rm A}=\Upsilon_{\rm A}(t)$ and $G_{\rm eff}=G_{\rm eff}(t)$ under the maximal spatial symmetry of the Universe, while $d_pS^{\rm (A)}$ represents the irreversible entropy production within $\Upsilon_{\rm A}$

$$\begin{aligned}d_pS^{\rm (A)}&=2\pi\Upsilon_{\rm A}\left(\frac{1}{2}\Upsilon_{\rm A}\frac{\dot G_{\rm eff}}{G_{\rm eff}^2}dt+V_{\rm A}\frac{\dot G_{\rm eff}}{G_{\rm eff}}\rho_{\rm eff}dt\right)\\&=2\pi\Upsilon_{\rm A}^2\frac{\dot G_{\rm eff}}{G_{\rm eff}^2}dt,\end{aligned}\tag{5.95}$$

where we have applied the following replacement

$$\frac{1}{2}\Upsilon_{\rm A}\frac{\dot G_{\rm eff}}{G_{\rm eff}^2}\;=\;V_{\rm A}\frac{\dot G_{\rm eff}}{G_{\rm eff}}\rho_{\rm eff},\tag{5.96}$$

whose validity is guaranteed by Eq.(5.78). Due to the extra entropy production element $d_pS^{\rm (A)}$, we regard Eq.(5.93) as the *nonequilibrium* Clausius equation, which depicts the heat transfer plus the extensive energy dissipation for the isochoric process of an arbitrary instantaneous $\Upsilon_{\rm A}$. With the nonequilibrium unified first law Eq.(5.87), Eq.(5.93) can be completed into the total energy differential

$$\begin{aligned}dE^{\rm A}_{\rm eff}\;&=\;A_{\rm A}\Psi_tdt+A_{\rm A}\left(\Psi_\Upsilon+\mathcal{W}\right)d\Upsilon_{\rm A}+\mathcal{E}_{\rm A}\\&=-T_{\rm A}(dS_{\rm A}+d_pS^{\rm (A)})+\rho_{\rm eff}dV_{\rm A}.\end{aligned}\tag{5.97}$$

5.6.4 The second law for the interiors of the apparent and the event horizons

For the cosmic entropy evolution, the second law of thermodynamics should still apply to the physical matter content $\{\rho_m,P_m\}$ rather than the mathematically effective $\{\rho_{\rm eff},P_{\rm eff}\}$. Under *minimal* geometry-matter couplings, the Noether compatible definition of $T^{(m)}_{\mu\nu}$ automatically guarantees $\nabla^\mu T^{(m)}_{\mu\nu}=0$, so the total continuity equation (5.91) can be decomposed into the ordinary one for the physical matter and the remaining part for the modified-gravity effect [64]:

$$\begin{aligned}&\dot\rho_m+3H(\rho_m+P_m)=0\\&\dot\rho_{\rm (MG)}+3H\Big(\rho_{\rm (MG)}+P_{\rm (MG)}\Big)=-\frac{\dot G_{\rm eff}}{G_{\rm eff}}\Big(\rho_m+\rho_{\rm (MG)}\Big).\end{aligned}\tag{5.98}$$

For the physical energy $E_m=\rho_mV=E_{\rm eff}-\rho_{\rm (MG)}V$ within an arbitrary volume, the positive-heat-out Gibbs equation (5.54) still yields $T_mdS_m=-d(\rho_mV)-P_mdV=-Vd\rho_m-(\rho_m+P_m)dV$, which together with

Eq.(5.98) leads to

$$T_m dS_m = 3H(\rho_m + P_m)Vdt - (\rho_m + P_m)Ad\Upsilon = \rho_m A(1+w_m)(H\Upsilon dt - d\Upsilon). \tag{5.99}$$

Hence, for the physical entropy $S_m^{(\mathrm{A})}$ inside the apparent horizon $\Upsilon_\mathrm{A}(t)$, Eq.(5.99) and the holographic-style dynamical equation (5.80) yield

$$\begin{aligned} T_m dS_m^{(\mathrm{A})} &= \rho_m A_\mathrm{A}(1+w_m)(\Upsilon_\mathrm{A} H - \dot{\Upsilon}_\mathrm{A})dt \\ &= -\frac{3}{2}\rho_m A_\mathrm{A}(1+w_m)H\Upsilon_\mathrm{A}(\frac{1}{3} + w_\mathrm{eff})dt \\ &= -\frac{9}{2}\rho_m V_\mathrm{A} H(1+w_m)(\frac{1}{3} + w_\mathrm{eff})dt. \end{aligned} \tag{5.100}$$

where $\rho_m A_\mathrm{A}$ cannot be simplified by Eq.(5.10) of GR. Recall that $-1/3 \le w_m \le 1$ in modified gravities, thus:

Theorem 4 *The physical entropy $S_m^{(A)}$ inside the cosmological apparent horizon satisfies $\dot{S}_m^{(A)} \ge 0$ only when $w_{eff} \le -1/3$.*

Moreover, inside the event horizon $\Upsilon_\mathrm{E}(t)$, Eq.(5.99) along with $\dot{\Upsilon}_\mathrm{E} = H\Upsilon_\mathrm{E} - 1$ give rise to

$$\begin{aligned} T_m dS_m^{(\mathrm{E})} &= \rho_m A_\mathrm{E}(1+w_m)(H\Upsilon_\mathrm{E} - \dot{\Upsilon}_\mathrm{E})dt \\ &= \rho_m A_\mathrm{E}(1+w_m)dt. \end{aligned} \tag{5.101}$$

Hence, for the FRW Universe governed by modified gravities and filled with ordinary matter $-1/3 \le w_m \le 1$:

Theorem 5 *The physical entropy $S_m^{(E)}$ inside the cosmological event horizon always satisfies $\dot{S}_m^{(E)} > 0$ regardless of the modified-gravity theories in use.*

5.6.5 GSL for the apparent-horizon system

Unlike the standard second law for the matter content $\{\rho_m, P_m\}$, GSLs further involve the modified-gravity effects $\{\rho_{(\mathrm{MG})}, P_{(\mathrm{MG})}\}$ which influence the horizon entropy. Compared with the ΛCDM situation in Sec. 5.5.5, there are three types of entropy for the apparent-horizon system in modified gravities: the physical $S_m^{(\mathrm{A})}$ for the internal matter content, the Wald entropy S_A of the horizon Υ_A, and the nonequilibrium extensive entropy production. From Eqs.(5.93) and (5.100), we have

$$\begin{aligned} &\dot{S}_m^{(\mathrm{A})} + \dot{S}_\mathrm{A} + \dot{S}_p^{(\mathrm{A})} \\ =& -\frac{1}{T_m}\frac{3}{2}\rho_m A_\mathrm{A}(1+w_m)H\Upsilon_\mathrm{A}(\frac{1}{3} + w_\mathrm{eff}) + \frac{2\pi\Upsilon_\mathrm{A}\dot{\Upsilon}_\mathrm{A}}{G_\mathrm{eff}} + \pi\Upsilon_\mathrm{A}^2\frac{\dot{G}_\mathrm{eff}}{G_\mathrm{eff}^2} \\ =& \frac{3}{2}\frac{\Upsilon_\mathrm{A}}{\Upsilon_\mathrm{H}}\left(-\frac{1}{T_m}\rho_m A_\mathrm{A}(1+w_m)(\frac{1}{3} + w_\mathrm{eff}) + \frac{1}{T_\mathrm{A}}\frac{1}{G_\mathrm{eff}}(1+w_\mathrm{eff}) + \frac{1}{T_\mathrm{A}}\frac{1}{3H}\frac{\dot{G}_\mathrm{eff}}{G_\mathrm{eff}^2}\right), \end{aligned} \tag{5.102}$$

where $\dot{S}_p^{(\mathrm{A})} := d_p S^{(\mathrm{A})}/dt$, $T_\mathrm{A} = 1/(2\pi\Upsilon_\mathrm{A})$, and $\dot{\Upsilon}_\mathrm{A} = \frac{3}{2}H\Upsilon_\mathrm{A}(1+w_\mathrm{eff})$. Generally the GSL for the apparent-horizon system does not hold because the region $\Upsilon \le \Upsilon_\mathrm{A}$ only comprises a finite portion of the Universe and is thermodynamically open with the absolute Hubble flow crossing $\Upsilon_{\rm A}$. However, Eq.(5.102) shows that $\dot{S}_m^{(\rm A)} + \dot{S}_{\rm A} + \dot{S}_p^{(\rm A)} \geq 0$ could validate when

$$\frac{T_m}{T_{\rm A}}\left(\frac{1+w_{\rm eff}}{G_{\rm eff}} + \frac{1}{3H}\frac{\dot{G}_{\rm eff}}{G_{\rm eff}^2}\right) \geq \rho_m A_{\rm A}(1+w_m)(\frac{1}{3}+w_{\rm eff}), \tag{5.103}$$

where $A_{\rm A}$ cannot be further replaced by $1/(\pi T_{\rm A}^2)$ to nonlinearize $T_{\rm A}$ since $T_{\rm A}$ is not an extensive quantity. Specifically for equilibrium theories with $G_{\rm eff}$ = constant, like the dynamical Chern-Simons gravity [61, 64], Eq.(5.103) reduces to become

$$(1+w_{\rm eff})\frac{T_m}{T_{\rm A}} \geq \rho_m A_{\rm A} G(1+w_m)(\frac{1}{3}+w_{\rm eff}), \tag{5.104}$$

which appears analogous to Eq.(5.63) of ΛCDM.

For the apparent-horizon GSL, these results have matured the pioneering investigations in [18] for generic modified gravities and other earlier results in e.g. [22, 24] for specific gravity theories by the nonequilibrium revision of the unified first law, selection of the Cai–Kim temperature, dropping of the artificial assumption $T_m = \mathcal{T}_{\rm A}^{(+)}$, and discovery of the explicit expression for the entropy production $d_p S^{(\rm A)}$.

5.6.6 GSL for the event-horizon system

For the event-horizon system, $dS_{\rm E} + d_p S^{(\rm E)}$ should be directly determined by the nonequilibrium unified first law Eq.(5.86),

$$\begin{aligned} &T_{\rm E}\left(dS_{\rm E} + d_p S^{(\rm E)}\right) \\ =&\delta Q_{(\rm E)} = -dE_{\rm eff}^{(\rm E)}\big|_{\Upsilon_{\rm E0}} = -(A_{\rm E}\Psi_t + \mathcal{E}_{\rm E}) \\ =&A_{\rm E}(1+w_{\rm eff})\rho_{\rm eff} H \Upsilon_{\rm E} dt + V_{\rm E}\frac{\dot{G}_{\rm eff}}{G_{\rm eff}}\rho_{\rm eff} dt. \end{aligned} \tag{5.105}$$

Then Eqs.(5.101) and (5.105) yield

$$\dot{S}_m^{(\rm E)} + \dot{S}_{\rm E} + \dot{S}_p^{(\rm E)} = \frac{1}{T_m}\rho_m A_{\rm E}(1+w_m) + \frac{1}{T_{\rm E}}\left(A_{\rm E}(1+w_{\rm eff})\rho_{\rm eff} H\Upsilon_{\rm E} + V_{\rm E}\frac{\dot{G}_{\rm eff}}{G_{\rm eff}}\rho_{\rm eff}\right). \tag{5.106}$$

Inspired by the validity of the event-horizon GSL for Sec. 5.5.6 and the standard second law Eq.(5.101), we a priori anticipate $\dot{S}_m^{(\rm E)} + \dot{S}_{\rm E} + \dot{S}_p^{(\rm E)} \geq 0$ to hold, which imposes the following viability constraint to modified gravities

$$\frac{T_m}{T_{\rm E}}\left((1+w_{\rm eff})H + \frac{\dot{G}_{\rm eff}}{G_{\rm eff}}\right)\rho_{\rm eff} \geq -\rho_m(1+w_m)\Upsilon_{\rm E}^{-1}. \tag{5.107}$$

Considering that $-1/3 \leq w_m \leq 1$, its right hand side is negative definite, so a sufficient (yet not necessary) condition to validate the GSL is

$$\left((1+w_{\rm eff})H + \frac{\dot{G}_{\rm eff}}{G_{\rm eff}}\right)\rho_{\rm eff} \geq 0. \tag{5.108}$$

These results improve the earlier investigations in e.g. [56] for the event-horizon GSL in modified gravities.

Note that the discussion in Sec. 5.6.3 is based on the holographic-style gravitational equations and only applies to the apparent-horizon system; if presuming a Wald entropy $A_{\rm E}/4G_{\rm eff}$ and employing the entropy production to balance all differential terms involving the evolution effect $\dot{G}_{\text{eff}}$, one would obtain

$$T_{\text{E}}\left(dS_{\text{E}}+d_pS^{(\text{E})}\right)=\left(T_{\text{E}}\frac{2\pi\Upsilon_{\text{E}}\dot{\Upsilon}_{\text{E}}}{G_{\text{eff}}}+V_{\text{E}}\frac{\dot{G}_{\text{eff}}}{G_{\text{eff}}}\rho_{\text{eff}}\right)dt, \tag{5.109}$$

with $d_pS^{(\text{E})}$ specified as

$$d_pS^{(\text{E})}=\left(T_{\text{E}}A_{\text{E}}\frac{\dot{G}_{\text{eff}}}{4G_{\text{eff}}^2}+V_{\text{E}}\frac{\dot{G}_{\text{eff}}}{G_{\text{eff}}}\rho_{\text{eff}}\right)dt. \tag{5.110}$$

Comparison of Eqs.(5.105) and (5.109) yields the condition

$$T_{\text{E}}\frac{2\pi\Upsilon_{\text{E}}(H\Upsilon_{\text{E}}-1)}{G_{\text{eff}}}=A_{\text{E}}(1+w_{\text{eff}})\rho_{\text{eff}}H\Upsilon_{\text{E}}, \tag{5.111}$$

and thus the whole discussion in Sec. 5.5.7 for ΛCDM can be parallelly applied to modified gravities with $G\mapsto G_{\text{eff}}$, $\rho_m\mapsto\rho_{\text{eff}}$ and $w_m\mapsto w_{\text{eff}}$, which again implies that the entropy $A/4G_{\text{eff}}$ and the Cai–Kim temperature $1/(2\pi\Upsilon)$ only unconditionally hold on the cosmological event horizon.

5.6.7 A note on existing methods of GSL

Existent papers on GSL of modified gravities (in the traditional positive-heat-in Gibbs equation $T_m d\widehat{S}_m = dE + P_m dV$) usually replace $\rho_m + P_m$ by $\widetilde{\rho}_{(\text{MG})}+\widetilde{P}_{(\text{MG})}$ in Eq.(5.99), with $\{\widetilde{\rho}_{(\text{MG})},\widetilde{P}_{(\text{MG})}\}$ set up in the field equation involving both Newton's constant G and the dynamic G_{eff}:

$$R_{\mu\nu}-\frac{1}{2}Rg_{\mu\nu}=8\pi G\widetilde{T}_{\mu\nu}^{(\text{eff})}=8\pi G\left(\widetilde{T}_{\mu\nu}^{(m)}+\widetilde{T}_{\mu\nu}^{(\text{MG})}\right), \tag{5.112}$$

where $\widetilde{T}^{\mu(\text{eff})}_{\ \nu}=\text{diag}\left[-\widetilde{\rho}_{\text{eff}},\widetilde{P}_{\text{eff}},\widetilde{P}_{\text{eff}},\widetilde{P}_{\text{eff}}\right]$, $\widetilde{\rho}_{\text{eff}}=\widetilde{\rho}_m+\widetilde{\rho}_{(\text{MG})}$, $\widetilde{P}_{\text{eff}}=\widetilde{P}_m+\widetilde{P}_{(\text{MG})}$, and the tilde ∼ means that the possibly dynamical aspect of G_{eff} in Eq.(5.75) has been absorbed into $\widetilde{T}_{\mu\nu}^{(\text{eff})}$ to formally maintain a constant coupling strength G; also note that for these tilded quantities the conservation equation becomes $\dot{\tilde{\rho}}_{\text{eff}}+3H\left(\tilde{\rho}_{\text{eff}}+\tilde{P}_{\text{eff}}\right)=0$ and $\dot{\rho}_m+3H(\rho_m+P_m)=0$ under minimal coupling (an energy exchange term between ρ_m and $\widetilde{\rho}_{(\text{MG})}$ was analyzed for minimal $f(R)$ gravity in [25], which however should be a feature of non-minimal coupling). This way, for the apparent-horizon system with $T_m\dot{\widehat{S}}_m=4\pi\Upsilon_{\text{A}}^2(\rho_m+P_m)\left(\Upsilon_{\text{A}}-H\dot{\Upsilon}_{\text{A}}\right)dt$, one would have the GSL (e.g. [22, 24, 25] for the $F(R,\mathcal{G})$, scalar-tensor-chameleon and interacting $f(R)$ gravities)

$$\dot{\widehat{S}}_m^{(\text{A})}+\dot{S}_{\text{A}}=\frac{1}{T_m}\frac{G}{G_{\text{eff}}}\left(\frac{\dot{\Upsilon}_{\text{A}}}{GH\Upsilon_{\text{A}}}-4\pi\Upsilon_{\text{A}}^2\left(\widetilde{\rho}_{(\text{MG})}+\widetilde{P}_{(\text{MG})}\right)\right)\left(\dot{\Upsilon}_{\text{A}}-\Upsilon_{\text{A}}H\right)+\frac{2\pi\Upsilon_{\text{A}}\dot{\Upsilon}_{\text{A}}}{G_{\text{eff}}}, \tag{5.113}$$

where G_{eff} is recognized from the coefficient of $G\widetilde{\rho}_m=G_{\text{eff}}\rho_m$ to utilize the Wald entropy $S_{\text{A}}=A_{\text{A}}/4G_{\text{eff}}$. In Eq.(5.113) we have incorporated the holographic-style gravitational equations [simply Eqs.(5.78)-(5.81) with $G_{\text{eff}}\mapsto G$ and $\rho_{\text{eff}}\mapsto\widetilde{\rho}_{\text{eff}}$, $P_{\text{eff}}\mapsto\widetilde{P}_{\text{eff}}$] for compactness, as well as the relation

$$\rho_m+P_m=\frac{G}{G_{\text{eff}}}\left(\widetilde{\rho}_m+\widetilde{P}_m\right). \tag{5.114}$$

However, Eq.(5.113) is not self-consistent, not just for the conflicting sign conventions encoded in $\widehat{S}_m^{(\text{A})}$ and S_{A}, but also because it uses two different coupling strength for $\{\widehat{S}_m^{(\text{A})},S_{\text{A}}\}$, and fails to capture the extra entropy production $d_p S^{(\mathrm{A})}$ which arises in all modified gravities with nontrivial G_{eff} [64, 67]. To overcome these flaws in this popular method, the adjusted Gibbs equation (5.54) along with the setups in Eqs.(5.75, 5.76) and the holographic-style Eqs.(5.78)-(5.81) lead to

$$\begin{aligned} T_m \dot{S}_m &= -\frac{1}{G_{\text{eff}}}\left(\frac{\dot{\Upsilon}_{\mathrm{A}}}{H\Upsilon_{\mathrm{A}}} - 4\pi\Upsilon_{\mathrm{A}}^2 G_{\text{eff}}\big(\rho_{(\mathrm{MG})} + P_{(\mathrm{MG})}\big)\right)\left(\dot{\Upsilon}_{\mathrm{A}} - \Upsilon_{\mathrm{A}} H\right) \\ &= -\frac{H\Upsilon_{\mathrm{A}}^5}{G_{\text{eff}}}\left(\dot{H} - \frac{k}{a^2} + 4\pi G_{\text{eff}}\big(\rho_{(\mathrm{MG})} + P_{(\mathrm{MG})}\big)\right)\left(\dot{H} + H^2\right), \end{aligned} \tag{5.115}$$

which together with Eq.(5.93) yields

$$\dot{S}_m^{(\mathrm{A})} + \dot{S}_{\mathrm{A}} + \dot{S}_p^{(\mathrm{A})} = -\frac{H\Upsilon_{\mathrm{A}}^5}{G_{\text{eff}}}\left(\dot{H} - \frac{k}{a^2} + 4\pi G_{\text{eff}}\big(\rho_{(\mathrm{MG})} + P_{(\mathrm{MG})}\big)\right)\left(\dot{H} + H^2\right) + \frac{2\pi\Upsilon_{\mathrm{A}}\dot{\Upsilon}_{\mathrm{A}}}{G_{\text{eff}}} + \pi\Upsilon_{\mathrm{A}}^2\frac{\dot{G}_{\text{eff}}}{G_{\text{eff}}^2}. \tag{5.116}$$

Eq.(5.116) improves Eq.(5.113) into a totally self-consistent and more natural method that employs a single gravitational coupling strength G_{eff} in accordance with the standard entropy $A_{\mathrm{A}}/4G_{\text{eff}}$. The approach by Eq.(5.116) looks more concentrative on $\{\rho_{(\mathrm{MG})}, P_{(\mathrm{MG})}\}$ of the modified-gravity effects; however, it has implicitly ignored the nonexotic character of the cosmic fluid $\rho_m + 3P_m \geq 0$, and complicated the mathematical calculations. Hence, in this paper we have chosen to work with Eqs.(5.100, 5.102) rather than Eqs.(5.115, 5.116) for the apparent-horizon system, and similarly Eq.(5.101, 5.106) for the event-horizon system.

5.6.8 Applications to concrete modified gravities

The formulation of gravitational thermodynamics in this section applies to all ordinary modified gravities of the form Eq.(5.75). One can just reverse the process and logic in [64] to see the detailed applications of the first laws for different gravity theories, and in this paper we will focus on the concretization of the second laws, for which we have drawn the following generic conclusions:

(1) $\dot{S}_m^{(\mathrm{E})} > 0$ always holds, while $\dot{S}_m^{(\mathrm{A})} \geq 0$ when $w_{\text{eff}} \leq -1/3$;

(2) $\dot{S}_m^{(\mathrm{E})} + \dot{S}_{\mathrm{E}} + \dot{S}_p^{(\mathrm{E})} \geq 0$ should hold with Eq.(5.107) as a validity constraint for modified gravities, while $\dot{S}_m^{(\mathrm{A})} + \dot{S}_{\mathrm{A}} + \dot{S}_p^{(\mathrm{A})} \geq 0$ could conditionally hold only when Eq.(5.103) is satisfied.

To concretize these conditions, one just needs to find out the effective gravitational coupling strength G_{eff}, the effective EoS parameter

$$\begin{aligned} w_{\text{eff}} &= \frac{(P_{\text{eff}} + \rho_{\text{eff}}) - \rho_{\text{eff}}}{\rho_{\text{eff}}} \\ &= -1 + \frac{(1 + w_m)\rho_m + \big(\rho_{(\mathrm{MG})} + P_{(\mathrm{MG})}\big)}{\rho_m + \rho_{(\mathrm{MG})}}, \end{aligned} \tag{5.117}$$

the "modified-gravity energy density" $\rho_{(\mathrm{MG})}$, and $\rho_{(\mathrm{MG})} + P_{(\mathrm{MG})}$.

$f(R)$ gravity

For the FRW Universe governed by the $\mathscr{L} = f(R) + 16\pi G\mathscr{L}_m$ gravity [59], we have $G_{\rm eff} = G/f_R$ and [64]

$$\rho_{\rm (MG)} = \frac{1}{8\pi G}\Big(\frac{1}{2}f_R R - \frac{1}{2}f - 3H\dot{f}_R\Big) \tag{5.118}$$

$$\rho_{\rm (MG)} + P_{\rm (MG)} = \frac{1}{8\pi G}\Big(\ddot{f}_R - H\dot{f}_R\Big) \tag{5.119}$$

$$w_{\rm eff} = -1 + \frac{8\pi G(1+w_m)\rho_m + \ddot{f}_R - H\dot{f}_R}{8\pi G\rho_m + \frac{1}{2}f_R R - \frac{1}{2}f - 3H\dot{f}_R}. \tag{5.120}$$

The GSL for the event-horizon system requires $f(R)$ gravity to respect the following viability condition

$$\frac{T_m}{T_{\rm E}}\left(\frac{8\pi G(1+w_m)\rho_m + \ddot{f}_R - H\dot{f}_R}{8\pi G\rho_m + \frac{1}{2}f_R R - \frac{1}{2}f - 3H\dot{f}_R}H - \frac{\dot{f}_R}{f_R}\right)\times \left(8\pi G\rho_m + \frac{1}{2}f_R R - \frac{1}{2}f - 3H\dot{f}_R\right) \geq -8\pi G\rho_m(1+w_m)\Upsilon_{\rm E}^{-1}, \tag{5.121}$$

while for the apparent-horizon open system, the second law and the GSL respectively hold in the situations

$$\frac{8\pi G(1+w_m)\rho_m + \ddot{f}_R - H\dot{f}_R}{8\pi G\rho_m + \frac{1}{2}f_R R - \frac{1}{2}f - 3H\dot{f}_R} \leq -\frac{2}{3}, \tag{5.122}$$

$$\frac{T_m}{T_{\rm A}}\left(f_R\frac{8\pi G(1+w_m)\rho_m + \ddot{f}_R - H\dot{f}_R}{8\pi G\rho_m + \frac{1}{2}f_R R - \frac{1}{2}f - 3H\dot{f}_R} - \frac{\dot{f}_R}{3H}\right) \geq G\rho_m A_{\rm A}(1+w_m)\left(\frac{8\pi G(1+w_m)\rho_m + \ddot{f}_R - H\dot{f}_R}{8\pi G\rho_m + \frac{1}{2}f_R R - \frac{1}{2}f - 3H\dot{f}_R} - \frac{2}{3}\right). \tag{5.123}$$

Scalar-tensor-chameleon gravity

For the scalar-tensor-chameleon gravity [24] with the Lagrangian density $\mathscr{L}_{\rm STC} = F(\phi)R - Z(\phi)\nabla_\alpha\phi\nabla^\alpha\phi - 2U(\phi) + 16\pi GE(\phi)\mathscr{L}_m$, we have $G_{\rm eff} = \frac{E(\phi)}{F(\phi)}G$ and [64]

$$\rho_{\rm (MG)} = \frac{1}{8\pi GE}\Big(-3H\dot{F} + \frac{1}{2}Z\dot{\phi}^2 + U\Big) \tag{5.124}$$

$$w_{\rm eff} = -1 + \frac{8\pi GE(1+w_m)\rho_m + \ddot{F} - H\dot{F} + Z\dot{\phi}^2}{8\pi GE\rho_m - 3H\dot{F} + \frac{1}{2}Z\dot{\phi}^2 + U}, \tag{5.125}$$

where in this subsection we temporarily adopt the abbreviations $E \equiv E(\phi)$, $F \equiv F(\phi)$, $U \equiv U(\phi)$ and $Z \equiv Z(\phi)$. Eq.(5.107) for the GSL of the event–horizon system imposes the constraint

$$\frac{T_m}{T_{\rm E}}\left(\frac{8\pi GE(1+w_m)\rho_m + \ddot{F} - H\dot{F} + Z\dot{\phi}^2}{8\pi GE\rho_m - 3H\dot{F} + \frac{1}{2}Z\dot{\phi}^2 + U}H + \frac{FE_\phi - EF_\phi}{EF}\dot{\phi}\right) \times\left(8\pi G\rho_m - 3H\frac{\dot{F}}{E} + \frac{Z}{E}\dot{\phi}^2 + \frac{U}{E}\right) \geq -8\pi G\rho_m(1+w_m)\Upsilon_{\rm E}^{-1}, \tag{5.126}$$

while $w_{\rm eff} \le -\frac{1}{3}$ and the apparent-horizon GSL Eq.(5.107) can be directly realized with Eq.(5.129) and $\rho_{\rm (MG)} + P_{\rm (MG)} = \frac{1}{8\pi GE}\left(\ddot F - H\dot F + Z\dot\phi^2\right)$. Moreover, in the specifications $E \mapsto 1$, $F \mapsto \phi$, $Z \mapsto \omega/\phi$, $U \mapsto \frac{1}{2}V$, we recover the generalized Brans-Dicke gravity [62] with a self-interacting potential, $\mathscr{L}_{\rm GBD} = \phi R - \frac{\omega}{\phi}\nabla_\alpha\phi\nabla^\alpha\phi - V(\phi) + 16\pi G\mathscr{L}_m$, and Eq.(5.130) reduces to become

$$\frac{T_m}{T_{\rm E}}\left(\frac{8\pi G(1+w_m)\rho_m + \ddot\phi - H\dot\phi + \frac{\omega}{\phi}\dot\phi^2}{8\pi G\rho_m - 3H\dot\phi + \frac{\omega}{2\phi}\dot\phi^2 + \frac{1}{2}V}H - \frac{\dot\phi}{\phi}\right)\times \left(8\pi G\rho_m - 3H\dot\phi + \frac{\omega}{2\phi}\dot\phi^2 + \frac{V}{2}\right) \ge -8\pi G\rho_m(1+w_m)\Upsilon_{\rm E}^{-1}. \tag{5.127}$$

Scalar-tensor-chameleon gravity

For the scalar-tensor-chameleon gravity [24] with the Lagrangian density $\mathscr{L}_{\rm STC} = F(\phi)R - Z(\phi)\nabla_\alpha\phi\nabla^\alpha\phi - 2U(\phi) + 16\pi GE(\phi)\mathscr{L}_m$ in the Jordan conformal frame, which generalizes the Brans-Dicke gravity, we have $G_{\rm eff} = \frac{E(\phi)}{F(\phi)}G$ and [64]

$$\rho_{\rm (MG)} = \frac{1}{8\pi GE}\Big(-3H\dot F + \frac{1}{2}Z\dot\phi^2 + U\Big) \tag{5.128}$$

$$w_{\rm eff} = -1 + \frac{8\pi GE(1+w_m)\rho_m + \ddot F - H\dot F + Z\dot\phi^2}{8\pi GE\rho_m - 3H\dot F + \frac{1}{2}Z\dot\phi^2 + U}, \tag{5.129}$$

where in this subsection we temporarily adopt the abbreviations $E \equiv E(\phi)$, $F \equiv F(\phi)$, $U \equiv U(\phi)$ and $Z \equiv Z(\phi)$, while H is still the Hubble parameter. Eq.(5.107) for the GSL of the event–horizon system imposes the constraint

$$\frac{T_m}{T_{\rm E}}\left(\frac{8\pi GE(1+w_m)\rho_m + \ddot F - H\dot F + Z\dot\phi^2}{8\pi GE\rho_m - 3H\dot F + \frac{1}{2}Z\dot\phi^2 + U}H + \frac{FE_\phi - EF_\phi}{EF}\dot\phi\right)\times\left(8\pi G\rho_m - 3H\frac{\dot F}{E} + \frac{Z}{2E}\dot\phi^2 + \frac{U}{E}\right) \ge -8\pi G\rho_m(1+w_m)\Upsilon_{\rm E}^{-1}, \tag{5.130}$$

while $w_{\rm eff} \le -\frac{1}{3}$ and the apparent-horizon GSL Eq.(5.107) can be directly realized with Eq.(5.129) and $\rho_{\rm (MG)} + P_{\rm (MG)} = \frac{1}{8\pi GE}\left(\ddot F - H\dot F + Z\dot\phi^2\right)$. Moreover, in the specifications $E \mapsto 1$, $F \mapsto \phi$, $Z \mapsto \omega/\phi$, $U \mapsto \frac{1}{2}V$, we recover the generalized Brans-Dicke gravity [62] with a self-interacting potential, $\mathscr{L}_{\rm GBD} = \phi R - \frac{\omega}{\phi}\nabla_\alpha\phi\nabla^\alpha\phi - V(\phi) + 16\pi G\mathscr{L}_m$, and Eq.(5.130) reduces to become

$$\frac{T_m}{T_{\rm E}}\left(\frac{8\pi G(1+w_m)\rho_m + \ddot\phi - H\dot\phi + \frac{\omega}{\phi}\dot\phi^2}{8\pi G\rho_m - 3H\dot\phi + \frac{\omega}{2\phi}\dot\phi^2 + \frac{1}{2}V}H - \frac{\dot\phi}{\phi}\right)\times\left(8\pi G\rho_m - 3H\dot\phi + \frac{\omega}{2\phi}\dot\phi^2 + \frac{1}{2}V\right) \ge -8\pi G\rho_m(1+w_m)\Upsilon_{\rm E}^{-1}. \tag{5.131}$$

Quadratic gravity

For the quadratic gravity $\mathscr{L}_{\rm QG} = R + aR^2 + bR_{\mu\nu}R^{\mu\nu} + 16\pi G\mathscr{L}_m$ whose Lagrangian density is an effective linear superposition of the quadratic independent Riemannian invariants [58, 60], with $\{a, b\}$ being constants, we have $G_{\rm eff}=\frac{G}{1+2aR}$ and [64]

$$\rho_{\rm (MG)}=\frac{1}{8\pi G}\left(\frac{a}{2}R^2-\frac{b}{2}R_c^2+\frac{b}{2}\ddot{R}-(4a+b)H\dot{R}+4bR^t{}_{\alpha t\beta}+2b\Box R_t{}^t\right),\tag{5.132}$$

$$w_{\rm eff}=-1+\frac{8\pi G(1+w_m)\rho_m+(2a+b)\ddot{R}-\frac{b}{2}H\dot{R}+4b(R^t{}_{\alpha t\beta}-R^r{}_{\alpha r\beta})R^{\alpha\beta}+2b\Box(R_t{}^t-R_r{}^r)}{8\pi G\rho_m+\frac{a}{2}R^2-\frac{b}{2}R_c^2+\frac{b}{2}\ddot{R}-(4a+b)H\dot{R}+4bR^t{}_{\alpha t\beta}+2b\Box R_t{}^t},\tag{5.133}$$

where $R_c^2:=R_{\mu\nu}R^{\mu\nu}$, $\Box=g^{\mu\nu}\nabla_\mu\nabla_\nu$, and we have used the compact geometric notations [64]. Hence, GSL of the event-horizon system requires

$$\begin{aligned}&\frac{T_m}{T_{\rm E}}\left(\frac{8\pi G(1+w_m)\rho_m+(2a+b)\ddot{R}-\frac{b}{2}H\dot{R}+4b(R^t{}_{\alpha t\beta}-R^r{}_{\alpha r\beta})R^{\alpha\beta}+2b\Box(R_t{}^t-R_r{}^r)}{8\pi G\rho_m+\frac{a}{2}R^2-\frac{b}{2}R_c^2+\frac{b}{2}\ddot{R}-(4a+b)H\dot{R}+4bR^t{}_{\alpha t\beta}+2b\Box R_t{}^t}H-\frac{2a\dot{R}}{1+2aR}\right)\\&\quad\times\left(8\pi G\rho_m+\frac{a}{2}R^2-\frac{b}{2}R_c^2+\frac{b}{2}\ddot{R}-(4a+b)H\dot{R}+4bR^t{}_{\alpha t\beta}+2b\Box R_t{}^t\right)\geq-8\pi G\rho_m(1+w_m)\Upsilon_{\rm E}^{-1},\end{aligned}\tag{5.134}$$

while $w_{\rm eff}\leq-\frac{1}{3}$ and Eq.(5.107) can be directly concretized with Eq.(5.133) and

$$\rho_{\rm (MG)}+P_{\rm (MG)}=\frac{1}{8\pi G}\left((2a+b)\ddot{R}-\frac{b}{2}H\dot{R}+4b(R^t{}_{\alpha t\beta}-R^r{}_{\alpha r\beta})R^{\alpha\beta}+2b\Box(R_t{}^t-R_r{}^r)\right).\tag{5.135}$$

Chern-Simons gravity

Finally let's analyze the dynamical Chern-Simons gravity $\mathscr{L}_{\rm CS}=R+\frac{a\vartheta}{\sqrt{-g}}{}^*\widehat{RR}-b\nabla_\mu\vartheta\nabla^\mu\vartheta-V(\vartheta)+16\pi G\mathscr{L}_m$ [61] which has a constant gravitational coupling strength $G_{\rm eff}=G$, where ${}^*\widehat{RR}={}^*R_{\alpha\beta\gamma\delta}R^{\alpha\beta\gamma\delta}$ denotes the Chern-Pontryagin invariant and $\{a,b\}$ are constants. We have [64]

$$\begin{aligned}\rho_{\rm (MG)}&=\frac{1}{16\pi G}\left(b\dot{\vartheta}^2+V(\vartheta)\right)&(5.136)\\ w_{\rm eff}=-1&+\frac{8\pi G\rho_m(1+w_m)+b\dot{\vartheta}^2}{8\pi G\rho_m+\frac{1}{2}b\dot{\vartheta}^2+\frac{1}{2}V(\vartheta)},&(5.137)\end{aligned}$$

and thus Eq.(5.107) leads to the viability condition

$$\frac{T_m}{T_{\rm E}}\left(8\pi G\rho_m(1+w_m)+b\dot{\vartheta}^2\right)\geq-8\pi G\rho_m(1+w_m)\frac{\Upsilon_{\rm H}}{\Upsilon_{\rm E}},\tag{5.138}$$

which, for $\dot{\vartheta}\neq0$, yields a constraint for b,

$$b\geq-8\pi G\rho_m(1+w_m)\left(\frac{\Upsilon_{\rm H}}{\Upsilon_{\rm E}}\frac{T_{\rm E}}{T_m}+1\right)\dot{\vartheta}^{-2}.\tag{5.139}$$

For the FRW cosmology, ${}^*\widehat{RR}$ makes no contribution to the gravitational equations, so $\mathscr{L}_{\rm CS}$ effectively acts as $\mathscr{L}=R-b\nabla_\mu\vartheta\nabla^\mu\vartheta-V(\vartheta)+16\pi G\mathscr{L}_m$, which formally resembles the scalarial dark energy [37, 39]. On the other hand, note that although Eqs.(5.138) and (5.139) are always satisfied for $b>0$, which corresponds to a canonical kinetic ϑ-field that is quintessence-like ($\mathscr{L}=-\frac{1}{2}\nabla_\mu\phi\nabla^\mu\phi-V(\phi)$), ϑ is allowed to be slightly phantom-like ($\mathscr{L} = \frac{1}{2}\nabla_\mu\phi\nabla^\mu\phi - V(\phi)$) for some $b < 0$ by Eq.(5.139). Hence, Eq.(5.139) does not coincide with the situation of ΛCDM in Sec. 5.5.6, where $\dot{S}_m^{(\mathrm{E})} + \dot{S}_\mathrm{E} \geq 0$ holds if and only if $w_m \geq -1$.

5.7 Conclusions and discussion

In this paper the thermodynamic implications of the holographic-style dynamical equations for the FRW Universe have been studied. We started from the ΛCDM model of GR to clearly build the whole framework of gravitational thermodynamics, and eventually extended it to modified gravities. A great advantage of our formulation is all constraints are expressed by the EoS parameters.

The holographic-style gravitational equations govern both the apparent-horizon dynamics and the cosmic spatial expansion. We have shown how they imply Hayward's unified first law of equilibrium thermodynamics $dE = A\boldsymbol{\psi} + WdV$ [46] and the isochoric-process Cai–Kim Clausius equation $T_\mathrm{A} dS_\mathrm{A} = \delta Q_\mathrm{A} = -A_\mathrm{A}\boldsymbol{\psi}_t$ [2, 8, 47]. The derivations of the Clausius equation in Sec. 5.3.2 actually involves a long standing confusion regarding the setup of the apparent-horizon temperature, and extensive comparisons in Sec. 5.4 have led to the argument that the Cai–Kim $T_\mathrm{A} = 1/(2\pi\Upsilon_\mathrm{A})$ is more appropriate than the Hayward $\mathcal{T}_\mathrm{A} = \kappa/2\pi$ and its partial absolute value $\mathcal{T}_\mathrm{A}^{(+)}$. Meanwhile, we have also introduced the "zero temperature divide" $w_m = 1/3$ for $\mathcal{T}_\mathrm{A} = \kappa/2\pi$, and proved the signs of both temperatures are independent of the inner or outer trappedness of the apparent horizon.

The "positive heat out" sign convention for the heat transfer and the horizon entropy has been decoded from $T_\mathrm{A} dS_\mathrm{A} = -dE$, provided that the third law of thermodynamics holds with a positive T_A. With the horizon temperature and entropy clarified, the cosmic entropy evolution has been investigated. We have adjusted the traditional matter entropy and Gibbs equation into $dE_m = -T_m dS_m - P_m dV_\mathrm{A}$ in accordance with the positive heat out convention of the horizon entropy. It turns out that the cosmic entropy is well behaved, specially for the event-horizon system, where both the second law and the GSL hold for nonexotic matter ($-1 \leq w_m \leq 1$). Also, we have clarified that the regions $\{\Upsilon \leq \Upsilon_\mathrm{A}, \Upsilon \leq \Upsilon_\mathrm{E}\}$ enveloped by the apparent and even horizons are simple open thermodynamic systems[2] so that one should not *a priori* expect the validity of nondecreasing entropy, and abandoned the local equilibrium assumptions restricting the interior and the boundary temperatures.

Finally we have generalized the whole formulations from the ΛCDM model to ordinary modified gravities whose field equations have been intrinsically compactified into the GR form $R_{\mu\nu} - Rg_{\mu\nu}/2 = 8\pi G_\mathrm{eff} T_{\mu\nu}^{(\mathrm{eff})}$. To our particular interest, we found that inside the apparent horizon the second law $\dot{S}_m \geq 0$ nontrivially holds if $w_\mathrm{eff} \leq -1/3$, while inside the event horizon $\dot{S}_m \geq 0$ always validates regardless of the gravity theories in use. These generic conclusions have been concretized in $f(R)$, scalar-tensor-chameleon, quadratic and dynamical Chern-Simons gravities.

Note that the volume V and surface area A used throughout this paper are interpreted as flat-space quantities in [26]. However, Υ and A are the proper radius and area for the standard sphere $\mathbb{S}^2$ in the 2 + 2 (rather than 3 + 1) decomposition $ds^2 = h_{\alpha\beta}dx^\alpha dx^\beta + \mathbb{S}^2$ of Eq.(5.1), while the role of V as a proper quantity is still not clear.

There are still some interesting problems arising in this paper and yet unsolved. For example, the discussion in Sec. 5.5.7 further raises the question that, what is the temperature T_E for the event horizon? Note

[2]Even the philosophical "whole Universe" would be an open system if there were matter creations which would cause irreversible extra entropy production, and one typical mechanism triggering this effect is nonminimal curvature-matter coupling [66].

that if $T_E \neq T_A$, there would be a spontaneous heat flow between Υ_A and Υ_E – would it affect the cosmic expansion? On the other hand, it is not clear whether or not the apparent and the event horizons could be heated by the absolute Hubble energy flow and consequently $T_E = T_m$ and $T_A = T_m$: this would avoid the temperature gradient between Υ_A and Υ_E, but throughout this paper we have not yet seen any evidence for T_A to be heated into T_m.

Moreover, besides the traditional GSLs, the "cosmic holographic principle" in [26] which argues that the physical entropy $\widehat{S}_m^{(A)}$ inside the apparent horizon Υ_A could never exceed the apparent-horizon entropy S_A, is also problematic in comparing $\widehat{S}_m^{(A)}$ with S_A – this principle should be restudied in the unified positive-heat-out sign convention. Moreover, is Υ_A the only hologram membrane for the FRW Universe? Can the relative evolution equation (5.17) be used in astrophysical and cosmological simulations? Also, how would the cosmic entropy evolve in a contracting Universe? We hope to find out the answers in prospective studies.

Acknowledgement

This work was financially supported by the Natural Sciences and Engineering Research Council of Canada.

Appendix: The minimum set of state functions and reversibility

Eqs.(5.29) and (5.30) clearly indicate that just like ordinary thermodynamics, the geometrically defined horizon temperature T_A and horizon entropy S_A remain as *state functions*, which are independent of thermodynamic processes that indeed correspond to the details of cosmic expansion $\dot{a}(t)$ and the apparent-horizon evolution $\dot{\Upsilon}_A$. Just like the regular temperatures of thermodynamic systems, the Cai–Kim T_A remains as an intensive property with $T_A = T_A(t) = 1/2\pi\Upsilon_A(t)$; one should not treat it as an extensive property by $T_A = T_A(V_A) = 1/(2\pi\sqrt[3]{\frac{3}{4\pi}V_A})$. Some other state functions involved here include the apparent-horizon radius Υ_A, the energy density $\rho_m(t)$, the pressure $P_m(t)$ and thus the EoS parameter $w_m = \rho_m/P_m$. These state quantities are not totally independent as they are related with one another by the Friedmann equations (5.7), the holographic-style dynamical equation (5.8), and the thermodynamic relations in Secs. 5.3.1 and 5.3.2. Here we select the following quantities to comprise a minimum set of *independent* state functions for Secs. 5.2 and 5.3:

$$\text{Minimum set} = \left\{\rho_m\,, w_m\,, T_A\right\}. \tag{5.140}$$

Based on this set, the product of ρ_m and w_m yields the pressure P_m. Through Eq.(5.10) ρ_m recovers the horizon area A_A and thus determines the entropy S_A. Treating T_A as an intensive property, we do not take the approach from Eq.(5.8) or Eq.(5.10) for the recovery $\rho_m \to A_A \to \Upsilon_A \to T_A$, and instead let T_A enter the minimum set directly as the Cai–Kim temperature ansatz. Similarly, for modified gravities with the dynamical equations (5.78)-(5.81), we choose the minimum set to be $\{\rho_{\text{eff}}, w_{\text{eff}}, G_{\text{eff}}, T_A\}$.

The fact that Eq.(5.31) is the Clausius equation for (quasi)equilibrium or reversible thermodynamic processes without extra entropy production raises the question that, what does reversibility mean from the perspective of cosmic and apparent-horizon dynamics? From the explicit expression of the heat transfer $\delta Q_A = T_A dS_A = A_A(1 + w_m)\rho_m H\Upsilon_A dt$ where the state quantity $T_A dS_A$ is balanced by the process quantity δQ_A, we naturally identify H as a *process quantity*; moreover, if one reverses the initial and final states of $T_A dS_A$, the state quantities $\{\rho_m(t)\,, w_m\,, \Upsilon_A\,, A_A\}$ can be automatically reversed. Hence, by reversibility we mean an imaginary negation $-H$ of the Hubble parameter that results in a spatial contraction process which directly evolves the Universe from a later state back to the earlier state of $T_{\rm A}dS_{\rm A}$ without reversing the time arrow and causing energy dissipation.

[68] suggests that since the energy-matter crossing the apparent horizon for the (accelerated) expanding Universe will not come back in the future, it should cause extra entropy production, and [68] further introduced the entropy flow vector and the entropy production density for it. In fact, the reversibility of $T_{\rm A}dS_{\rm A} = \delta Q_{\rm A}$ simply allows for such a possibility in principle, rather than the realistic occurrence of the reverse process, so we believe that the entropy-production treatment in [68] is inappropriate. As shown in Sec. 5.6.3, irreversibility and entropy production is a common feature for such (minimally coupled) modified gravities with a *nontrivial* effective gravitational coupling strength ($G_{\rm eff} \neq$ constant) when their field equations are cast into the GR form $R_{\mu\nu} - Rg_{\mu\nu}/2 = 8\pi G_{\rm eff} T^{(\rm eff)}_{\mu\nu}$, and the time evolution of $G_{\rm eff}$ causes irreversible energy dissipation and constitutes the only source of entropy production.

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Chapter 6. Lovelock-Brans-Dicke gravity [*Class. Quantum Grav.* **33** (2016), 045001]

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Abstract

According to Lovelock's theorem, the Hilbert-Einstein and the Lovelock actions are indistinguishable from their field equations. However, they have different scalar-tensor counterparts, which correspond to the Brans-Dicke and the *Lovelock-Brans-Dicke* (LBD) gravities, respectively. In this paper the LBD model of alternative gravity with the Lagrangian density $\mathscr{L}_{\text{LBD}} = \frac{1}{16\pi}\Big[\phi\Big(R + \frac{a}{\sqrt{-g}}\,{}^*RR + b\mathcal{G}\Big) - \frac{\omega_{\text{L}}}{\phi}\nabla_\alpha\phi\nabla^\alpha\phi\Big]$ is developed, where ${}^*RR$ and $\mathcal{G}$ respectively denote the topological Chern-Pontryagin and Gauss-Bonnet invariants. The field equation, the kinematical and dynamical wave equations, and the constraint from energy-momentum conservation are all derived. It is shown that, the LBD gravity reduces to general relativity in the limit $\omega_{\text{L}} \to \infty$ unless the "topological balance condition" holds, and in vacuum it can be conformally transformed into the dynamical Chern-Simons gravity and the generalized Gauss-Bonnet dark energy with Horndeski-like or Galileon-like kinetics. Moreover, the LBD gravity allows for the late-time cosmic acceleration without dark energy. Finally, the LBD gravity is generalized into the Lovelock-scalar-tensor gravity, and its equivalence to fourth-order modified gravities is established. It is also emphasized that the standard expressions for the contributions of generalized Gauss-Bonnet dependence can be further simplified.

Key words: Lovelock's theorem, topological effects, modified gravity
PACS numbers: 04.20.Cv , 04.20.Fy , 04.50.Kd

6.1 Introduction

As an alternative to the various models of dark energy with large negative pressure that violates the standard energy conditions, the accelerated expansion of the Universe has inspired the reconsideration of relativistic gravity and modifications of general relativity (GR), which can explain the cosmic acceleration and reconstruct the entire expansion history without dark energy.

Such alternative and modified gravities actually encode the possible ways to go beyond Lovelock's theorem and its necessary conditions [1], which limit the second-order field equation in four dimensions to $R_{\mu\nu} - Rg_{\mu\nu}/2 + \Lambda g_{\mu\nu} = 8\pi G T^{(\text{m})}_{\mu\nu}$, i.e. Einstein's equation supplemented by the cosmological constant Λ. These directions can allow for, for example, fourth and even higher order gravitational field equations [2–5], more than four spacetime dimensions [6, 7], extensions of pure pseudo-Riemannian geometry and metric gravity [7, 8], extra physical degrees of freedom [9–12], and nonminimal curvature-matter couplings [13, 14]. From

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a variational approach, these violations manifest themselves as different modifications of the Hilbert-Einstein action, such as extra curvature invariants, scalar fields, and non-Riemannian geometric variables.

For the Lovelock action in Lovelock's theorem and the Hilbert-Einstein-Λ action, it is well known that they yield the same field equation and thus are indistinguishable by their gravitational effects. When reconsidering Lovelock's theorem, we cannot help but ask whether the effects of these two actions are really the same in all possible aspects. Is there any way for the two topological sources in the Lovelock action to show nontrivial consequences? As a possible answer to this question, we propose the Lovelock-Brans-Dicke gravity.

This paper is organized as follows. In Sec. 6.2, the Lovelock-Brans-Dicke gravity is introduced based on Lovelock's theorem, and its gravitational and wave equations are derived in Sec. 6.3. Section 6.4 studies the behaviors at the infinite-Lovelock-parameter limit $\omega_{\rm L} \to \infty$, and Sec. 6.5 derives the constraint from energy-momentum conservation. Section 6.6 shows that in vacuum the Lovelock-Brans-Dicke gravity can be conformally transformed into the dynamical Chern-Simon gravity and the generalized Gauss-Bonnet dark energy with Horndeski-like or Galileon-like kinetics. Then the possibility of realizing the acceleration phase for the late-time Universe is discussed in Sec. 6.7. Finally, in Sec. 6.8 the Lovelock-Brans-Dicke theory is extended to the Lovelock-scalar-tensor gravity, and its equivalence to fourth-order modified gravities is analyzed. Throughout this paper, we adopt the sign conventions $\Gamma^{\alpha}_{\beta\gamma} = \Gamma^{\alpha}{}_{\beta\gamma}$, $R^{\alpha}{}_{\beta\gamma\delta} = \partial_\gamma \Gamma^{\alpha}_{\delta\beta} - \partial_\delta \Gamma^{\alpha}_{\gamma\beta} \cdots$ and $R_{\mu\nu} = R^{\alpha}{}_{\mu\alpha\nu}$ with the metric signature $(-,+++)$.

6.2 Lovelock-Brans-Dicke action

An algebraic Riemannian invariant $\widetilde{\mathcal{R}} = \widetilde{\mathcal{R}}\left(g_{\alpha\beta}\,, R_{\alpha\mu\beta\nu}\right)$ in the action $\int d^4x\sqrt{-g}\,\widetilde{\mathcal{R}}$ generally leads to fourth-order gravitational field equations by the variational derivative

$$\frac{\delta\left(\sqrt{-g}\widetilde{\mathcal{R}}\right)}{\delta g^{\mu\nu}} = \frac{\partial\left(\sqrt{-g}\widetilde{\mathcal{R}}\right)}{\partial g^{\mu\nu}} - \partial_\alpha \frac{\partial\left(\sqrt{-g}\widetilde{\mathcal{R}}\right)}{\partial(\partial_\alpha g^{\mu\nu})} + \partial_\alpha\partial_\beta \frac{\partial\left(\sqrt{-g}\widetilde{\mathcal{R}}\right)}{\partial(\partial_\alpha\partial_\beta g^{\mu\nu})}. \tag{6.1}$$

Lovelock found out that in *four* dimensions the most general action leading to second-order field equations is [1]

$$\begin{aligned} \mathcal{S} &= \int d^4x\sqrt{-g}\,\mathscr{L} + \mathcal{S}_m \quad \text{with} \\ \mathscr{L} &= \frac{1}{16\pi G}\left(R - 2\Lambda + \frac{a}{2\sqrt{-g}}\epsilon_{\alpha\beta\mu\nu}R^{\mu\nu}{}_{\gamma\delta}R^{\alpha\beta\gamma\delta} + b\mathcal{G}\right), \end{aligned} \tag{6.2}$$

where Λ is the cosmological constant, $\{a\,,b\}$ are dimensional coupling constants, and without any loss of generality we have set the coefficient of R equal to one. Also, $\epsilon_{\alpha\beta\mu\nu}$ refers to the totally antisymmetric Levi-Civita pseudotensor with $\epsilon_{0123} = \sqrt{-g}$, $\epsilon^{0123} = \frac{1}{\sqrt{-g}}$, and $\{\epsilon_{\alpha\beta\mu\nu}, \epsilon^{\alpha\beta\mu\nu}\}$ can be obtained from each other by raising or lowering the indices with the metric tensor. In Eq.(6.2), $\epsilon_{\alpha\beta\mu\nu}R^{\mu\nu}{}_{\gamma\delta}R^{\alpha\beta\gamma\delta}$ and $\mathcal{G}$ respectively refer to the Chern-Pontryagin density and the Gauss-Bonnet invariant, with

$$\mathcal{G} := R^2 - 4R_{\mu\nu}R^{\mu\nu} + R_{\mu\alpha\nu\beta}R^{\mu\alpha\nu\beta}. \tag{6.3}$$

The variational derivatives $\delta(\epsilon_{\alpha\beta\mu\nu}R^{\mu\nu}{}_{\gamma\delta}R^{\alpha\beta\gamma\delta})/\delta g^{\mu\nu}$ and $\delta(\sqrt{-g}\mathcal{G})/\delta g^{\mu\nu}$ yield total derivatives which serve as boundary terms in varying the full action Eq.(6.2). The Chern-Pontryagin scalar $\epsilon_{\alpha\beta\mu\nu}R^{\mu\nu}{}_{\gamma\delta}R^{\alpha\beta\gamma\delta}$ is proportional to the divergence of the topological Chern-Simons four-current K^μ [11],

$$\begin{aligned} &\epsilon_{\alpha\beta\mu\nu}R^{\mu\nu}{}_{\gamma\delta}R^{\alpha\beta\gamma\delta} = -8\,\partial_\mu K^\mu \quad \text{with} \\ &K^\mu = \epsilon^{\mu\alpha\beta\gamma}\left(\frac{1}{2}\Gamma^\xi_{\alpha\tau}\partial_\beta\Gamma^\tau_{\gamma\xi} + \frac{1}{3}\Gamma^\xi_{\alpha\tau}\Gamma^\tau_{\beta\eta}\Gamma^\eta_{\gamma\xi}\right), \end{aligned} \tag{6.4}$$

and similarly, the topological current for the Gauss-Bonnet invariant is (see Refs.[15, 16] for earlier discussion and Ref.[17] for further clarification)

$$\begin{aligned} &\sqrt{-g}\,\mathcal{G} = -\partial_\mu J^\mu \quad \text{with} \\ &J^\mu = \sqrt{-g}\,\epsilon^{\mu\alpha\beta\gamma}\epsilon_{\rho\sigma}{}^{\xi\zeta}\Gamma^\rho_{\xi\alpha}\left(\frac{1}{2}R^\sigma{}_{\zeta\beta\gamma} - \frac{1}{3}\Gamma^\sigma_{\lambda\beta}\Gamma^\lambda_{\zeta\gamma}\right). \end{aligned} \tag{6.5}$$

Hence, the covariant densities $\epsilon_{\alpha\beta\mu\nu}R^{\mu\nu}{}_{\gamma\delta}R^{\alpha\beta\gamma\delta}$ and $\sqrt{-g}\mathcal{G}$ in Eq.(6.2) make no contribution to the field equation $\delta\mathcal{S}/\delta g^{\mu\nu} = 0$.

According to Lovelock's theorem, one cannot tell whether Einstein's equation $R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} = 8\pi G T^{(\mathrm{m})}_{\mu\nu}$ comes from the customary Hilbert-Einstein action

$$\mathcal{S}_{\mathrm{HE}} = \frac{1}{16\pi G}\int d^4x\,\sqrt{-g}\,R + \mathcal{S}_m\,, \tag{6.6}$$

or from the induced Lovelock action[1]

$$\begin{aligned} &\mathcal{S}_{\mathrm{L}} = \int d^4x\,\sqrt{-g}\,\mathscr{L}_{\mathrm{L}} + \mathcal{S}_m \quad \text{with} \\ &\mathscr{L}_{\mathrm{L}} = \frac{1}{16\pi G}\left(R + \frac{a}{\sqrt{-g}}{}^*RR + b\mathcal{G}\right), \end{aligned} \tag{6.7}$$

where for simplicity we switch to the denotation

$${}^*RR := \frac{1}{2}\epsilon_{\alpha\beta\mu\nu}R^{\mu\nu}{}_{\gamma\delta}R^{\alpha\beta\gamma\delta} \tag{6.8}$$

for the Chern-Pontryagin density, as the symbol ${}^*RR$ has been widely used in the literature of Chern-Simons gravity [11, 18, 19]. In Eqs.(6.2), (6.6) and (6.7), the matter action $\mathcal{S}_m$ is given in terms of the matter Lagrangian density $\mathscr{L}_m$ by $\mathcal{S}_m = \int d^4x\,\sqrt{-g}\,\mathscr{L}_m$, and the stress-energy-momentum density tensor $T^{(\mathrm{m})}_{\mu\nu}$ is defined in the usual way by [20]

$$\delta\mathcal{S}_m = -\frac{1}{2}\int d^4x\,\sqrt{-g}\,T^{(\mathrm{m})}_{\mu\nu}\delta g^{\mu\nu} \quad \text{with} \quad T^{(\mathrm{m})}_{\mu\nu} := \frac{-2}{\sqrt{-g}}\frac{\delta\left(\sqrt{-g}\,\mathscr{L}_m\right)}{\delta g^{\mu\nu}}. \tag{6.9}$$

The indistinguishability between $\mathcal{S}_{\mathrm{L}}$ and $\mathcal{S}_{\mathrm{HE}}$ from their field equations begs the question: Does Einstein's equation come from $\mathcal{S}_{\mathrm{L}}$ or $\mathcal{S}_{\mathrm{HE}}$? Is there any way to discriminate them?

[1] Note that not to confuse with the more common "Lovelock action" for the topological generalizations of the Hilbert-Einstein action to generic N dimensions that still preserves second-order field equations, as in Ref.[6].

Recall that GR from $\mathcal{S}_{\text{HE}}$ has a fundamental scalar-tensor counterpart, the Brans-Dicke gravity [9],

$$\begin{aligned} \mathcal{S}_{\text{BD}} &= \int d^4x \sqrt{-g}\, \mathscr{L}_{\text{BD}} + \mathcal{S}_m \quad \text{with} \\ \mathscr{L}_{\text{BD}} &= \frac{1}{16\pi}\left(\phi R - \frac{\omega_{\text{BD}}}{\phi}\, \nabla_\alpha \phi \nabla^\alpha \phi\right), \end{aligned} \tag{6.10}$$

which proves to be a successful alternative to GR that passes all typical GR tests [21], and it is related to GR by

$$\begin{aligned} \mathscr{L}_{\text{HE}} &= \frac{R}{16\pi G} \\ \Rightarrow\ \mathscr{L}_{\text{BD}} &= \frac{1}{16\pi}\left(\phi R - \frac{\omega_{\text{BD}}}{\phi}\, \nabla_\alpha \phi \nabla^\alpha \phi\right). \end{aligned} \tag{6.11}$$

That is to say, Brans-Dicke firstly replaces the matter-gravity coupling constant G with a pointwise scalar field $\phi(x^\alpha)$ in accordance with the spirit of Mach's principle, $G \mapsto \phi^{-1}$, and further adds to the action a formally canonical kinetic term $-\frac{\omega_{\text{BD}}}{\phi} \nabla_\alpha \phi \nabla^\alpha \phi$ governing the kinetics of $\phi(x^\alpha)$. Applying this prescription to the Lovelock action Eq.(6.7), we obtain

$$\begin{aligned} \mathscr{L}_{\text{L}} &= \frac{1}{16\pi G}\left(R + \frac{a}{\sqrt{-g}}{}^*RR + b\mathcal{G}\right) \\ \Rightarrow \mathscr{L}_{\text{LBD}} &= \frac{1}{16\pi}\left[\phi\left(R + \frac{a}{\sqrt{-g}}{}^*RR + b\mathcal{G}\right) - \frac{\omega_{\text{L}}}{\phi}\nabla_\alpha\phi\nabla^\alpha\phi\right], \end{aligned} \tag{6.12}$$

where the Lovelock parameter ω_{L} is a dimensionless constant. Based on Eq.(6.12), we obtain what we dub as the *Lovelock-Brans-Dicke* (henceforth LBD) gravity with the action

$$\mathcal{S}_{\text{LBD}} = \int d^4x \sqrt{-g}\, \mathscr{L}_{\text{LBD}} + \mathcal{S}_m\,, \tag{6.13}$$

or the *Lanczos-Lovelock-Brans-Dicke gravity*, as Lovelock's theorem is based on Lanczos' discovery that an isolated ${}^*RR$ or $\mathcal{G}$ in the action does not affect the field equation [22].

Unlike the $\delta({}^*RR)/\delta g^{\mu\nu}$ and $\delta(\sqrt{-g}\mathcal{G})/\delta g^{\mu\nu}$ in $\delta\mathcal{S}_{\text{L}}/\delta g^{\mu\nu}$, the $[\phi\delta({}^*RR)]/\delta g^{\mu\nu}$ and $\left[\phi\delta(\sqrt{-g}\mathcal{G})\right]/\delta g^{\mu\nu}$ for $\delta\mathcal{S}_{\text{LBD}}/\delta g^{\mu\nu}$ are no longer pure divergences, because the scalar field $\phi(x^\alpha)$ as a nontrivial coefficient will be absorbed into the variations of ${}^*RR$ and $\sqrt{-g}\mathcal{G}$ when integrating by parts. Hence, although $\mathcal{S}_{\text{L}}$ and $\mathcal{S}_{\text{HE}}$ are indistinguishable, their respective scalar-tensor counterparts $\mathcal{S}_{\text{LBD}}$ and $\mathcal{S}_{\text{BD}}$ are different.

Note that the cosmological-constant term -2Λ in Eq.(6.2) is temporarily abandoned in $\mathscr{L}_{\text{L}}$; otherwise, it would add an extra term $-2\Lambda\phi$ to $\mathscr{L}_{\text{LBD}}$, which serves as a simplest linear potential. This is primarily for a better analogy between the LBD and the Brans-Dicke gravities, as the latter in its standard form does not contain a potential term $V(\phi)$, and an unspecified potential $V(\phi)$ would cause too much arbitrariness to $\mathscr{L}_{\text{LBD}}$.

Also, Lovelock's original action Eq.(6.2) concentrates on the *algebraic* curvature invariants; in fact, one can further add to Eq.(6.2) the relevant differential terms $\Box R$, $\Box{}^*RR$, and $\Box\mathcal{G}$ ($\Box = g^{\alpha\beta}\nabla_\alpha\nabla_\beta$ denoting the covariant d'Alembertian), while the field equation will remain unchanged. This way, the gravitational Lagrangian density in Eq.(6.7) is enriched into

$$\mathscr{L} = \frac{1}{16\pi G}\left(R + \frac{a^*RR}{\sqrt{-g}} + b\mathcal{G} + c\Box R + d\Box^*RR + e\Box\mathcal{G}\right), \tag{6.14}$$

with $\{c, d, e\}$ being constants, and its Brans-Dicke-type counterpart extends Eq.(6.12) into

$$\mathscr{L} = \frac{1}{16\pi}\left[\phi\left(R + \frac{a}{\sqrt{-g}}{}^*RR + b\mathcal{G}\right) - \frac{\omega_{\rm L}}{\phi}\nabla_\alpha\phi\nabla^\alpha\phi + \phi\left(c\Box R + d\Box^*RR + e\Box\mathcal{G}\right)\right], \tag{6.15}$$

where $\phi\cdot(c\Box R + d\Box^*RR + e\Box\mathcal{G})$ have nontrivial contributions to the field equation. However, unlike $*RR$ and $\sqrt{-g}\mathcal{G}$ which are divergences of their respective topological current as in Eqs.(6.4) and (6.5), $\{\Box R$, $\Box^*RR$, $\Box\mathcal{G}\}$ are total derivatives simply because the d'Alembertian $\Box$ satisfies $\sqrt{-g}\Box\Theta = \partial_\alpha\left(\sqrt{-g}\, g^{\alpha\beta}\partial_\beta\Theta\right)$ when acting on an arbitrary scalar field Θ; in this sense, these differential boundary terms which contain fourth-order derivatives of the metric are less interesting than $*RR$ and $\mathcal{G}$. In this paper, we will focus on the LBD gravity $\mathscr{L}_{\rm LBD}$ Eq.(6.12) built upon the original Lovelock action and Lovelock's theorem, rather than Eq.(6.15) out of the modified action Eq.(6.14).

6.3 Gravitational and wave equations

In this section we will work out the gravitational field equation $\delta\mathcal{S}_{\rm LBD}/\delta g^{\mu\nu} = 0$ and the wave equation $\delta\mathcal{S}_{\rm LBD}/\delta\phi = 0$ for the LBD gravity. First of all, with $\delta g_{\alpha\beta} = -g_{\alpha\mu}g_{\beta\nu}\delta g^{\mu\nu}$, $\delta\Gamma^\lambda_{\alpha\beta} = \frac{1}{2}g^{\lambda\sigma}\left(\nabla_\alpha\delta g_{\sigma\beta} + \nabla_\beta\delta g_{\sigma\alpha} - \nabla_\sigma\delta g_{\alpha\beta}\right)$, and the Palatini identity $\delta R^\lambda{}_{\alpha\beta\gamma} = \nabla_\beta\left(\delta\Gamma^\lambda_{\gamma\alpha}\right) - \nabla_\gamma\left(\delta\Gamma^\lambda_{\beta\alpha}\right)$ [23], for the first term ϕR in $\mathscr{L}_{\rm LBD}$ it is easy to work out that

$$\frac{1}{\sqrt{-g}}\frac{\delta(\sqrt{-g}\,\phi R)}{\delta g^{\mu\nu}} \cong -\frac{1}{2}\phi R g_{\mu\nu} + \phi R_{\mu\nu} + \left(g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu\right)\phi, \tag{6.16}$$

where $\cong$ means equality by neglecting all total-derivative terms which are boundary terms for the action.

6.3.1 Coupling to the Chern-Pontryagin invariant

The Chern-Pontryagin density ${}^*RR$ in $\mathscr{L}_{\rm LBD}$ measures the gravitational effects of parity violation through $\int d^4x\,\phi^*RR$ for its dependence on the Levi-Civita pseudotensor. In addition to Eq.(6.8), ${}^*RR$ is related to the left dual of the Riemann tensor via

$${}^*RR = \frac{1}{2}\left(\epsilon_{\alpha\beta\mu\nu}R^{\mu\nu}{}_{\gamma\delta}\right)R^{\alpha\beta\gamma\delta} = {}^*R_{\alpha\beta\gamma\delta}R^{\alpha\beta\gamma\delta}\,. \tag{6.17}$$

Applying the Ricci decomposition $R_{\alpha\beta\gamma\delta} = C_{\alpha\beta\gamma\delta} + \frac{1}{2}\left(g_{\alpha\gamma}R_{\beta\delta} - g_{\alpha\delta}R_{\beta\gamma} + g_{\beta\delta}R_{\alpha\gamma} - g_{\beta\gamma}R_{\alpha\delta}\right) - \frac{1}{6}\left(g_{\alpha\gamma}g_{\beta\delta} - g_{\alpha\delta}g_{\beta\gamma}\right)R$ to Eq.(6.17) and using the cyclic identity $C_{\alpha\beta\gamma\delta} + C_{\alpha\gamma\delta\beta} + C_{\alpha\delta\beta\gamma} = 0$ for the traceless Weyl tensor, one could find the equivalence

$${}^*RR = {}^*CC := \frac{1}{2}\left(\epsilon_{\alpha\beta\mu\nu}C^{\mu\nu}{}_{\gamma\delta}\right)C^{\alpha\beta\gamma\delta} = {}^*C_{\alpha\beta\gamma\delta}C^{\alpha\beta\gamma\delta}\,, \tag{6.18}$$

which indicates that the Chern-Pontryagin density is conformally invariant [15] under a rescaling $g_{\mu\nu} \mapsto \Omega(x^\alpha)^2\cdot g_{\mu\nu}$ of the metric tensor.

With the Chern-Simons topological current K^μ in Eq.(6.4), one can integrate by parts and obtain $\int d^4x\,\phi^*RR = -4\int d^4x\,\phi\left(\partial_\mu K^\mu\right) = -4\int d^4x\,\partial_\mu\left(\phi K^\mu\right) + 4\int d^4x\left(\partial_\mu\phi\right)K^\mu$. Hence, instead of directly varying ϕ^*RR with respect to the inverse metric, we firstly vary the four-current K^μ by the Levi-Civita connection. It follows that

$$
\begin{aligned}
& \delta \int d^4x\, \phi\, {}^*RR \;\cong\; 4\int d^4x \left(\partial_\mu\phi\right)\delta K^\mu \\
= \quad & 2\int d^4x \left(\partial_\mu\phi\right)\epsilon^{\mu\alpha\beta\gamma} R^\xi{}_{\rho\beta\gamma}\,\delta\Gamma^\rho_{\alpha\xi} \\
= \quad & 2\int d^4x \left(\partial_\mu\phi\right)\epsilon^{\mu\alpha\beta\gamma} R^{\xi\nu}{}_{\beta\gamma}\left(\nabla_\xi\delta g_{\alpha\nu}-\nabla_\nu\delta g_{\alpha\xi}\right) \\
\cong \; - & 2\int d^4x \left[\left(\partial_\mu\phi\right)\epsilon^{\mu\alpha\beta\gamma}\nabla_\xi R^{\xi\nu}{}_{\beta\gamma}+\left(\partial_\mu\partial_\xi\phi\right)\epsilon^{\mu\alpha\beta\gamma}R^{\xi\nu}{}_{\beta\gamma}\right]\delta g_{\alpha\nu} \\
= \; - & 4\int d^4x \left[\left(\partial_\mu\phi\right)\epsilon^{\mu\alpha\beta\gamma}\nabla_\beta R_\gamma{}^\nu+\left(\partial_\mu\partial_\xi\phi\right){}^*R^{\mu\alpha\xi\nu}\right]\delta g_{\alpha\nu} \qquad (6.19)\\
= \quad & 4\int d^4x \left[\left(\partial^\mu\phi\right)\epsilon_{\mu\alpha\beta\gamma}\nabla^\beta R^\gamma{}_\nu+\left(\partial_\mu\partial_\xi\phi\right){}^*R^{\mu}{}_{\alpha}{}^{\xi}{}_{\nu}\right]\delta g^{\alpha\nu}, \qquad (6.20)
\end{aligned}
$$

where, in the third row we expanded $\delta\Gamma^\rho_{\alpha\xi}$ and made use of the cancelation $R^{\xi\nu}{}_{\beta\gamma}\nabla_\alpha\delta g_{\xi\nu}=0$ due to the skew-symmetry for the indices $\xi\leftrightarrow\nu$; in the fourth row, we applied the replacement $\nabla_\xi R^{\xi\nu}{}_{\beta\gamma}=\nabla_\beta R_\gamma{}^\nu-\nabla_\gamma R_\beta{}^\nu$ in accordance with the relation

$$\nabla^\alpha R_{\alpha\mu\beta\nu}=\nabla_\beta R_{\mu\nu}-\nabla_\nu R_{\mu\beta}, \qquad (6.21)$$

which is an implication of the second Bianchi identity $\nabla_\gamma R_{\alpha\mu\beta\nu}+\nabla_\nu R_{\alpha\mu\gamma\beta}+\nabla_\beta R_{\alpha\mu\nu\gamma}=0$; in the last step, we raised the indices of $\delta g_{\alpha\nu}$ to $\delta g^{\alpha\nu}$ and thus had the overall minus sign dropped. In Eq.(6.20) we adopted the usual notation $\partial^\mu\phi\equiv g^{\hat\mu\mu}\partial_{\hat\mu}\phi$, and note that $\left(\partial_\mu\partial_\xi\phi\right){}^*R^{\mu}{}_{\alpha}{}^{\xi}{}_{\nu}\neq\left(\partial^\mu\partial^\xi\phi\right){}^*R_{\mu\alpha\xi\nu}$ since in general the metric tensor does not commute with partial derivatives and thus $\partial^\mu\partial^\xi\phi=g^{\mu\hat\mu}\partial_{\hat\mu}\left(g^{\xi\hat\xi}\partial_{\hat\xi}\phi\right)\neq g^{\mu\hat\mu}g^{\xi\hat\xi}\partial_{\hat\mu}\partial_{\hat\xi}\phi$. Relabel the indices of Eq.(6.19) and we obtain the variational derivative

$$\frac{1}{\sqrt{-g}}\frac{\delta\left(\phi\,{}^*RR\right)}{\delta g^{\mu\nu}} \;=:\; H^{(\mathrm{CP})}_{\mu\nu} \quad \text{and}$$

$$\sqrt{-g}\,H^{(\mathrm{CP})}_{\mu\nu}=2\partial^\xi\phi\cdot\left(\epsilon_{\xi\mu\alpha\beta}\nabla^\alpha R^\beta{}_\nu+\epsilon_{\xi\nu\alpha\beta}\nabla^\alpha R^\beta{}_\mu\right)+2\partial_\alpha\partial_\beta\phi\cdot\left({}^*R^\alpha{}_\mu{}^\beta{}_\nu+{}^*R^\alpha{}_\nu{}^\beta{}_\mu\right). \qquad (6.22)$$

Compared with Eq.(6.16), $H^{(\mathrm{CP})}_{\mu\nu}$ does not contain a $-\frac{1}{2}\phi\,{}^*RRg_{\mu\nu}$ term, because ${}^*RR$ by itself already serves as a covariant density as opposed to the usual form $\sqrt{-g}\,\mathcal{R}$ for other curvature invariants.

Note that the nonminimal coupling between a scalar field and ${}^*RR$ is crucial to the Chern-Simons gravity; however, its original proposal Ref. [11] had adopted the opposite geometric system which uses the metric signature $(+,-\,-\,-)$, the conventions $\{R^\alpha{}_{\beta\gamma\delta}=\partial_\delta\Gamma^\alpha{}_{\gamma\beta}\cdots,\ R_{\mu\nu}=R^\alpha{}_{\mu\alpha\nu}\}$, Einstein's equation $R_{\mu\nu}-\frac{1}{2}Rg_{\mu\nu}=-8\pi GT^{(\mathrm{m})}_{\mu\nu}$, and the definition ${}^*RR=-{}^*R_{\alpha\beta\gamma\delta}R^{\alpha\beta\gamma\delta}=-\frac{1}{2}\left(\epsilon_{\alpha\beta\mu\nu}R^{\mu\nu}{}_{\gamma\delta}\right)R^{\alpha\beta\gamma\delta}$. This has caused quite a few mistakes in the subsequent Chern-Simons literature that adopt different conventions, and we hope the details in this subsection could correct these misunderstandings. Also, in Eq. (6.22), the quantities $\{\epsilon_{\xi\mu\alpha\beta},\ K^\mu,\ {}^*RR,\ R^\beta{}_\nu,\ {}^*R_{\beta\mu\alpha\nu}\}$ have the same values in both sets of sign conventions. See our note Ref.[24] for further clarification of this issue.

6.3.2 Coupling to the Gauss-Bonnet invariant

The third term $\phi\mathcal{G}$ in $\mathscr{L}_{\text{LBD}}$ represents the nonminimal coupling between the scalar field and the Gauss-Bonnet invariant $\mathcal{G} = R^2 - 4R_c^2 + R_m^2$, where we have employed the straightforward abbreviations $R_c^2 := R_{\alpha\beta}R^{\alpha\beta}$ and $R_m^2 := R_{\alpha\mu\beta\nu}R^{\alpha\mu\beta\nu}$ to denote the Ricci and Riemann tensor squares. Following the standard procedures of variational derivative as before in $\delta\left(\sqrt{-g}\phi R\right)/\delta g^{\mu\nu}$, we have

$$\frac{\delta\left(\sqrt{-g}\phi\mathcal{G}\right)}{\sqrt{-g}\;\delta g^{\mu\nu}} = \frac{\delta(\phi R^2)}{\delta g^{\mu\nu}} - 4\frac{\delta(\phi R_c^2)}{\delta g^{\mu\nu}} + \frac{\delta(\phi R_m^2)}{\delta g^{\mu\nu}} - \frac{1}{2}\phi\mathcal{G}g_{\mu\nu}, \tag{6.23}$$

with

$$\begin{aligned}
\frac{\delta\left(\phi R^2\right)}{\delta g^{\mu\nu}} &\cong 2\phi R R_{\mu\nu} + 2\left(g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu\right)(\phi R) &(6.24)\\
\frac{\delta\left(\phi R_c^2\right)}{\delta g^{\mu\nu}} &\cong 2\phi R_\mu{}^\alpha R_{\alpha\nu} + \Box\left(\phi R_{\mu\nu}\right) - \nabla_\alpha\nabla_\nu\left(\phi R_\mu{}^\alpha\right)\\
&\quad -\nabla_\alpha\nabla_\mu\left(\phi R_\nu{}^\alpha\right) + g_{\mu\nu}\nabla_\alpha\nabla_\beta\left(\phi R^{\alpha\beta}\right) &(6.25)\\
\frac{\delta\left(\phi R_m^2\right)}{\delta g^{\mu\nu}} &\cong 2\phi R_{\mu\alpha\beta\gamma}R_\nu{}^{\alpha\beta\gamma} + 4\nabla^\beta\nabla^\alpha\left(\phi R_{\alpha\mu\beta\nu}\right), &(6.26)
\end{aligned}$$

where total-derivative terms have been removed. Recall that besides Eq.(6.21), the second Bianchi identity also has the following implications which transform the derivative of a high-rank curvature tensor into that of lower-rank tensors plus nonlinear algebraic terms:

$$\begin{aligned}
\nabla^\alpha R_{\alpha\beta} &= \frac{1}{2}\nabla_\beta R &(6.27)\\
\nabla^\beta\nabla^\alpha R_{\alpha\beta} &= \frac{1}{2}\Box R &(6.28)\\
\nabla^\beta\nabla^\alpha R_{\alpha\mu\beta\nu} = \Box R_{\mu\nu} &- \frac{1}{2}\nabla_\mu\nabla_\nu R + R_{\alpha\mu\beta\nu}R^{\alpha\beta} - R_\mu{}^\alpha R_{\alpha\nu} &(6.29)\\
\nabla^\alpha\nabla_\mu R_{\alpha\nu} + \nabla^\alpha\nabla_\nu R_{\alpha\mu} &= \nabla_\mu\nabla_\nu R - 2R_{\alpha\mu\beta\nu}R^{\alpha\beta} + 2R_\mu{}^\alpha R_{\alpha\nu}. &(6.30)
\end{aligned}$$

Using Eq.(6.21) and Eqs.(6.27)-(6.30) to expand the second-order covariant derivatives in Eqs.(6.24)-(6.26), and putting them back into Eq.(6.23), we obtain

$$\frac{1}{\sqrt{-g}}\frac{\delta(\sqrt{-g}\,\phi\,\mathcal{G})}{\delta g^{\mu\nu}} =: H_{\mu\nu}^{(\text{GB})} \quad \text{with}$$

$$\begin{aligned}
H_{\mu\nu}^{(\text{GB})} =&\phi\left(2RR_{\mu\nu} - 4R_\mu{}^\alpha R_{\alpha\nu} - 4R_{\alpha\mu\beta\nu}R^{\alpha\beta} + 2R_{\mu\alpha\beta\gamma}R_\nu{}^{\alpha\beta\gamma}\right)\\
&+ 2R\left(g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu\right)\phi + 4R_\mu{}^\alpha\nabla_\alpha\nabla_\nu\phi + 4R_\nu{}^\alpha\nabla_\alpha\nabla_\mu\phi\\
&- 4R_{\mu\nu}\Box\phi - 4g_{\mu\nu}R^{\alpha\beta}\nabla_\alpha\nabla_\beta\phi + 4R_{\alpha\mu\beta\nu}\nabla^\beta\nabla^\alpha\phi - \frac{1}{2}\phi\mathcal{G}g_{\mu\nu},
\end{aligned} \tag{6.31}$$

where the second-order derivatives $\{\Box, \nabla_\alpha\nabla_\nu, \text{etc}\}$ only act on the scalar field ϕ.

However, we realize that Eq.(6.31) is still not the ultimate expression. In four dimensions, $\sqrt{-g}\,\mathcal{G}$ is proportional to the Euler-Poincaré topological density, $\mathcal{G} = \left(\frac{1}{2}\epsilon_{\alpha\beta\gamma\zeta}R^{\gamma\zeta\eta\xi}\right)\cdot\left(\frac{1}{2}\epsilon_{\eta\xi\rho\sigma}R^{\rho\sigma\alpha\beta}\right) = {}^*R_{\alpha\beta}{}^{\eta\xi}\cdot{}^*R_{\eta\xi}{}^{\alpha\beta}$, and the integral $\frac{1}{32\pi^2}\int dx^4\sqrt{-g}\,\mathcal{G}$ equates the Euler characteristic $\chi(\mathcal{M})$ of the spacetime. Thus $\frac{\delta}{\delta g^{\mu\nu}}\int dx^4\sqrt{-g}\,\mathcal{G} = 32\pi^2\frac{\delta}{\delta g^{\mu\nu}}\chi(\mathcal{M}) \equiv 0$. Based on Eqs.(6.24)-(6.26), one could easily obtain the Bach-Lanczos identity from the explicit variational derivative $\delta\left(\sqrt{-g}\,\mathcal{G}\right)/\delta g^{\mu\nu}$,

$$2RR_{\mu\nu} - 4R_{\mu}{}^{\alpha}R_{\alpha\nu} - 4R_{\alpha\mu\beta\nu}R^{\alpha\beta} + 2R_{\mu\alpha\beta\gamma}R_{\nu}{}^{\alpha\beta\gamma} \equiv \frac{1}{2}\mathcal{G}g_{\mu\nu}, \tag{6.32}$$

with which Eq.(6.31) can be best simplified into

$$\begin{aligned} H^{(\mathrm{GB})}_{\mu\nu} &= 2R\left(g_{\mu\nu}\Box - \nabla_{\mu}\nabla_{\nu}\right)\phi + 4R_{\mu}{}^{\alpha}\nabla_{\alpha}\nabla_{\nu}\phi + 4R_{\nu}{}^{\alpha}\nabla_{\alpha}\nabla_{\mu}\phi \\ &\quad - 4R_{\mu\nu}\Box\phi - 4g_{\mu\nu}\cdot R^{\alpha\beta}\nabla_{\alpha}\nabla_{\beta}\phi + 4R_{\alpha\mu\beta\nu}\nabla^{\beta}\nabla^{\alpha}\phi, \end{aligned} \tag{6.33}$$

whose trace is

$$g^{\mu\nu}H^{(\mathrm{GB})}_{\mu\nu} = 2R\Box\phi - 4R^{\alpha\beta}\nabla_{\alpha}\nabla_{\beta}\phi. \tag{6.34}$$

In the existent literature, the effects of the generalized and thus nontrivial Gauss-Bonnet dependence for the field equations are generally depicted in the form analogous to Eq.(6.31), such as the string-inspired Gauss-Bonnet effective dark energy [12] with $\mathscr{L} = \frac{1}{16\pi G}R - \frac{\gamma}{2}\partial_{\mu}\varphi\partial^{\mu}\varphi - V(\varphi) + f(\varphi)\mathcal{G}$, as well as the $R + f(\mathcal{G})$ [3], the $f(R,\mathcal{G})$ [4] and the $f(R,\mathcal{G},\mathscr{L}_m)$ [14] generalized Gauss-Bonnet gravities. Here we emphasize that the Gauss-Bonnet effects therein could all be simplified into the form of Eq.(6.33).

6.3.3 Gravitational field equation

Collecting the results in Eqs.(6.16), (6.22), and (6.33), we finally obtain the gravitational field equation

$$\begin{aligned} &\phi\left(R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu}\right) - \frac{\omega_{\mathrm{L}}}{\phi}\left(\nabla_{\mu}\phi\nabla_{\nu}\phi - \frac{1}{2}g_{\mu\nu}\nabla_{\alpha}\phi\nabla^{\alpha}\phi\right) \\ &+ \left(g_{\mu\nu}\Box - \nabla_{\mu}\nabla_{\nu}\right)\phi + aH^{(\mathrm{CP})}_{\mu\nu} + bH^{(\mathrm{GB})}_{\mu\nu} = 8\pi T^{(\mathrm{m})}_{\mu\nu}, \end{aligned} \tag{6.35}$$

where $H^{(\mathrm{CP})}_{\mu\nu}$ vanishes for all spherically symmetric or conformal flat spacetimes. Eq.(6.35) yields the trace equation

$$-\phi R + \frac{\omega_{\mathrm{L}}}{\phi}\nabla_{\alpha}\phi\nabla^{\alpha}\phi + (3 + 2bR)\,\Box\phi - 4bR^{\alpha\beta}\nabla_{\alpha}\nabla_{\beta}\phi = 8\pi T^{(\mathrm{m})}, \tag{6.36}$$

where $H^{(\mathrm{CP})}_{\mu\nu}$ is always traceless, $g^{\mu\nu}H^{(\mathrm{CP})}_{\mu\nu} \equiv 0$ – this is not a surprise because it equivalently traces back to the effects of the dual square ${}^*CC$ of the traceless Weyl tensor.

Note that in existent studies the invariants ${}^*RR$ and $\mathcal{G}$ have demonstrated their importance in various aspects. For example, as shown by Eq.(6) of Ref.[25] [recall the equivalence ${}^*RR = {}^*CC$ in Eq.(6.18)], in the effective field theory for the initial cosmic inflation, the only leading-order fluctuations to the standard inflation action in the tensor modes are the parity-violation Chern-Pontryagin and the topological Gauss-Bonnet effects.

6.3.4 Wave equations

Straightforward extremization of $\mathcal{S}_{\text{LBD}}$ with respect to the scalar field yields the *kinematical* wave equation

$$\frac{2\omega_{\text{L}}}{\phi}\Box\phi = -R + \frac{\omega_{\text{L}}}{\phi^2}\nabla_\alpha\phi\nabla^\alpha\phi - \left(\frac{a}{\sqrt{-g}}{}^*RR + b\mathcal{G}\right), \tag{6.37}$$

with $\Box\phi = \frac{1}{\sqrt{-g}}\partial_\alpha\left(\sqrt{-g}\,g^{\alpha\beta}\partial_\beta\phi\right)$. We regard Eq.(6.37) as "kinematical" because it does not explicitly relate the propagation of ϕ to the matter distribution $\mathscr{L}_m$ or $T^{(\text{m})} = g^{\mu\nu}T^{(\text{m})}_{\mu\nu}$.

Combine Eq.(6.37) with the gravitational trace equation (6.36), and it follows that

$$(2\omega_{\text{L}} + 3 + 2bR)\,\Box\phi = -\left(\frac{a}{\sqrt{-g}}{}^*RR + b\mathcal{G}\right)\phi + 8\pi T^{(\text{m})} + 4bR^{\alpha\beta}\nabla_\alpha\nabla_\beta\phi, \tag{6.38}$$

which serves as the generalized Klein-Gordon equation that governs the dynamics of the scalar field.

6.4 The $\omega_{\text{L}} \to \infty$ limit and GR

From the dynamical equation (6.38), we obtain

$$\Box\phi = \frac{1}{2\omega_{\text{L}} + 3 + 2bR}\left\{-\left(\frac{a}{\sqrt{-g}}{}^*RR + b\mathcal{G}\right)\phi + 8\pi T^{(\text{m})} + 4bR^{\alpha\beta}\nabla_\alpha\nabla_\beta\phi\right\}. \tag{6.39}$$

The topology-gravity coupling strengths $\{a, b\}$ should take finite values – just like the Newtonian constant G for matter-gravity coupling. Similarly the curvature invariants $\{R, {}^*RR, \mathcal{G}\}$ for a physical spacetime should be finite, and we further assume the scalar field ϕ to be nonsingular. Thus, in the limit $\omega_{\text{L}} \to \infty$, Eq.(6.39) yields $\Box\phi = \mathbb{O}\left(\frac{1}{\omega_{\text{L}}}\right)$ and

$$\phi = \langle\phi\rangle + \mathbb{O}\left(\frac{1}{\omega_{\text{L}}}\right) = \frac{1}{G} + \mathbb{O}\left(\frac{1}{\omega_{\text{L}}}\right), \tag{6.40}$$

where $\langle\phi\rangle$ denotes the expectation value of the scalar field and we expect it to be the inverse of the Newtonian constant $1/G$. Under the behaviors Eq.(6.40) in the infinite ω_{L} limit, we have $H^{(\text{CP})}_{\mu\nu} = 0 = H^{(\text{GB})}_{\mu\nu}$, and the field equation (6.35) reduces to become Einstein's equation $R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} = 8\pi GT^{(\text{m})}_{\mu\nu}$.

On the other hand, from Eq.(6.39) we can also observe that $\Box\phi \equiv 0$ in the special situation

$$-4bR^{\alpha\beta}\nabla_\alpha\nabla_\beta\phi + \left(\frac{a}{\sqrt{-g}}{}^*RR + b\mathcal{G}\right)\phi = 8\pi T^{(\text{m})}, \tag{6.41}$$

and the scalar field becomes undeterminable from the dynamical equation (6.39).

The term $-4bR^{\alpha\beta}\nabla_\alpha\nabla_\beta\phi$ comes from the trace $g^{\mu\nu}H^{(\text{GB})}_{\mu\nu}$, while ${}^*RR$ and $\mathcal{G}$ are respectively related to the topological instanton number [15] and the Euler characteristic. Thus, all terms on the left hand side of Eq.(6.41) are related to topological effects nonminimally coupled with ϕ, and they cancel out the trace of the matter tensor. In this sense, we call Eq.(6.41) the *topological balance condition*.

Putting $\Box\phi \equiv 0$ and the condition Eq.(6.41) back into the trace equation (6.36), we obtain

$$\frac{\omega_L}{\phi^2}\nabla_\alpha\phi\nabla^\alpha\phi = R + \frac{a}{\sqrt{-g}}{}^*RR + b\mathcal{G} \tag{6.42}$$

$$= -\omega_L \Box \ln\phi, \tag{6.43}$$

where in the second step we further made use of the expansion $\Box \ln\phi = \nabla^\alpha\left(\frac{1}{\phi}\nabla_\alpha\phi\right) = -\frac{1}{\phi^2}\nabla_\alpha\phi\nabla^\alpha\phi + \frac{1}{\phi}\Box\phi = -\frac{1}{\phi^2}\nabla_\alpha\phi\nabla^\alpha\phi$ for $\Box\phi \equiv 0$. Thus it follows that

$$\omega_L \nabla_\alpha (\ln\phi)\, \nabla^\alpha (\ln\phi) = R + \frac{a}{\sqrt{-g}}{}^*RR + b\mathcal{G}\,. \tag{6.44}$$

For $\omega_L \to \infty$, this equation gives the estimate

$$\left\| \nabla_\alpha(\ln\phi) \right\| \sim \sqrt{\frac{R + \frac{a}{\sqrt{-g}}{}^*RR + b\mathcal{G}}{\omega_L}} \sim \mathbb{O}\left(\frac{1}{\sqrt{\omega_L}}\right), \tag{6.45}$$

which integrates to yield $\ln\phi = \text{constant} + \mathbb{O}\left(\frac{1}{\sqrt{\omega_L}}\right)$. Hence, ϕ satisfies

$$\phi \sim \phi_0 + \mathbb{O}\left(\frac{1}{\sqrt{\omega_L}}\right), \tag{6.46}$$

where the constant ϕ_0 is the average value of ϕ. In accordance with Eq.(6.42) and the estimate Eq.(6.46), the term $-\frac{\omega_L}{\phi}\left(\nabla_\mu\phi\nabla_\nu\phi - \frac{1}{2}g_{\mu\nu}\nabla_\alpha\phi\nabla^\alpha\phi\right)$ in the field equation (6.35), which arises from the source $-\frac{\omega_L}{\phi}\nabla_\alpha\phi\nabla^\alpha\phi$ in $\mathcal{S}_{LBD}$, will not vanish. This way, the $\omega_L \to \infty$ limit could not recover Einstein's equation and GR in situations where the topological balance condition Eq.(6.41) holds, although the existence of such solutions remains to be carefully checked.

This is similar to the Brans-Dicke theory given by the action Eq.(6.10), which recovers GR in the limit $\omega_{BD} \to \infty$, unless the stress-energy-momentum tensor has a vanishing trace $T^{(m)} = 0$ [26], such as the matter content being radiation with $P_{rad} = \frac{1}{3}\rho_{rad}$ and $T^{(m)}_{rad} = -\rho_{rad} + 3P_{rad} = 0$.

6.5 Energy-momentum conservation

In modified gravities with the generic Lagrangian density $\mathscr{L} = f(R, \mathcal{R}_i, \cdots)$, where $\mathcal{R}_i = \mathcal{R}_i(g_{\alpha\beta}, R_{\alpha\mu\beta\nu}, \nabla_\gamma R_{\alpha\mu\beta\nu}, \cdots, \nabla_{\gamma_1}\nabla_{\gamma_2}\ldots\nabla_{\gamma_n}R_{\alpha\mu\beta\nu})$ and the "$\cdots$" in $\mathscr{L} = f$ refer to arbitrary curvature invariants beyond the Ricci scalar, the energy-momentum conservation is naturally guaranteed by Noether's law or the generalized contracted Bianchi identities [27]

$$\nabla^\mu\left(\frac{1}{\sqrt{-g}}\frac{\delta\left[\sqrt{-g}\, f(R, \mathcal{R}_i, \cdots)\right]}{\delta g^{\mu\nu}}\right) = 0, \tag{6.47}$$

which can be expanded into

$$f_R R_{\mu\nu} + \sum f_{\mathcal{R}_i}\mathcal{R}^{(i)}_{\mu\nu} - \frac{1}{2}f(R, \mathcal{R}_i, \cdots)\, g_{\mu\nu} = 0, \tag{6.48}$$

where $f_R := \partial f(R, \mathcal{R}_i, \cdots)/\partial R$, $f_{\mathcal{R}_i} := \partial f(R, \mathcal{R}_i, \cdots)/\partial \mathcal{R}_i$, and $\mathcal{R}^{(i)}_{\mu\nu} \cong (f_{\mathcal{R}_i} \delta \mathcal{R}_i)/\delta g^{\mu\nu}$. However, in the more generic situations of scalar-tensor-type gravities with $\mathscr{L} = f(\phi, R, \mathcal{R}_i, \cdots) + \varpi(\phi, \nabla_\alpha\phi\nabla^\alpha\phi)$ where nonminimal couplings between the scalar fields and the curvature invariants are involved, such as the LBD proposal under discussion, the conservation problem is more complicated than pure tensorial gravity.

Now let's get back to the LBD field equation (6.35). By the coordinate invariance or the diffeomorphism invariance of the matter action $\mathcal{S}_m$ in which $\mathscr{L}_m$ is neither coupled with the curvature invariants nor the scalar field ϕ, naturally we have the energy-momentum conservation $\nabla^\mu T^{(\mathrm{m})}_{\mu\nu} = 0$ for the matter content. Thus, the covariant derivative of the left hand side of Eq.(6.35) should also vanish. With the Bianchi identity $\nabla^\mu \left(R_{\mu\nu} - \frac{1}{2} R g_{\mu\nu}\right) = 0$ and the third-order-derivative commutator $(\nabla_\nu \Box - \Box \nabla_\nu)\phi = -R_{\mu\nu}\nabla^\mu\phi$, it follows that

$$\nabla^\mu \left[\phi\left(R_{\mu\nu} - \frac{1}{2} R g_{\mu\nu}\right) + \left(g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu\right)\phi\right] = -\frac{1}{2} R\, \nabla_\nu \phi. \tag{6.49}$$

Moreover, for the scalar field, we have

$$\begin{aligned}\nabla^\mu \left[-\frac{\omega_{\mathrm{L}}}{\phi}\left(\nabla_\mu\phi\nabla_\nu\phi - \frac{1}{2} g_{\mu\nu}\nabla_\alpha\phi\nabla^\alpha\phi\right)\right] &= \frac{1}{2}\nabla_\nu\phi \cdot \left(\frac{\omega_{\mathrm{L}}}{\phi^2}\nabla_\alpha\phi\nabla^\alpha\phi - \frac{2\omega_{\mathrm{L}}}{\phi}\Box\phi\right) \\ &= \frac{1}{2}\nabla_\nu\phi \cdot \left(R + \frac{a}{\sqrt{-g}}{}^*RR + b\mathcal{G}\right),\end{aligned} \tag{6.50}$$

where the kinematical wave equation (6.37) has been employed.

For the Chern-Pontryagin and the Gauss-Bonnet parts in Eq.(6.35), consider the componential actions $\mathcal{S}_{\mathrm{CP}} = \int d^4x\, \phi\, {}^*RR$ and $\mathcal{S}_{\mathrm{GB}} = \int d^4x \sqrt{-g}\phi\mathcal{G}$. Under an arbitrary infinitesimal coordinate transformation $x^\mu \mapsto x^\mu + \delta x^\mu$, where $\delta x^\mu = \xi^\mu$ is an infinitesimal vector field which vanishes on the boundary, so that the spacetime manifold is mapped onto itself. Then $\mathcal{S}_{\mathrm{CP}}$ and $\mathcal{S}_{\mathrm{GB}}$ vary by

$$\delta\mathcal{S}_{\mathrm{CP}} = -\int d^4x\, \phi\, \partial_\mu\left(\xi^{\mu *}RR\right) \cong \int d^4x\, {}^*RR\left(\partial_\mu\phi\right)\xi^\mu, \tag{6.51}$$

$$\delta\mathcal{S}_{\mathrm{GB}} = -\int d^4x\, \phi\, \partial_\mu\left(\xi^\mu \sqrt{-g}\mathcal{G}\right) \cong \int d^4x \sqrt{-g}\mathcal{G}\left(\partial_\mu\phi\right)\xi^\mu. \tag{6.52}$$

For the first step in Eqs.(6.51) and Eqs.(6.52), one should note that $x^\mu \mapsto x^\mu + \xi^\mu$ is a particle/active transformation, under which the dynamical tensor fields transform, while the background scalar field $\phi(x^\alpha)$ and the coordinate system parameterizing the spacetime manifold remain unchanged [28]. On the other hand, the inverse metric transforms by $g^{\mu\nu} \mapsto g^{\mu\nu} + \delta g^{\mu\nu}$ with $\delta g^{\mu\nu} = -\pounds_{\vec{\xi}} g^{\mu\nu} = \nabla^\mu\xi^\nu + \nabla^\nu\xi^\mu$, and thus we have

$$\delta\mathcal{S}_{\mathrm{CP}} = 2\int d^4x \sqrt{-g}\, H^{(\mathrm{CP})}_{\mu\nu}\, \nabla^\mu\xi^\nu \cong -2\int d^4x \sqrt{-g}\, \left(\nabla^\mu H^{(\mathrm{CP})}_{\mu\nu}\right)\xi^\nu, \tag{6.53}$$

$$\delta\mathcal{S}_{\mathrm{GB}} = 2\int d^4x \sqrt{-g}\, H^{(\mathrm{GB})}_{\mu\nu}\nabla^\mu\xi^\nu \cong -2\int d^4x \sqrt{-g}\, \left(\nabla^\mu H^{(\mathrm{GB})}_{\mu\nu}\right)\xi^\nu. \tag{6.54}$$

Comparing Eqs.(6.51) with (6.53), and Eqs.(6.52) with (6.54), we obtain the relations

$$\nabla^\mu H^{(\mathrm{CP})}_{\mu\nu} = -\frac{1}{2}\frac{{}^*RR}{\sqrt{-g}} \cdot \partial_\nu\phi\,, \tag{6.55}$$

$$\nabla^\mu H^{(\mathrm{GB})}_{\mu\nu} = -\frac{1}{2}\mathcal{G}\cdot\partial_\nu\phi\,. \tag{6.56}$$

Adding up Eqs.(6.49), (6.50), (6.55), and (6.56), one could find that the covariance divergence for the left hand side of the field equation (6.35) vanishes, which confirms the energy-momentum conservation in the LBD gravity.

Eqs.(6.55) and (6.56) for the nontrivial divergences of $H^{(\mathrm{CP})}_{\mu\nu}$ and $H^{(\mathrm{GB})}_{\mu\nu}$, by their derivation process, reflect the breakdown of diffeomorphism invariance for $\mathcal{S}_{\mathrm{CP}}$ and $\mathcal{S}_{\mathrm{GB}}$ in $\mathcal{S}_{\mathrm{LBD}}$. They have clearly shown the influences of nonminimal ϕ-topology couplings to the covariant conservation, as opposed to the straightforward generalized Bianchi identities

$$\nabla^\mu\left(\frac{1}{\sqrt{-g}}\frac{\delta\,{}^*RR}{\delta g^{\mu\nu}}\right)=0 \quad \text{and} \quad \nabla^\mu\left(\frac{1}{\sqrt{-g}}\frac{\delta(\sqrt{-g}\,\mathcal{G})}{\delta g^{\mu\nu}}\right)=0. \tag{6.57}$$

6.6 Conformal transformations

The standard LBD action $\mathcal{S}_{\mathrm{LBD}}$ in Eq.(6.12) can be transformed into different representations by conformal rescaling of the spacetime line element, which geometrically preserves the angles between spacetime vectors and physically retains local causality structures.

6.6.1 Dynamical Chern-Simons gravity

As a simplest example, consider the specialized $\mathcal{S}_{\mathrm{LBD}}$ in vacuum and for spacetimes of negligible gravitational effects from the nonminimally ϕ−coupled Gauss-Bonnet term. With $\mathcal{S}_m = 0$ and $b = 0$, Eq.(6.12) reduces to become

$$\mathcal{S} = \frac{1}{16\pi}\int d^4x\left[\sqrt{-g}\left(\phi R - \frac{\omega_{\mathrm{L}}}{\phi}\nabla_\alpha\phi\nabla^\alpha\phi\right) + a\phi\,{}^*RR\right]. \tag{6.58}$$

For a pointwise scaling field $\Omega = \Omega(x^\alpha) > 0$, we can rescale the metric $g_{\mu\nu}$ of the original frame into $\tilde{g}_{\mu\nu}$ via $\tilde{g}_{\mu\nu} = \Omega^2 g_{\mu\nu}$; it follows that $g_{\mu\nu} = \Omega^{-2}\tilde{g}_{\mu\nu}$, $g^{\mu\nu} = \Omega^2\tilde{g}^{\mu\nu}$, $\sqrt{-g} = \Omega^{-4}\sqrt{-\tilde{g}}$, and[2] [10]

$$R = \Omega^2\left[\tilde{R} + 6\Box(\ln\Omega) - 6\tilde{g}^{\alpha\beta}\partial_\alpha(\ln\Omega)\,\partial_\beta(\ln\Omega)\right]. \tag{6.59}$$

Hence, for the reduced LBD action Eq.(6.58), the conformal transformation

$$g_{\mu\nu} = \frac{1}{G\phi}\cdot\tilde{g}_{\mu\nu} \tag{6.60}$$

along with the redefinition of the scalar field $\{\vartheta = \vartheta(x^\alpha),\ \phi = \phi(\vartheta)\}$ lead to

$$\mathcal{S} \cong \frac{1}{16\pi G}\int d^4x\left[\sqrt{-\tilde{g}}\left(\tilde{R} - \frac{2\omega_{\mathrm{L}}+3}{2\phi(\vartheta)^2}\left(\frac{d\phi}{d\vartheta}\right)^2\tilde{\nabla}_\alpha\vartheta\tilde{\nabla}^\alpha\vartheta\right) + a\,\phi(\vartheta)\,{}^*RR\right], \tag{6.61}$$

[2] Compared with $R = \Omega^2\left[\tilde{R} + 6\Box\Omega/\Omega - 12\tilde{g}^{\alpha\beta}\partial_\alpha\Omega\partial_\beta\Omega/\Omega^2\right]$, Eq.(6.59) best isolates pure-divergence terms and thus most simplifies the action once the coefficient of R is reset into unity. Moreover, by employing $\ln\Omega$ instead of Ω, the transformations $R\to\tilde{R}$ becomes skew-symmetric to $\tilde{R}\to R$.

where the scalar field ϑ no longer directly couples to the Ricci scalar $\tilde{R}$, and thus the $6\Box(\ln\Omega)$ component in Eq.(6.59) has been removed as it simply yields a boundary term $6\int\partial_\alpha\left[\sqrt{-g}\partial^\alpha(\ln\Omega)\right]d^4x$ for the action. Also, Eq.(6.61) has utilized the fact that the (1, 3)-type Weyl tensor $C^\alpha{}_{\beta\gamma\delta}$ and thus ${}^*RR = {}^*CC = {}^*\widetilde{CC} = {}^*\widetilde{RR}$ are conformally invariant. It is straightforward to observe from Eq.(6.61) that the kinetics of ϑ is canonical for $\omega_{\rm L} > -3/2$, noncanonical for $\omega_{\rm L} < -3/2$, and nondynamical for $\omega_{\rm L} = -3/2$; here we are interested in the canonical case. For the specialization

$$d\vartheta = \pm\sqrt{2\omega_{\rm L}+3}\,\frac{d\phi}{\phi}, \tag{6.62}$$

which integrates to yield

$$\vartheta = \pm\sqrt{2\omega_{\rm L}+3}\,\ln\frac{\phi}{\phi_0}, \tag{6.63}$$

where ϕ_0 is an integration constant, or inversely

$$\phi = \phi_0\exp\left(\pm\frac{\vartheta}{\sqrt{2\omega_{\rm L}+3}}\right), \tag{6.64}$$

the action Eq.(6.65) finally becomes

$$\mathcal{S} = \frac{1}{16\pi G}\int d^4x\left[\sqrt{-\tilde{g}}\left(\tilde{R}-\frac{1}{2}\tilde{\nabla}_\alpha\vartheta\tilde{\nabla}^\alpha\vartheta\right)+a\phi_0\exp\left(\pm\frac{\vartheta}{\sqrt{2\omega_{\rm L}+3}}\right){}^*\widetilde{RR}\right]. \tag{6.65}$$

Hence, the conformal rescaling $g_{\mu\nu} = \tilde{g}_{\mu\nu}/G\phi$ along with the new scalar field $\vartheta(x^\alpha)$ recast the reduced LBD action Eq.(6.58) into Eq.(6.65), which is an action for the dynamical Chern-Simons gravity [19], though the nonminimal ϑ–${}^*\widetilde{RR}$ coupling is slightly more complicated than the straightforward $\vartheta{}^*\widetilde{RR}$ as in the popular Chern-Simons literature. Moreover, the conformal invariance of ${}^*RR$ guarantees that the effect of $\int d^4x\,\phi{}^*RR$ could never be removed by conformal transformations.

Note that the matter action $\mathcal{S}_m(g_{\mu\nu},\psi_m)$ would be transformed into $\mathcal{S}_m(\tilde{g}_{\mu\nu}/G\phi,\psi_m)$ (in general S_m does not contain derivatives of the metric tensor [20]), which are different in the ϕ–$\mathcal{S}_m$ or ϕ–$\mathscr{L}_m$ couplings; consequently $T^{(\rm m)}_{\mu\nu}$ fails to be conformally invariant unless it is traceless $T^{(\rm m)} = 0$ [10]. This is why we focus on the vacuum situation.

6.6.2 Generalized Gauss-Bonnet dark energy

Similarly, in vacuum and for spacetimes of negligible Chern-Simons parity-violation effect, $\mathcal{S}_{\rm LBD}$ reduces into

$$\mathcal{S} = \frac{1}{16\pi}\int d^4x\left[\sqrt{-g}\left(\phi R + b\phi\mathcal{G} - \frac{\omega_{\rm L}}{\phi}\nabla_\alpha\phi\nabla^\alpha\phi\right)\right]. \tag{6.66}$$

Under the local rescaling $g_{\mu\nu}\mapsto\tilde{g}_{\mu\nu} = \Omega^2 g_{\mu\nu}$ for the metric, the Gauss-Bonnet scalar satisfies [29]

$$\begin{aligned}\mathcal{G} = \Omega^4\Big\{&\widetilde{\mathcal{G}} - 8\tilde{R}^{\alpha\beta}\tilde{\nabla}_\alpha\tilde{\nabla}_\beta(\ln\Omega) - 8\tilde{R}^{\alpha\beta}\tilde{\nabla}_\alpha(\ln\Omega)\tilde{\nabla}_\beta(\ln\Omega) + 4\tilde{R}\,\Box(\ln\Omega) - 8\Box(\ln\Omega)\cdot\tilde{\nabla}_\alpha(\ln\Omega)\tilde{\nabla}^\alpha(\ln\Omega)\\ &+ 8\left[\Box(\ln\Omega)\right]^2 - 8\tilde{\nabla}_\alpha\tilde{\nabla}_\beta(\ln\Omega)\cdot\tilde{\nabla}^\alpha\tilde{\nabla}^\beta(\ln\Omega) - 16\tilde{\nabla}_\alpha\tilde{\nabla}_\beta(\ln\Omega)\cdot\tilde{\nabla}^\alpha(\ln\Omega)\tilde{\nabla}^\beta(\ln\Omega)\Big\}.\end{aligned} \tag{6.67}$$

Set the factor of conformal transformation to be $\Omega = \sqrt{G\phi}$ so that the Ricci scalar decouples from the scalar field, and redefine the scalar field via $\phi(x^\alpha) \mapsto \varphi(x^\alpha) = \sqrt{2\omega_L + 3}\,\ln\frac{\phi}{\phi_0}$ or equivalently $\phi = \phi_0 \exp\left(\frac{\varphi}{\sqrt{2\omega_L+3}}\right)$; then it follows that

$$
\begin{aligned}
\ln\Omega &= \frac{1}{2}\ln\phi + \frac{1}{2}\ln G \\
&= \frac{1}{2}\frac{\varphi}{\sqrt{2\omega_L + 3}} + \frac{1}{2}\ln\phi_0 + \frac{1}{2}\ln G\,.
\end{aligned}
\tag{6.68}
$$

With $\{\ln\phi_0, \ln G\}$ being constants, substitution of Eq.(6.68) into Eq.(6.67) yields

$$
\sqrt{-g}\,\mathcal{G} = \sqrt{-\tilde{g}}\left(\tilde{\mathcal{G}} + \frac{\mathcal{K}(\tilde{\nabla}\varphi)}{\sqrt{2\omega_L + 3}}\right) \quad \text{and} \tag{6.69}
$$

$$
\begin{aligned}
\mathcal{K}(\tilde{\nabla}\varphi) = &-2\tilde{R}^{\alpha\beta}\left(2\tilde{\nabla}_\alpha\tilde{\nabla}_\beta\varphi + \tilde{\nabla}_\alpha\varphi\tilde{\nabla}_\beta\varphi\right) + \Box\varphi\cdot\left(2\tilde{R} + 2\Box\varphi - \tilde{\nabla}_\alpha\varphi\tilde{\nabla}^\alpha\varphi\right) \\
&-2\tilde{\nabla}_\alpha\tilde{\nabla}_\beta\varphi\cdot\left(\tilde{\nabla}^\alpha\tilde{\nabla}^\beta\varphi + \tilde{\nabla}^\alpha\varphi\tilde{\nabla}^\beta\varphi\right).
\end{aligned}
\tag{6.70}
$$

Here one can observe that since the coefficient Ω^{-4} in $\sqrt{-g} = \Omega^{-4}\sqrt{-g}$ exactly neutralizes the Ω^4 in Eq.(6.67), the nonminimally ϕ-coupled Gauss-Bonnet effect $\int d^4x\,\sqrt{-g}\phi\mathcal{G}$ could never be canceled by a conformal rescaling $g_{\mu\nu} = \Omega^{-2}\tilde{g}_{\mu\nu}$. Hence, the reduced LBD action Eq.(6.66) is finally transformed into

$$
\mathcal{S} = \frac{1}{16\pi G}\int d^4x\,\sqrt{-\tilde{g}}\left\{\tilde{R} - \frac{1}{2}\tilde{\nabla}_\alpha\varphi\tilde{\nabla}^\alpha\varphi + b\phi_0\exp\left(\frac{\varphi}{\sqrt{2\omega_L + 3}}\right)\left[\tilde{\mathcal{G}} + \mathcal{K}(\tilde{\nabla}\varphi)\right]\right\}, \tag{6.71}
$$

which generalizes the canonical Gauss-Bonnet dark energy in vacuum $\mathcal{S} = \frac{1}{16\pi G}\int d^4x\,\sqrt{-g}\left(R - \frac{1}{2}\nabla_\alpha\varphi\nabla^\alpha\varphi + f(\varphi)\mathcal{G}\right)$ [12] by the Horndeski-like [30] or Galileon-like [31] kinetics in $\mathcal{K}(\tilde{\nabla}\varphi)$ for the scalar field.

Note that in the two examples just above, because of the nonminimal coupling to the scalar field $\phi(x^\alpha)$, negligible Gauss-Bonnet effect does not imply a zero Euler characteristic $\chi(\mathcal{M}) = \frac{1}{32\pi^2}\int\sqrt{-g}\,\mathcal{G}d^4x = 0$ for the spacetime, and similarly, negligibility of the Chern-Simons effect does not indicate a vanishing instanton number $\int {}^*RR\,d^4x = 0$, either.

Also, for the actions of the Chern-Simons gravity and the Gauss-Bonnet dark energy in the Jordan frame, in which a scalar field is respectively coupled to ${}^*RR$ and $\mathcal{G}$, we cannot help but ask that why the scalar field is not simultaneously coupled to the Ricci scalar? We have previously seen from Eq.(6.47) that all algebraic and differential Riemannian invariants stand equal in front of the generalized Bianchi identities, so are there any good reasons for the scalar field to discriminate among different curvature invariants? We hope that the LBD gravity help release this tension (at least in empty spacetimes), as the scalar field ϕ indiscriminately couples to all the LBD invariants $\{R, {}^*RR, \mathcal{G}\}$, and the LBD gravity takes the Chern-Simons gravity and the Gauss-Bonnet dark energy as its reduced representations in the Einstein frame.

6.7 Cosmological applications

Having extensively discussed the theoretical structures of the LBD gravity, in this section we will apply this theory to the Friedman-Robertson-Walker (FRW) Universe and investigate the possibility to realize the late-time cosmic acceleration.

6.7.1 Generalized Friedmann and Klein-Gordon equations

The field equation (6.35) can be recast into a GR form,

$$R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} = \kappa^2 G_{\text{eff}}\left(T^{(\text{m})}_{\mu\nu} + T^{(\phi)}_{\mu\nu} + T^{(\text{CP})}_{\mu\nu} + T^{(\text{GB})}_{\mu\nu}\right), \tag{6.72}$$

where $\kappa^2 = 8\pi$, and $G_{\text{eff}} = 1/\phi$ denotes the effective gravitational coupling strength. $T^{(\text{m})}_{\mu\nu} + T^{(\phi)}_{\mu\nu} + T^{(\text{CP})}_{\mu\nu} + T^{(\text{GB})}_{\mu\nu} =: T^{(\text{eff})}_{\mu\nu}$ compromises the total effective stress-energy-momentum tensor, with

$$\begin{aligned} \kappa^2 T^{(\text{CP})}_{\mu\nu} &= -aH^{(\text{CP})}_{\mu\nu} \quad , \quad \kappa^2 T^{(\text{GB})}_{\mu\nu} = -bH^{(\text{GB})}_{\mu\nu}, \text{ and} \\ \kappa^2 \qquad T^{(\phi)}_{\mu\nu} &= \left(\nabla_\mu\nabla_\nu - g_{\mu\nu}\Box\right)\phi + \frac{\omega_{\text{L}}}{\phi}\left(\nabla_\mu\phi\nabla_\nu\phi - \frac{1}{2}g_{\mu\nu}\nabla_\alpha\phi\nabla^\alpha\phi\right). \end{aligned} \tag{6.73}$$

Note that besides the effects of the source term $-\frac{\omega_{\text{L}}}{\phi}\nabla_\alpha\phi\nabla^\alpha\phi$ in $\mathscr{L}_{\text{LBD}}$ via $\delta\left(-\sqrt{-g}\,\frac{\omega_{\text{L}}}{\phi}\nabla_\alpha\phi\nabla^\alpha\phi\right)/\delta g^{\mu\nu}$, the $\left(\nabla_\mu\nabla_\nu - g_{\mu\nu}\Box\right)\phi$ part from $\delta\left(\sqrt{-g}\phi R\right)/\delta g^{\mu\nu}$ is also packed into $T^{(\phi)}_{\mu\nu}$. Moreover, with the four distinct components of $T^{(\text{eff})}_{\mu\nu}$ sharing the same gravitational strength $1/\phi$, Eq.(6.72) implicitly respects the equivalence principle that the gravitational interaction is independent of the internal structures and compositions of a test body or self-gravitating object [21].

For the FRW metric of the flat Universe with a vanishing spatial curvature index,

$$ds^2 = -dt^2 + a(t)^2\sum_{i=1}^{3}\left(dx^i\right)^2, \tag{6.74}$$

${}^*RR = 0$ due to the maximal spatial symmetry, while the Ricci and Gauss-Bonnet scalars are respectively

$$\begin{aligned} R &= 6\frac{a\ddot{a} + \dot{a}^2}{a^2} = 6\left(\dot{H} + 2H^2\right) \\ \mathcal{G} &= 24\frac{\dot{a}^2\ddot{a}}{a^3} = 24H^2\left(\dot{H} + H^2\right), \end{aligned} \tag{6.75}$$

where overdot denotes the derivative over the cosmic comoving time, and $H := \dot{a}/a$ represents the time-dependent Hubble parameter. Thus, an accelerated/decelerated flat Universe has a positive/negative Euler-Poincaré topological density. With a perfect-fluid form $T^\mu{}_\nu = \text{diag}\left[-\rho, P, P, P\right]$ assumed for each component in $T^{(\text{eff})}_{\mu\nu}$ [in consistency with the metric signature $(-,+++)$], the cosmic expansion satisfies the generalized Friedmann equations

$$\left(\frac{\dot{a}}{a}\right)^2 = \frac{1}{3\phi}\left(\kappa^2\rho_m - 3H\dot{\phi} + \frac{\omega_{\text{L}}}{2\phi}\dot{\phi}^2 - 12bH^3\dot{\phi}\right), \tag{6.76}$$

$$\frac{\ddot{a}}{a} = -\frac{1}{6\phi}\left\{\kappa^2\left(\rho_m + 3P_m\right) + 3\ddot{\phi} + 3H\dot{\phi} + \frac{2\omega_{\text{L}}}{\phi}\dot{\phi}^2 + 12bH^2\ddot{\phi} + 12b\left(2\dot{H} + H^2\right)H\dot{\phi}\right\}, \tag{6.77}$$

where $T^{(\mathrm{CP})}_{\mu\nu} = 0$ for FRW. Moreover, the kinematical wave equation (6.37) and the dynamical wave equation (6.38) respectively lead to

$$\frac{2\omega_{\mathrm{L}}}{\phi}\left(\ddot{\phi} + 3H\dot{\phi}\right) = 6\frac{a\ddot{a} + \dot{a}^2}{a^2} + \frac{\omega_{\mathrm{L}}}{\phi^2} + \ddot{\phi} + 24bH^2\frac{\ddot{a}}{a}, \tag{6.78}$$

$$\left(2\omega_{\mathrm{L}} + 3 + 12b\frac{a\ddot{a} + \dot{a}^2}{a^2}\right)\left(\ddot{\phi} + 3H\dot{\phi}\right) = 24bH^2\frac{\ddot{a}}{a}\phi - 8\pi\left(3P_m - \rho_m\right) + 12b\left(\frac{\ddot{a}}{a}\ddot{\phi} + \frac{a\ddot{a} + 2\dot{a}^2}{a^2}H\dot{\phi}\right). \tag{6.79}$$

In principle, one could understand the evolutions of the scale factor $a(t)$ and the homogeneous scalar field $\phi(t)$ by (probably numerically) solving Eqs.(6.76)-(6.79). However the solutions will be complicated, so we will start with some solution ansatz for $\{a(t), \phi(t)\}$, which are easier to work with.

6.7.2 Cosmic acceleration in the late-time approximation

The physical matter satisfies the continuity equation

$$\dot{\rho}_m + 3H(\rho_m + P_m) = 0, \tag{6.80}$$

and for pressureless dust $P_m = 0$, it integrates to yield

$$\rho_m = \rho_0^{(m)} a^{-3} = \frac{\rho_0^{(m)}}{a_0^3} t^{-3\beta}, \tag{6.81}$$

where we have assumed a power-law scale factor

$$a = a_0 t^{\beta} \quad \text{with} \;\; \beta > 1. \tag{6.82}$$

Here $\{a_0, \beta\}$ are constants, and $\beta > 1$ so that $\ddot{a} > 0$. Similarly, we also take a power-law ansatz for the scalar field,

$$\phi = \phi_0 t^{\gamma}. \tag{6.83}$$

Based on Eqs.(6.81)-(6.83), the dynamical wave equation (6.38) with $T^{(\mathrm{m})} = -\rho_m$ for dust yields

$$\gamma\left(2\omega_{\mathrm{L}} + 3\right)\left(3\beta - 1 + \gamma\right) = \frac{\kappa^2 \rho_0^{(\mathrm{m})}}{\phi_0 a_0^3} t^{2-3\beta-\gamma} + 24b\frac{\beta^3(\beta - 1)}{t^2} - 12b\beta^2\gamma\frac{(3\beta - 3 + \gamma)}{t^2}, \tag{6.84}$$

and in the late-time (large t) approximation it reduces to

$$\gamma\left(\gamma + 3\beta - 1\right) = \frac{1}{\phi_0}\frac{\kappa^2 \rho_0^{(\mathrm{m})}}{a_0^3\left(2\omega_{\mathrm{L}} + 3\right)} t^{2-3\beta-\gamma}, \tag{6.85}$$

which can be satisfied by

$$\gamma = 2 - 3\beta \quad \text{and} \quad \phi_0 = \frac{\kappa^2 \rho_0^{(\mathrm{m})}}{a_0^3\left(2\omega_{\mathrm{L}} + 3\right)\left(2 - 3\beta\right)}. \tag{6.86}$$

Moreover, the first Friedmann equation (6.76) leads to

$$3\beta^2 = \kappa^2 \frac{\rho_0^{(m)}}{a_0^3 \phi_0} t^{2-3\beta-\gamma} - 3\beta\gamma + \frac{\omega_L}{2}\gamma^2 - 12b\frac{\beta^3\gamma}{t^2}, \tag{6.87}$$

and with Eq.(6.86), in the late-time approximation it becomes

$$3\beta^2 = (2-3\beta)(2\omega_L+3) - 3\beta(2-3\beta) + \frac{\omega_L}{2}(2-3\beta)^2. \tag{6.88}$$

For $\beta = 2$, Eq.(6.88) trivially holds for an arbitrary ω_L, while for $\beta \neq 2$, we have β in terms of ω_L via

$$\beta = \frac{2(\omega_L+1)}{3\omega_L+4}. \tag{6.89}$$

Note that Eqs.(6.86) and (6.89) reuire $\omega_L \neq -4/3$, $\omega_L \neq -3/2$ ($\beta \neq 2$), and $\beta \neq 2/3$; they are simply consequences of the power-law-solution ansatz and the late-time approximations rather than universal constraints on ω_L, and according to Eq.(6.89), the last condition $\beta \neq 2/3$ trivially holds with $\beta \to 2/3$ for $\omega_L \to \infty$. As a consistency test, the kinematical equation (6.37) yields

$$\omega_L\left(\frac{1}{2}\gamma^2 - \gamma + 3\beta\gamma\right) = 3\beta(2\beta-1) + 12b\frac{\beta^3(\beta-1)}{t^2} \tag{6.90}$$

with the late-time approximation

$$\omega_L\left(\frac{1}{2}\gamma^2 - \gamma + 3\beta\gamma\right) = 3\beta(2\beta-1), \tag{6.91}$$

which holds for Eqs.(6.86) and (6.89). Substituting Eqs.(6.81), (6.82), (6.83), (6.86) and (6.89) into the second Friedmann equation (6.77), we obtain

$$\frac{\ddot{a}}{a} = -\frac{2(\omega_L+1)(\omega_L+2)}{(3\omega_L+4)^2}t^{-2}, \tag{6.92}$$

and the deceleration parameter reads

$$q := -\frac{\ddot{a}a}{\dot{a}^2} = \frac{1}{2}\left(1 + 3\frac{P_{\text{eff}}}{\rho_{\text{eff}}}\right) = \frac{\omega_L+2}{2(\omega_L+1)}. \tag{6.93}$$

Eqs.(6.92) and (6.93) clearly indicate that the late-time acceleration could be realized for $-2 < \omega_L < -1$ ($\omega_L \neq -4/3$, $\omega_L \neq -3/2$), although this domain of ω_L makes the kinetics of the scalar field noncanonical.

6.8 Lovelock-scalar-tensor gravity

6.8.1 From LBD to Lovelock-scalar-tensor gravity

The LBD gravity can be generalized into the Lovelock-scalar-tensor (LST) gravity with the action

$$\mathcal{S}_{\rm LST} = \int d^4x\, \sqrt{-g}\, \mathscr{L}_{\rm LST} + \mathcal{S}_m \quad \text{and}$$
$$\mathscr{L}_{\rm LST} = \frac{1}{16\pi G}\left(f_1(\phi) R + f_2(\phi)\frac{{}^*RR}{\sqrt{-g}} + f_3(\phi)\mathcal{G} - \frac{\omega(\phi)}{\phi}\nabla_\alpha\phi\nabla^\alpha\phi - V(\phi)\right), \tag{6.94}$$

where $\{f_i(\phi), \omega(\phi)\}$ are generic functions of the scalar field, and $V(\phi)$ is the self-interaction potential. Note that this time Newton's constant G is included in the overall coefficient $1/16\pi G$ of $\mathscr{L}_{\rm LST}$, as is the case of the ordinary scalar-tensor gravity. The gravitational field equation is

$$f_1(\phi)\left(R_{\mu\nu} - \frac{1}{2}R g_{\mu\nu}\right) + \left(g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu\right) f_1(\phi) - \frac{\omega(\phi)}{\phi}\left(\nabla_\mu\phi\nabla_\nu\phi - \frac{1}{2}g_{\mu\nu}\nabla_\alpha\phi\nabla^\alpha\phi\right)$$
$$+ \frac{1}{2}V(\phi) g_{\mu\nu} + \widetilde{H}^{\rm (CP)}_{\mu\nu} + \widetilde{H}^{\rm (GB)}_{\mu\nu} = 8\pi T^{\rm (m)}_{\mu\nu}, \tag{6.95}$$

where $\widetilde{H}^{\rm (CP)}_{\mu\nu}$ denotes the contribution from $f_2(\phi)^*RR$,

$$\sqrt{-g}\,\widetilde{H}^{\rm (CP)}_{\mu\nu} = 2\partial^\xi f_2(\phi)\cdot\left(\epsilon_{\xi\mu\alpha\beta}\nabla^\alpha R^\beta{}_\nu + \epsilon_{\xi\nu\alpha\beta}\nabla^\alpha R^\beta{}_\mu\right) + 2\partial_\alpha\partial_\beta f_2(\phi)\cdot\left({}^*R^\alpha{}_\mu{}^\beta{}_\nu + {}^*R^\alpha{}_\nu{}^\beta{}_\mu\right), \tag{6.96}$$

and $\widetilde{H}^{\rm (GB)}_{\mu\nu}$ attributes to the effect of $\sqrt{-g} f_3(\phi)\mathcal{G}$,

$$\widetilde{H}^{\rm (GB)}_{\mu\nu} = 2R\left(g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu\right) f_3(\phi) - 4R_{\mu\nu}\Box f_3(\phi) + 4R_\mu{}^\alpha\nabla_\alpha\nabla_\nu f_3(\phi) + 4R_\nu{}^\alpha\nabla_\alpha\nabla_\mu f_3(\phi)$$
$$- 4g_{\mu\nu}R^{\alpha\beta}\nabla_\alpha\nabla_\beta f_3(\phi) + 4R_{\alpha\mu\beta\nu}\nabla^\beta\nabla^\alpha f_3(\phi). \tag{6.97}$$

It is straightforward to derive the kinematical wave equation by $\delta\mathcal{S}_{\rm LST}/\delta\phi = 0$, which along with the trace of Eq.(6.95) could yield the dynamical wave equation, and they generalize the wave equations (6.37, 6.38) in the LBD gravity. The wave equations however will not be listed here as the interest of this section is only the field equation $\delta\mathcal{S}/\delta g^{\mu\nu} = 0$.

6.8.2 Equivalence of LST with fourth-order gravities

It is well known that the $f(R)$ gravity is equivalent to the nondynamical (i.e. $\omega_{\rm BD} = 0$) Brans-Dicke gravity [27], and such equivalence holds for the LBD gravity as well. Consider the fourth-order modified gravity

$$\mathscr{L} = \frac{1}{16\pi G}\left[f(R,\mathcal{G}) + h\left(\frac{{}^*RR}{\sqrt{-g}}\right)\right], \tag{6.98}$$

for which the field equation is

$$f_R R_{\mu\nu} + \left(g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu\right) f_R - \frac{1}{2} f(R,\mathcal{G}) g_{\mu\nu} + \mathcal{H}^{\rm (CP)}_{\mu\nu} + \mathcal{H}^{\rm (GB)}_{\mu\nu} = 8\pi T^{\rm (m)}_{\mu\nu}, \tag{6.99}$$

where

$$\sqrt{-g}\,\mathcal{H}^{(\mathrm{CP})}_{\mu\nu} = 2\partial^{\xi} h_{^*RR}\cdot\left(\epsilon_{\xi\mu\alpha\beta}\nabla^{\alpha}R^{\beta}{}_{\nu} + \epsilon_{\xi\nu\alpha\beta}\nabla^{\alpha}R^{\beta}{}_{\mu}\right) + 2\partial_{\alpha}\partial_{\beta}h_{^*RR}\cdot\left({}^*R^{\alpha}{}_{\mu}{}^{\beta}{}_{\nu} + {}^*R^{\alpha}{}_{\nu}{}^{\beta}{}_{\mu}\right), \tag{6.100}$$

and

$$\begin{aligned}\mathcal{H}^{(\mathrm{GB})}_{\mu\nu} = 2R\left(g_{\mu\nu}\Box - \nabla_{\mu}\nabla_{\nu}\right)f_{\mathcal{G}} - 4R_{\mu\nu}\Box f_{\mathcal{G}} + 4R_{\mu}{}^{\alpha}\nabla_{\alpha}\nabla_{\nu}f_{\mathcal{G}} + 4R_{\nu}{}^{\alpha}\nabla_{\alpha}\nabla_{\mu}f_{\mathcal{G}} \\ - 4g_{\mu\nu}R^{\alpha\beta}\nabla_{\alpha}\nabla_{\beta}f_{\mathcal{G}} + 4R_{\alpha\mu\beta\nu}\nabla^{\beta}\nabla^{\alpha}f_{\mathcal{G}},\end{aligned} \tag{6.101}$$

with $f_R = f_R(R,\mathcal{G}) = \partial f(R,\mathcal{G})/\partial R$, $f_{\mathcal{G}} = f_{\mathcal{G}}(R,\mathcal{G}) = \partial f(R,\mathcal{G})/\partial\mathcal{G}$, and $h_{^*RR} = dh({}^*RR/\sqrt{-g})/d({}^*RR/\sqrt{-g})$. For the nondynamical LST gravity with $\omega(\phi)\equiv 0$ in Eq.(6.95), compare it with Eq.(6.99) and at the level of the gravitational equation, one could find the equivalence

$$\begin{aligned} f_1(\phi) = f_R\ ,\ \ f_3(\phi) = f_{\mathcal{G}}\ ,\ \ f_2(\phi) = h_{^*RR}, \\ V(\phi) = -f(R,\mathcal{G}) + f_R R\,. \end{aligned} \tag{6.102}$$

In the $V(\phi)$ relation we have applied the replacement $f_1(\phi) = f_R$, and note that $V(\phi)$ does not contain a $f_{\mathcal{G}}\mathcal{G}$ term which has been removed from $\mathcal{H}^{(\mathrm{GB})}_{\mu\nu}$ because of the Bach-Lanczos identity Eq.(6.32).

6.8.3 Partial equivalence for "multi-scalar LBD gravity"

Removing the ω_{L} term in Eq.(6.35) and then comparing it with Eq.(6.99), one could find that an equivalence between the nondynamical LBD gravity (now equipped with an extra potential $-U(\phi)$ in $\mathscr{L}_{\mathrm{LBD}}$) and the $f(R,\mathcal{G}) + h\left(\frac{{}^*RR}{\sqrt{-g}}\right)$ gravity would require $f_R = f_{\mathcal{G}} = \phi = h_{^*RR}$, and $U(\phi) = -f(R,\mathcal{G}) + f_R R$. These conditions are so restrictive that the $f(R,\mathcal{G}) + h\left(\frac{{}^*RR}{\sqrt{-g}}\right)$ gravity would totally lose its generality. Instead, introduce three auxiliary fields $\{\chi_1,\chi_2,\chi_3\}$ and consider the dynamically equivalent action

$$\begin{aligned}\mathcal{S} = &\frac{1}{16\pi}\int d^4x\sqrt{-g}\Big[f(\chi_1,\chi_2) + f_{\chi_1}\cdot(R-\chi_1) + f_{\chi_2}\cdot(\mathcal{G}-\chi_2) \\ &+ h(\chi_3) + h_{\chi_3}\cdot\left(\frac{{}^*RR}{\sqrt{-g}} - \chi_3\right)\Big] + \mathcal{S}_m\,;\end{aligned} \tag{6.103}$$

its variation with respect to χ_1, χ_2, and χ_3 separately yields the constraints

$$f_{\chi_1\chi_1}(R-\chi_1) = 0\,,\quad f_{\chi_2\chi_2}(\mathcal{G}-\chi_2) = 0\,,\quad \text{and}\quad h_{\chi_3\chi_3}\Big(\frac{{}^*RR}{\sqrt{-g}} - \chi_3\Big) = 0\,, \tag{6.104}$$

where $f_{\chi_j} := \partial f(\chi_1,\chi_2)/\partial\chi_j$, $f_{\chi_j\chi_j} := \partial^2 f(\chi_1,\chi_2)/\partial\chi_j^2$, $h_{\chi_3} := \partial h(\chi_3)/\partial\chi_3$ and $h_{\chi_3\chi_3} := \partial^2 f(\chi_3)/\partial\chi_3^2$. If $f_{\chi_1\chi_1}$, $f_{\chi_2\chi_2}$ and $h_{\chi_3\chi_3}$ do not vanish identically, Eq.(6.104) leads to $\chi_1 = R$, $\chi_2 = \mathcal{G}$ and $\chi_3 = \frac{{}^*RR}{\sqrt{-g}}$. Redefining the fields $\{\chi_1,\chi_2,\chi_3\}$ by

$$\phi = f_{\chi_1}\,,\quad \psi = f_{\chi_2}\,,\quad \varphi = h_{\chi_3} \tag{6.105}$$

and setting

$$V(\phi,\psi,\varphi)=\phi\cdot R(\phi,\psi)+\psi\cdot\mathcal{G}(\phi,\psi)+\varphi\cdot\frac{{}^*RR}{\sqrt{-g}}(\varphi)-f\Big(R(\phi,\psi),\mathcal{G}(\phi,\psi)\Big)-h\left(\frac{{}^*RR}{\sqrt{-g}}(\varphi)\right), \tag{6.106}$$

then the $f(R,\mathcal{G})+h\left(\frac{{}^*RR}{\sqrt{-g}}\right)$ gravity is partially equivalent to the following "multi-scalar LBD gravity" carrying three nondynamical scalar fields

$$\mathscr{L}=\frac{1}{16\pi}\left(\phi R+\varphi\frac{{}^*RR}{\sqrt{-g}}+\psi\mathcal{G}-V(\phi,\psi,\varphi)\right), \tag{6.107}$$

where the coupling coefficients $\{a,b\}$ appearing in $\mathscr{L}_{\text{LBD}}$ have been absorbed into the scalar fields $\{\varphi,\psi\}$. Also, by "partially equivalent" we mean that Eq.(6.106) as is stands is only partially on-shell; to recover Eq.(6.98) from the multi-field action of Eq.(6.107), one would have to add extra Lagrange multipliers identifying the different fields, but this would break the exact equivalence between such modified Eq.(6.107) and Eq.(6.98).

6.9 Conclusions and discussion

The Hilbert-Einstein action $\mathcal{S}_{\text{HE}}$ and the Lovelock action $\mathcal{S}_{\text{L}}$ yield identical field equations and thus are observationally indistinguishable. However, the former takes the Brans-Dicke gravity as its scalar-tensor counterpart, while the latter's companion is the LBD gravity, and these two theories are different.

We have extensively studied the theoretical structures of the LBD gravity, including the gravitational and wave equations, the ordinary $\omega_{\text{L}}\to\infty$ limit that recovers GR, the unusual $\omega_{\text{L}}\to\infty$ limit satisfying the topology balance condition Eq.(6.41) and thus departing from GR, the energy-momentum conservation, the conformal transformations into the dynamical Chern-Simons gravity and the generalized Gauss-Bonnet dark energy, as well as the extensions to LST gravity with its equivalence to fourth-order modified gravity.

We have taken the opportunity of deriving the field equation to look deeper into the properties of the Chern-Pontryagin and Gauss-Bonnet topological invariants. Especially, for the $f(\phi)\mathcal{G}$ Gauss-Bonnet dark energy as well as the $f(R,\mathcal{G})$ and $f(R,\mathcal{G},\mathscr{L}_m)$ gravities, the contributions of the generalized Gauss-Bonnet dependence could be simplified from the popular form like Eq.(6.31) into our form like Eq.(6.33).

An important goal of alternative and modified gravities is to explain the accelerated expansion of the Universe, and we have applied the LBD theory to this problem, too. It turned out that the acceleration could be realized for $-2<\omega_{\text{L}}<-1$ under our solution ansatz. Note that our estimate of cosmic acceleration in Sec. 6.7 is not satisfactory. For example, the kinematical equation (6.90) clearly shows that because of the higher-order time derivative terms arising from the $\phi\mathcal{G}$ dependence, the simplest solution ansatz $\{\phi=\phi_0 t^{\gamma},\ a=a_0 t^{\beta}\}$ with $\{\beta=\text{constant},\ \gamma=\text{constant}\}$ are not compatible with each other unless the late-time approximation is imposed, while such approximations further lead to the behaviors analogous to the Brans-Dicke cosmology [32].

Section 6.7 has shown that, the effects from the parity-violating Chern-Pontryagin term ϕ^*RR are ineffective for the FRW cosmology because of its spatial homogeneity and isotropy. However, it is believed that ϕ^*RR could have detectable consequences on leptogenesis and gravitational waves in the initial inflation epoch [33] where ϕ acts as the inflaton field. The inflation problem usually works with the slow-roll approximations $\ddot{\phi}\ll\dot{\phi}\ll H$ and requires the existence of a potential well $V(\phi)$; thus, at least for the description of the initial inflation, the LBD gravity should be generalized to carry a potential:

$$\widehat{\mathscr{L}}_{\mathrm{LBD}} = \frac{1}{16\pi}\left[\phi\left(R + a\frac{{}^{*}RR}{\sqrt{-g}} + b\mathcal{G}\right) - \frac{\omega_{\mathrm{L}}}{\phi}\nabla_{\alpha}\phi\nabla^{\alpha}\phi - V(\phi)\right], \tag{6.108}$$

with $V(\phi) = 2\Lambda\phi$ being the simplest possibility.

Our prospective studies aim to construct the complete history of cosmic expansion in LBD gravity [probably equipped with $V(\phi)$], throughout the dominance of radiation, dust, and effective dark energy. Moreover, it is well known that primordial gravitational waves can trace back to the Planck era of the Universe and serve as one of the most practical and efficient tests for modified gravities, so it is very useful to find out whether the gravitational-wave polarizations carry different intensities in this gravity. There are also some other problems from the LBD gravity attracting our attention, such as its relation to the low-energy effective string theory. We will look for the answers in future.

Acknowledgement

DWT is very grateful to Prof. Christian Cherubini (Università Campus Bio-Medico) for helpful discussion on the topological current for the Gauss-Bonnet invariant. Also, we are very grateful to the anonymous referees for constructive suggestions to improve the manuscript. This work was financially supported by the Natural Sciences and Engineering Research Council of Canada, under the grant 261429-2013.

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[24] Switching from the sign convention in Ref.[11] to the convention in our paper and Ref.[20], the signs for the following quantities are changed: $g_{\mu\nu}$, $\Gamma_{\alpha\beta\gamma}$, $R^{\alpha}{}_{\mu\beta\nu}$, $R_{\mu\nu} = R^{\alpha}{}_{\mu\alpha\nu}$, $G_{\mu\nu} = R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu}$, $T^{(\mathrm{m})}_{\mu\nu}$, Λ (cosmological constant) while the following quantities take unchanging values: $\sqrt{-g}$, $\epsilon^{\alpha\beta\mu\nu}$, $\epsilon_{\alpha\beta\mu\nu}$, $\Gamma^{\alpha}_{\mu\nu}$, $R_{\alpha\mu\beta\nu}$, $R = g^{\mu\nu}R_{\mu\nu}$. Moreover, Ref.[11] defined ${}^*RR$ by $\left(\epsilon_{\alpha\beta\mu\nu}R^{\mu\nu}{}_{\gamma\delta}\right)R^{\alpha\beta\gamma\delta} = 2{}^*R_{\alpha\beta\gamma\delta}R^{\alpha\beta\gamma\delta} = -2{}^*RR$, differing from ours by a minus sign, as we choose to follow Lovelock's usage which is more popular and standard.

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Chapter 7. Traversable wormholes and energy conditions in Lovelock-Brans-Dicke gravity [arXiv:1507.07448]

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Abstract

This paper studies traversable wormholes and the states of energy conditions in Lovelock-Brans-Dicke gravity, which involves the nonminimal couplings of a background scalar field with the Chern-Pontryagin density and the Gauss-Bonnet invariant. The flaring-out condition indicates that a Morris-Thorne-type wormhole can be maintained by violating the generalized null energy condition, and thus also breaking down the generalized weak, strong, and dominant energy conditions; meanwhile, analyses of the zero-tidal-force solution show that the standard null energy condition in general relativity can still be respected by the physical matter threading the wormhole. This way, the topological sources of gravity have to dominate over the effects of ordinary matter, and the scalar field is preferred to be noncanonical. By treating Brans-Dicke gravity as a reduced situation of Lovelock-Brans-Dicke gravity, we also examine the Brans-Dicke wormholes and energy conditions.

PACS numbers: 04.50.Kd, 04.20.Cv, 04.90.+e
Key words: traversable wormhole; Lovelock-Brans-Dicke gravity; Chern-Pontryagin density; Gauss-Bonnet invariant; flaring-out condition; generalized and standard energy conditions

7.1 Introduction

A wormhole is a fascinating passage as a shortcut connecting two distant regions in a spacetime or bridging two distinct universes. Pioneering investigations of wormholes can date back to the Einstein-Rosen bridge [1] in general relativity (GR), and earlier constructions of wormholes, such as those converted from the Kerr-Newman family of black holes, suffer from severe instability against small perturbations and immediate collapse of the throat after formation [2].

Modern interest in wormholes are mainly based on the seminal work of Morris and Thorne on traversable Lorentzian wormholes [3], and the way to convert them into time machines [4]. Morris and Thorne firstly designed the metric with the desired structures of a traversable wormhole, and then recovered the matter fields through Einstein's equation. It turns out that the energy-momentum tensor has to violate the null energy condition, and thus it needs exotic matter to maintain the wormhole tunnel [3]. The standard energy conditions, however, are a cornerstone in many areas in GR, such as the classical black hole thermodynamics [5, 6]. Thus, much effort has been made to minimize the violation of the energy conditions and reduce the encounter of exotic matter at the throat (e.g. [3, 7, 8]).

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The search for promising candidates of exotic matter is not an easy job, and only a small handful situations are recognized, such as the quantum Casimir effect and the semiclassical Hawking radiation, while all classical matter fields obey the standard energy conditions. With the development of precision cosmology and the discovery of cosmic acceleration, various models of dark energy with exotic equations of state have been proposed, which provide new possibilities to support wormholes, such as those supported by the cosmological constant [9], phantom- or quintom-type energy [10, 11], generalized or modified Chaplygin gas [12, 13], and interacting dark sectors [14].

On the other hand, as an alternative to the mysterious dark energy, modified and alternative theories of relativistic gravity beyond GR have been greatly developed to explain the accelerated expansion of the Universe. The higher order terms or extra degrees of freedom in these theories yield antigravity effects, which overtake the gravitational attraction of ordinary matter at the cosmic scale. Lobo took Weyl conformal gravity as an example and suggested that modified gravities provide another possibility to support traversable wormholes [15]: it is the generalized energy conditions that are violated, while the standard energy conditions as in GR may remain valid. To date, this proposal has been applied to exact solutions of Morris-Thorne-type wormholes in various modified gravities, such as the metric $f(R)$ [16], nonminimal curvature-matter coupling [17], braneworld scenario [18], Brans-Dicke [19], modified teleparallel [20], metric-Palatini hybrid $f(R)$ [21], and Einstein-Gauss-Bonnet gravities [22].

In this paper, we will look into traversable wormholes and the standard energy conditions in Lovelock-Brans-Dicke gravity [23], which takes into account the gravitational effects of spacetime parity and topology by the nonminimal couplings of a background scalar field to the Chern-Pontryagin density and the Gauss-Bonnet invariant. This paper is organized as follows. We firstly review the gravity theory in Sec. 7.2, and derive its generalized energy conditions in Sec. 7.3. Then the conditions to support Morris-Thorne-type wormholes are investigated in Sec. 7.4, which are extensively examined by a zero-tidal-force solution in Sec. 7.5. Also, comparison with wormholes in Brans-Dicke gravity is studied in Sec. 7.6. Throughout this paper, we adopt the geometric conventions $\Gamma^{\alpha}_{\beta\gamma} = \Gamma^{\alpha}{}_{\beta\gamma}$, $R^{\alpha}{}_{\beta\gamma\delta} = \partial_\gamma \Gamma^{\alpha}_{\delta\beta} - \partial_\delta \Gamma^{\alpha}_{\gamma\beta} \cdots$ and $R_{\mu\nu} = R^{\alpha}{}_{\mu\alpha\nu}$ with the metric signature $(-,+++)$.

7.2 Lovelock-Brans-Dicke gravity

Recently we have discussed a new theory of alternative gravity which has been dubbed as Lovelock-Brans-Dicke (LBD) gravity [23]. This theory is given by the action

$$\begin{aligned} \mathcal{S}_{\text{LBD}} &= \int d^4x \sqrt{-g}\, \mathscr{L}_{\text{LBD}} + \mathcal{S}_m \quad \text{with} \\ \mathscr{L}_{\text{LBD}} &= \frac{1}{16\pi}\left[\phi\left(R + \frac{a}{\sqrt{-g}}{}^*RR + \hat{b}\mathcal{G}\right) - \frac{\omega_{\text{L}}}{\phi}\nabla_\alpha\phi\nabla^\alpha\phi - 2V(\phi)\right], \end{aligned} \tag{7.1}$$

where $\phi = \phi(x^\alpha)$ is a background scalar field, $\{a, \hat{b}\}$ are dimensional coupling constants (note: $\hat{b}$ is hatted to be distinguished from $b = b(r)$ in Secs. 7.4, 7.5 and 7.6, which is a standard denotation for the shape function in wormhole physics), ω_{L} denotes the dimensionless Lovelock parameter tuning the kinetics of $\phi(x^\alpha)$, $V(\phi)$ refers to a self-interaction potential, and as usual the matter action is given by the matter Lagrangian density via $\mathcal{S}_m = \int d^4x \sqrt{-g}\, \mathscr{L}_m$. In Eq.(7.1), ${}^*RR$ and $\mathcal{G}$ denote the Chern-Pontryagin density and the Gauss-Bonnet invariant, respectively,

$$
\begin{aligned}
{}^*RR &:= {}^*R_{\alpha\beta\gamma\delta}R^{\alpha\beta\gamma\delta} = \frac{1}{2}\epsilon_{\alpha\beta\mu\nu}R^{\mu\nu}{}_{\gamma\delta}R^{\alpha\beta\gamma\delta}\,, \\
\mathcal{G} &:= R^2 - 4R_{\mu\nu}R^{\mu\nu} + R_{\mu\alpha\nu\beta}R^{\mu\alpha\nu\beta}\,,
\end{aligned}
\tag{7.2}
$$

where ${}^*R_{\alpha\beta\gamma\delta} := \frac{1}{2}\epsilon_{\alpha\beta\mu\nu}R^{\mu\nu}{}_{\gamma\delta}$ is the left dual of Riemann tensor, and $\epsilon_{\alpha\beta\mu\nu}$ represents the totally antisymmetric Levi-Civita pseudotensor with $\epsilon_{0123} = \sqrt{-g}$ and $\epsilon^{0123} = 1/\sqrt{-g}$. Note that unlike the other two curvature invariants $\{R,\ \mathcal{G}\}$, the term ${}^*RR$ in $\mathscr{L}_{\text{LBD}}$ is divided by $\sqrt{-g}$; this is because ${}^*RR$ itself already serves as a covariant density for $\mathcal{S}_{\text{LBD}}$, as opposed to $\sqrt{-g}\,R$ and $\sqrt{-g}\,\mathcal{G}$ therein.

$\mathcal{S}_{\text{LBD}}$ is inspired by the connection between GR and Brans-Dicke gravity, and proposed as the Brans-Dicke-type counterpart for the classic Lovelock action in Lovelock's theorem [24], i.e. $\mathcal{S}_{\text{L}} = \frac{1}{16\pi G}\int d^4x\,\sqrt{-g}\left(R - 2\Lambda + \frac{a}{\sqrt{-g}}{}^*RR + b\mathcal{G}\right) + \mathcal{S}_m$. $\mathcal{S}_{\text{L}}$ is the most general action made up of algebraic curvature invariants that yields second-order field equations in four dimensions, and limits the field equation to be Einstein's equation equipped with a cosmological constant Λ. The Chern-Pontryagin and the Gauss-Bonnet invariants in $\mathcal{S}_{\text{L}}$ do not influence the field equation, because ${}^*RR$ and $\sqrt{-g}\,\mathcal{G}$ are equal to the divergences of their respective topological currents (see Ref.[23] and the relevant references therein); instead, the nonminimally ϕ–coupled covariant densities $\phi{}^*RR$ and $\sqrt{-g}\,\phi\mathcal{G}$ in the LBD action Eq.(7.1) will have nontrivial contributions to the field equation. Recall that for the two invariants ${}^*RR$ and $\mathcal{G}$, the former is related to the spacetime parity with $\int d^4x\,{}^*RR$ proportional to the instanton number of the spacetime, while the latter's integral $\frac{1}{32\pi^2}\int dx^4\,\sqrt{-g}\,\mathcal{G}$ equates the Euler characteristic of the spacetime. Hence, LBD gravity has taken into account the gravitational effects of the spacetime parity and the Euler topology.

The extremized variational derivative $\delta\mathcal{S}_{\text{LBD}}/\delta g^{\mu\nu} = 0$ yields the gravitational field equation

$$
\begin{aligned}
&\phi\left(R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu}\right) + \left(g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu\right)\phi + aH^{(\text{CP})}_{\mu\nu} + \hat{b}H^{(\text{GB})}_{\mu\nu} \\
&- \frac{\omega_{\text{L}}}{\phi}\left(\nabla_\mu\phi\nabla_\nu\phi - \frac{1}{2}g_{\mu\nu}\nabla_\alpha\phi\nabla^\alpha\phi\right) + V(\phi)g_{\mu\nu} = 8\pi T^{(\text{m})}_{\mu\nu},
\end{aligned}
\tag{7.3}
$$

where $H^{(\text{CP})}_{\mu\nu} := \frac{1}{\sqrt{-g}}\frac{\delta(\phi{}^*RR)}{\delta g^{\mu\nu}}$ collects the contributions from the Chern-Pontryagin density with nonminimal coupling to $\phi(x^\alpha)$,

$$
\sqrt{-g}\,H^{(\text{CP})}_{\mu\nu} = 2\partial^\xi\phi\cdot\left(\epsilon_{\xi\mu\alpha\beta}\nabla^\alpha R^\beta{}_\nu + \epsilon_{\xi\nu\alpha\beta}\nabla^\alpha R^\beta{}_\mu\right) + 2\partial_\alpha\partial_\beta\phi\cdot\left({}^*R^\alpha{}_\mu{}^\beta{}_\nu + {}^*R^\alpha{}_\nu{}^\beta{}_\mu\right)\,,
\tag{7.4}
$$

and $H^{(\text{GB})}_{\mu\nu} := \frac{1}{\sqrt{-g}}\frac{\delta(\sqrt{-g}\,\phi\mathcal{G})}{\delta g^{\mu\nu}}$ refers to the effect of extra degrees of freedom from the nonminimally $\phi-$coupled Gauss-Bonnet invariant,

$$
\begin{aligned}
H^{(\text{GB})}_{\mu\nu} &= 2R\left(g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu\right)\phi + 4R_\mu{}^\alpha\nabla_\alpha\nabla_\nu\phi + 4R_\nu{}^\alpha\nabla_\alpha\nabla_\mu\phi \\
&\quad - 4R_{\mu\nu}\Box\phi - 4g_{\mu\nu}\cdot R^{\alpha\beta}\nabla_\alpha\nabla_\beta\phi + 4R_{\alpha\mu\beta\nu}\nabla^\beta\nabla^\alpha\phi\,,
\end{aligned}
\tag{7.5}
$$

with $\Box := g^{\alpha\beta}\nabla_\alpha\nabla_\beta$ denoting the covariant d'Alembertian. Compared to the field equations of the $f(R,\mathcal{G})$ and $f(R,\mathcal{G},\mathscr{L}_m)$ generalized Gauss-Bonnet gravities with generic $\mathcal{G}-$dependence [25, 26], we have removed the algebraic terms in $H^{(\text{GB})}_{\mu\nu}$ by the Bach-Lanczos identity $2RR_{\mu\nu} - 4R_\mu{}^\alpha R_{\alpha\nu} - 4R_{\alpha\mu\beta\nu}R^{\alpha\beta} + 2R_{\mu\alpha\beta\gamma}R_\nu{}^{\alpha\beta\gamma} \equiv \frac{1}{2}\mathcal{G}g_{\mu\nu}$.

Immediately, the trace of the field equation (7.3) is found to be

$$-\phi R + \frac{\omega_{\rm L}}{\phi}\nabla_\alpha\phi\nabla^\alpha\phi + \left(3 + 2\hat{b}R\right)\Box\phi - 4\hat{b}R^{\alpha\beta}\nabla_\alpha\nabla_\beta\phi + 4V(\phi) = 8\pi T^{(\rm m)}, \tag{7.6}$$

where $g^{\mu\nu}H_{\mu\nu}^{(\rm GB)} = 2R\Box\phi - 4R^{\alpha\beta}\nabla_\alpha\nabla_\beta\phi$, $T^{(\rm m)} = g^{\mu\nu}T_{\mu\nu}^{(\rm m)}$, and $H_{\mu\nu}^{(\rm CP)}$ is always traceless.

On the other hand, for the scalar field $\phi(x^\alpha)$, the extremization $\delta\mathcal{S}_{\rm LBD}/\delta\phi = 0$ directly leads to the *kinematical* wave equation

$$2\omega_{\rm L}\Box\phi = -\left(R + \frac{a}{\sqrt{-g}}{}^*RR + \hat{b}\mathcal{G}\right)\phi + \frac{\omega_{\rm L}}{\phi}\nabla_\alpha\phi\nabla^\alpha\phi + 2V_\phi\phi\,, \tag{7.7}$$

with $\Box\phi = g^{\alpha\beta}\nabla_\alpha\nabla_\beta\phi = \frac{1}{\sqrt{-g}}\partial_\alpha\left(\sqrt{-g}\,g^{\alpha\beta}\partial_\beta\phi\right)$, and $V_\phi := dV(\phi)/d\phi$. Along with the trace equation (7.6), it yields the *dynamical* wave equation

$$\left(2\omega_{\rm L} + 3 + 2\hat{b}R\right)\Box\phi = -\left(\frac{a}{\sqrt{-g}}{}^*RR + \hat{b}\mathcal{G}\right)\phi + 8\pi T^{(\rm m)} + 4\hat{b}R^{\alpha\beta}\nabla_\alpha\nabla_\beta\phi + 2V_\phi\phi - 4V(\phi)\,, \tag{7.8}$$

which explicitly relates the propagation of $\phi(x^\alpha)$ to the trace $T^{(\rm m)}$ of the matter tensor for the energy-momentum distribution.

In this paper, we will work out the conditions to support traversable wormholes and examine the energy conditions in LBD gravity; especially, we will pay attention to the gravitational effects of the scalar field and $H_{\mu\nu}^{(\rm GB)}$, while $H_{\mu\nu}^{(\rm CP)}$ does not influence Morris-Thorne-type wormholes. To begin with, we firstly derive the generalized energy conditions for LBD gravity.

7.3 Generalized LBD energy conditions

In a region of a spacetime, for the expansion rate $\theta_{(\ell)}$ of a null congruence along its null tangent vector field ℓ^μ, and the expansion rate $\theta_{(u)}$ of a timelike congruence along its timelike tangent u^μ, $\theta_{(\ell)}$ and $\theta_{(u)}$ respectively satisfy the Raychaudhuri equations [6]

$$\ell^\mu\nabla_\mu\theta_{(\ell)} = \frac{d\theta_{(\ell)}}{d\lambda} = \kappa_{(\ell)}\theta_{(\ell)} - \frac{1}{2}\theta_{(\ell)}^2 - \sigma_{\mu\nu}^{(\ell)}\sigma_{(\ell)}^{\mu\nu} + \omega_{\mu\nu}^{(\ell)}\omega_{(\ell)}^{\mu\nu} - R_{\mu\nu}\ell^\mu\ell^\nu\,, \tag{7.9}$$

$$u^\mu\nabla_\mu\theta_{(u)} = \frac{d\theta_{(u)}}{d\tau} = \kappa_{(u)}\theta_{(u)} - \frac{1}{3}\theta_{(u)}^2 - \sigma_{\mu\nu}^{(u)}\sigma_{(u)}^{\mu\nu} + \omega_{\mu\nu}^{(u)}\omega_{(u)}^{\mu\nu} - R_{\mu\nu}u^\mu u^\nu\,. \tag{7.10}$$

The inaffinity coefficients are zero $\kappa_{(\ell)} = 0 = \kappa_{(u)}$ under affine parameterizations, the twist vanishes $\omega_{\mu\nu}\omega^{\mu\nu} = 0$ for hypersurface-orthogonal foliations, and being spatial tensors $\left(\sigma_{\mu\nu}^{(\ell)}\ell^\mu = 0 = \sigma_{\mu\nu}^{(u)}u^\mu\right)$ the shears always satisfy $\sigma_{\mu\nu}\sigma^{\mu\nu} \geq 0$. Thus, to guarantee $d\theta_{(\ell)}/d\lambda \leq 0$ and $d\theta_{(u)}/d\tau \leq 0$ under all circumstances – even in the occasions $\theta_{(\ell)} = 0 = \theta_{(u)}$, so that the congruences focus and gravity is always an attractive force, the following geometric nonnegativity conditions are expected to hold:

$$R_{\mu\nu}\ell^\mu\ell^\nu \geq 0 \qquad , \qquad R_{\mu\nu}u^\mu u^\nu \geq 0\,. \tag{7.11}$$

Note that although this is the most popular approach to derive Eq.(7.11) for its straightforwardness and simplicity, it is not perfect. In general $\theta_{(\ell)}$ and $\theta_{(u)}$ are nonzero and one could only obtain $\frac{1}{2}\theta_{(\ell)}^2 + R_{\mu\nu}\ell^\mu\ell^\nu \geq 0$

and $\frac{1}{3}\theta^2_{(u)}+R_{\mu\nu}u^\mu u^\nu \geq 0$. Thus, it is only safe to say that Eq.(7.11) provides the sufficient rather than necessary conditions to ensure $d\theta_{(\ell)}/d\lambda \leq 0$ and $d\theta_{(u)}/d\tau \leq 0$. Fortunately, this imperfectness is not a disaster and does not negate the conditions in Eq.(7.11); for example, one can refer to Ref. [27] for a rigorous derivation of the first inequality in Eq.(7.11) from the Virasoro constraint in the worldsheet string theory.

On the other hand, consider generic relativistic gravities with the Lagrangian density $\mathscr{L}_{\text{total}} = \frac{1}{16\pi G}\mathscr{L}_G$ $(R, R_{\mu\nu}R^{\mu\nu}, \mathcal{R}_i, \cdots, \vartheta, \nabla_\mu\vartheta\nabla^\mu\vartheta)+\mathscr{L}_m$, where $\mathcal{R}_i = \mathcal{R}_i\,(g_{\alpha\beta}\,, R_{\mu\alpha\nu\beta}\,, \nabla_\gamma R_{\mu\alpha\nu\beta}\,, \ldots)$ refers to a generic curvature invariant beyond the Ricci scalar, and ϑ denotes a scalarial extra degree of freedom unabsorbed by $\mathscr{L}_m$. The field equation reads

$$\mathcal{H}_{\mu\nu} = 8\pi G T^{(\text{m})}_{\mu\nu} \quad \text{with} \quad \mathcal{H}_{\mu\nu} \coloneqq \frac{1}{\sqrt{-g}}\frac{\delta\left(\sqrt{-g}\,\mathscr{L}_G\right)}{\delta g^{\mu\nu}}\,, \tag{7.12}$$

where total-derivative terms should be removed in the derivation of $\mathcal{H}_{\mu\nu}$. In the spirit of reconstructing an effective dark energy, Eq.(7.12) can be intrinsically recast into a compact GR form by isolating the Ricci tensor $R_{\mu\nu}$ out of $\mathcal{H}_{\mu\nu}$:

$$R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} = 8\pi G_{\text{eff}} T^{(\text{eff})}_{\mu\nu} \quad \text{with} \quad \mathcal{H}_{\mu\nu} = \frac{G}{G_{\text{eff}}}G_{\mu\nu} - 8\pi G T^{(\text{MG})}_{\mu\nu}\,, \tag{7.13}$$

where G_{eff} denotes the effective gravitational coupling strength, and it is recognized from the coefficient of the matter tensor $T^{(\text{m})}_{\mu\nu}$. $T^{(\text{eff})}_{\mu\nu}$ refers to the total effective energy-momentum tensor, and $T^{(\text{MG})}_{\mu\nu} = T^{(\text{eff})}_{\mu\nu} - T^{(\text{m})}_{\mu\nu}$, with $T^{(\text{MG})}_{\mu\nu}$ collecting all the modified-gravity nonlinear and higher-order effects. Thus, all terms beyond GR have been packed into $T^{(\text{MG})}_{\mu\nu}$ and G_{eff}.

Following Eq.(7.13) along with its trace equation $R = -8\pi G_{\text{eff}} T^{(\text{eff})}$ and the equivalent form $R_{\mu\nu} = 8\pi G_{\text{eff}}\left(T^{(\text{eff})}_{\mu\nu} - \frac{1}{2}g_{\mu\nu}T^{(\text{eff})}\right)$, the geometric nonnegativity conditions in Eq.(7.11) can be translated into the generalized null and strong energy conditions (GNEC and GSEC for short)

$$G_{\text{eff}} T^{(\text{eff})}_{\mu\nu}\,\ell^\mu\ell^\nu \geq 0 \quad (\text{GNEC}) \quad , \quad G_{\text{eff}}\left(T^{(\text{eff})}_{\mu\nu}u^\mu u^\nu + \frac{1}{2}T^{(\text{eff})}\right) \geq 0 \quad (\text{GSEC})\,, \tag{7.14}$$

where $\ell^\mu\ell_\mu = 0$ for the GNEC, and $u_\mu u^\mu = -1$ in the GSEC for compatibility with the metric signature $(-,+++)$. We further supplement Eq.(7.14) by the generalized weak energy condition

$$G_{\text{eff}} T^{(\text{eff})}_{\mu\nu}u^\mu u^\nu \geq 0 \quad (\text{GWEC})\,, \tag{7.15}$$

and the generalized dominant energy condition (GDEC) that $G_{\text{eff}} T^{(\text{eff})}_{\mu\nu}u^\mu u^\nu \geq 0$ with $G_{\text{eff}} T^{(\text{eff})}_{\mu\nu}u^\mu$ being a causal vector.

Note that for the common pattern of the field equations in modified gravities, we have chosen to adopt Eq.(7.13) rather than $R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} = 8\pi G\widehat{T}^{(\text{eff})}_{\mu\nu}$, where G is Newton's constant. That is to say, we do not absorb G_{eff} into $T^{(\text{eff})}_{\mu\nu}$ so that $G_{\text{eff}} T^{(\text{eff})}_{\mu\nu} = G\widehat{T}^{(\text{eff})}_{\mu\nu}$; as a consequence, G_{eff} shows up in the generalized energy conditions as well. This is because the effective matter-gravity coupling strength G_{eff} plays important roles in many physics problems, such as the Wald entropy of black-hole horizons [28] and the cosmological gravitational thermodynamics (e.g.[29]), although the meanings and applications of G_{eff} have not been fully understood (say the relations between G_{eff} and the weak, Einstein, and strong equivalence principles).

G_{eff} and $T^{(\text{eff})}_{\mu\nu}$ vary among different theories of modified gravity, which concretize Eqs.(7.14) and (7.15) into different sets of generalized energy conditions. For LBD gravity summarized in Sec. 7.2, we have

$$G_{\text{eff}} = \phi^{-1} \quad \text{and} \quad T^{(\text{eff})}_{\mu\nu} = T^{(\text{m})}_{\mu\nu} + T^{(\phi)}_{\mu\nu} + T^{(\text{CP})}_{\mu\nu} + T^{(\text{GB})}_{\mu\nu}, \tag{7.16}$$

with the components of $T^{(\text{eff})}_{\mu\nu}$ given by

$$\begin{aligned} 8\pi T^{(\text{CP})}_{\mu\nu} = -aH^{(\text{CP})}_{\mu\nu} \quad , \quad 8\pi T^{(\text{GB})}_{\mu\nu} = -\hat{b}H^{(\text{GB})}_{\mu\nu}\,, \\ 8\pi T^{(\phi)}_{\mu\nu} = \left(\nabla_\mu\nabla_\nu - g_{\mu\nu}\Box\right)\phi + \frac{\omega_{\text{L}}}{\phi}\left(\nabla_\mu\phi\nabla_\nu\phi - \frac{1}{2}g_{\mu\nu}\nabla_\alpha\phi\nabla^\alpha\phi\right) - Vg_{\mu\nu}\,. \end{aligned} \tag{7.17}$$

Hence, for LBD gravity, the GNEC, GWEC and GSEC are respectively

$$\phi^{-1}\ell^\mu\ell^\nu\left(8\pi T^{(\text{m})}_{\mu\nu} + \nabla_\mu\nabla_\nu\phi + \frac{\omega_{\text{L}}}{\phi}\nabla_\mu\phi\nabla_\nu\phi - aH^{(\text{CP})}_{\mu\nu} - \hat{b}H^{(\text{GB})}_{\mu\nu}\right) \geq 0\,, \tag{7.18}$$

$$\phi^{-1}u^\mu u^\nu\left(8\pi T^{(\text{m})}_{\mu\nu} + \nabla_\mu\nabla_\nu\phi + \frac{\omega_{\text{L}}}{\phi}\nabla_\mu\phi\nabla_\nu\phi - aH^{(\text{CP})}_{\mu\nu} - \hat{b}H^{(\text{GB})}_{\mu\nu}\right) + \phi^{-1}\left(\Box\phi + \frac{\omega_{\text{L}}}{2\phi}\nabla_\alpha\phi\nabla^\alpha\phi + V\right) \geq 0, \tag{7.19}$$

and

$$\begin{aligned} &\phi^{-1}u^\mu u^\nu\left(8\pi T^{(\text{m})}_{\mu\nu} + \nabla_\mu\nabla_\nu\phi + \frac{\omega_{\text{L}}}{\phi}\nabla_\mu\phi\nabla_\nu\phi - aH^{(\text{CP})}_{\mu\nu} - \hat{b}H^{(\text{GB})}_{\mu\nu}\right) \\ &+\frac{1}{2}\phi^{-1}\left(8\pi T^{(\text{m})} + 4\hat{b}R^{\alpha\beta}\nabla_\alpha\nabla_\beta\phi - (1+2\hat{b}R)\Box\phi - 2V\right) \geq 0\,, \end{aligned} \tag{7.20}$$

while the GDEC can be concretized in the same way. Among all generalized energy conditions, Eq.(7.18) clearly shows that the GNEC is not influenced by the background potential $V = V(\phi)$ of the scalar field.

Particularly, LBD gravity reduces to become GR for the situation $\phi(x^\alpha) \equiv G^{-1} = \text{constant}$ and $V(\phi) = 0$, as ${}^*RR$ and $\sqrt{-g}\mathcal{G}$ in Lovelock's action $\mathcal{S}_{\text{L}}$ do not affect the field equation. Then Eqs.(7.14) and (7.15) reduce to become the standard energy conditions for classical matter fields [5]:

$$T^{(\text{m})}_{\mu\nu}\,\ell^\mu\ell^\nu \geq 0 \quad (\text{NEC}) \quad , \quad T^{(\text{m})}_{\mu\nu}\,u^\mu u^\nu \geq 0 \quad (\text{WEC}) \quad , \quad T^{(\text{m})}_{\mu\nu}u^\mu u^\nu \geq \frac{1}{2}T^{(\text{eff})}u_\mu u^\mu \quad (\text{SEC})\,. \tag{7.21}$$

7.4 Conditions to support wormholes in LBD graity

7.4.1 Generic conditions supporting static, spherically symmetric wormholes

It has been nearly three decades since the classical work of Morris and Thorne, and nowadays the Morris-Thorne metric for static spherically symmetric wormholes is still the most useful and popular ansatz to study traversable wormholes. The metric reads [3]

$$ds^2 = -e^{2\Phi(r)}dt^2 + \left(1 - \frac{b(r)}{r}\right)^{-1} dr^2 + r^2\left(d\theta^2 + \sin^2\theta d\varphi^2\right)\,, \tag{7.22}$$

where $\Phi(r)$ and $b(r)$ are the redshift and the shape functions, respectively, and the radial coordinate $r \geq r_0$ ranges from a minimum value r_0 at the wormhole throat to infinity. $\Phi(r)$ is related to the gravitational redshift of an infalling body, and it must be finite everywhere to avoid the behavior $e^{2\Phi(r)} \to 0$ and consequently the existence of an event horizon. $b(r)$ determines the shape of the 2-slice $\{t = \text{constant}, \theta = \pi/2\}$ in the embedding diagram; it satisfies $b(r) < r$ to keep the wormhole Lorentzian, $b(r_0) = r_0$ at the throat, and $b(r)/r \to 0$ at $r \to \infty$ if asymptotically flat. Moreover, the embedding of the 2-slice $ds^2 = \left(1 - \frac{b(r)}{r}\right)^{-1} dr^2 + r^2 d\varphi^2$ yields the geometrical "flaring-out condition" $(b - b'r)/b^2 > 0$, which reduces to become $b'(r_0) < 1$ at the throat $r = r_0$ with $b(r_0) = r_0$ [3]. Here and hereafter the prime denotes the derivative with respect to the radial coordinate r.

Following the metric Eq.(7.22), in the null tetrad adapted to the spherical symmetry and the null radial congruence,

$$l^\mu = \left(e^{-\Phi(r)}, \sqrt{1 - \frac{b(r)}{r}}, 0, 0\right), \quad n^\mu = \frac{1}{2}\left(e^{-\Phi(r)}, -\sqrt{1 - \frac{b(r)}{r}}, 0, 0\right), \quad m^\mu = \frac{1}{\sqrt{2}\, r}\left(0, 0, 1, \frac{i}{\sin\theta}\right), \tag{7.23}$$

one could find the outgoing expansion rate $\theta_{(l)}$ and the ingoing expansion rate $\theta_{(n)}$ to be

$$\theta_{(l)} = -(\rho_{\rm NP} + \bar{\rho}_{\rm NP}) = \frac{2}{r}\sqrt{1 - \frac{b(r)}{r}}, \qquad \theta_{(n)} = \mu_{\rm NP} + \bar{\mu}_{\rm NP} = -\frac{1}{r}\sqrt{1 - \frac{b(r)}{r}}, \tag{7.24}$$

where $\rho_{\rm NP} := -m^\mu \bar{m}^\nu \nabla_\nu \ell_\mu$ and $\mu_{\rm NP} := \bar{m}^\mu m^\nu \nabla_\nu n_\mu$ are two Newman-Penrose spin coefficients. Thus the metric ansatz Eq.(7.22) guarantees that the spacetime is everywhere untrapped as $\theta_{(l)} = 2\theta_{(n)} > 0$, which is a characteristic property of traversable wormholes [30]. Also, Eq.(7.24) shows that the expansion rates are independent of the redshift function $\Phi(r)$, and the spacetime is free of apparent horizons for $r > r_0$.

Since the outward-flaring constraint $(b - b'r)/b^2 > 0$ solely comes from the embedding geometry, it is independent of and applicable to all gravity theories. In GR through Einstein's equation, this condition implies that all infalling observers threading a Morris-Thorne wormhole will experience the violation of the standard null energy condition $T^{(\rm m)}_{\mu\nu}\ell^\mu\ell^\nu \geq 0$ [3, 4]. Similarly, according to the GR form of the field equation (7.13), the flaring-out condition implies that wormholes in LBD gravity are supported by the breakdown of the LBD generalized energy conditions as in Eqs.(7.18) and (7.19). On the other hand, in principle it may still be possible to preserve the standard energy conditions in Eq.(7.21). Thus, to fulfill the constraint $(b - b'r)/b^2 > 0$ in LBD gravity, a possible way to violate the GNEC while keeping the standard NEC, i.e. $\phi^{-1}T^{(\rm eff)}_{\mu\nu}\ell^\mu\ell^\nu < 0$ and $T^{(\rm m)}_{\mu\nu}\ell^\mu\ell^\nu \geq 0$, can be

$$0 \leq 8\pi\ell^\mu\ell^\nu T^{(\rm m)}_{\mu\nu} \leq \ell^\mu\ell^\nu\left(aH^{(\rm CP)}_{\mu\nu} + \hat{b}H^{(\rm GB)}_{\mu\nu} - \nabla_\mu\nabla_\nu\phi - \frac{\omega_{\rm L}}{\phi}\nabla_\mu\phi\nabla_\nu\phi\right). \tag{7.25}$$

As another example, violation of the GWEC and preservation of the WEC, i.e. $\phi^{-1}T^{(\rm eff)}_{\mu\nu}u^\mu u^\nu < 0$ and $T^{(\rm m)}_{\mu\nu}u^\mu u^\nu \geq 0$, can be realized if

$$0 < 8\pi T^{(\rm m)}_{\mu\nu}u^\mu u^\nu < u^\mu u^\nu\left(aH^{(\rm CP)}_{\mu\nu} + \hat{b}H^{(\rm GB)}_{\mu\nu} - \nabla_\mu\nabla_\nu\phi - \frac{\omega_{\rm L}}{\phi}\nabla_\mu\phi\nabla_\nu\phi\right) - \left(\frac{\omega_{\rm L}}{2\phi}\nabla_\alpha\phi\nabla^\alpha\phi + \Box\phi + V\right). \tag{7.26}$$

Eqs.(7.25) and (7.26) indicate that $H^{(\rm CP)}_{\mu\nu}$ and $H^{(\rm GB)}_{\mu\nu}$, which represent the effects of the spacetime parity and topology, jointly with $T^{(\phi)}_{\mu\nu}$ should dominate over the material source of gravity. Also, a noncanonical scalar field ($\omega_{\rm L} < 0$) is preferred than a canonical one ($\omega_{\rm L} > 0$) to help support the wormhole.

Note that in Eqs.(7.25) and (7.26) we have assumed $\phi^{-1} = G_{\rm eff} > 0$. This is inspired by the fact in $f(R)$

gravity that the effective coupling strength $G_{\text{eff}} = df(R)/dR =: f_R$ has to satisfy $f_R > 0$ to guarantee that in the particle content via the spin projectors, the graviton itself and the induced scalar particle are not ghosts [31]. Similarly, in scalar-tensor gravity $\mathscr{L} = \frac{1}{16\pi G}\left[f(\phi)R - h(\phi)\nabla_\alpha\phi\nabla^\alpha\phi - 2U(\phi)\right] + \mathscr{L}_m$ in the Jordan frame, $G_{\text{eff}} = f(\phi)^{-1}$ should also be positive definite so that the graviton is not a ghost [32]. More generally, for modified gravities of the field equation (7.13), an assumption $G_{\text{eff}} > 0$ can not only simplify the generalized energy conditions Eqs.(7.14) and (7.15), but also help reduce the violation of these conditions.

In Sec. 7.5, we will demonstrate by a zero-tidal-force solution that Eq.(7.25) can really be satisfied while Eq.(7.26) is partially falsified for the same numerical setups. To facilitate the discussion, we further concretize the tensorial inequalities Eqs.(7.25) and (7.26) into an anisotropic perfect fluid form.

7.4.2 Supporting conditions in anisotropic fluid scenario

In accordance with the nonzero and unequal components of the Einstein tensor $G^\mu{}_\nu$, one can assume an anisotropic perfect-fluid form $T^\mu{}_\nu = \text{diag}\left[-\rho(r), P^r(r), P^T(r), P^T(r)\right]$ for $T^{\mu\,(\text{eff})}_{\ \nu}$ and each of its components. Here $T^\mu{}_\nu$ is adapted to the metric signature $(-,+++)$, with ρ standing for the energy density, P^r for the radial pressure, and P^T for the transverse pressure orthogonal to the radial direction. In wormhole physics, it is P^r that helps to open and maintain the wormhole tunnel, so in the context below we will be more concentrative on P^r rather than P^T. Then the generalized energy conditions in Sec. 7.3 imply $G_{\text{eff}}(\rho_{\text{eff}} + P^r_{\text{eff}}) \geq 0$ for the GNEC, $G_{\text{eff}}\rho_{\text{eff}} \geq 0$ and $G_{\text{eff}}(\rho_{\text{eff}} + P^r_{\text{eff}}) \geq 0$ for the GWEC, $G_{\text{eff}}(\rho_{\text{eff}} + P^r_{\text{eff}} + 2P^T_{\text{eff}}) \geq 0$ and $G_{\text{eff}}(\rho_{\text{eff}} + P^r_{\text{eff}}) \geq 0$ for the GSEC, as well as $G_{\text{eff}}\rho_{\text{eff}} \geq 0$ and $G_{\text{eff}}\rho_{\text{eff}} \geq \left|G_{\text{eff}}P^r_{\text{eff}}\right|$ for the GDEC, with G_{eff} removable when $G_{\text{eff}} > 0$.

In fact, the perfect-fluid form of $T^\mu{}_\nu$ clearly shows that violation of the null energy condition – that is to say, giving up the dominance of the energy density over the pressure, will imply the simultaneous violations of the weak, strong, and dominant energy conditions. This chain of violation happens for both the standard and the generalized energy conditions, and in this sense, it is sufficient to consider the violation of the null energy condition. According to the GNEC in LBD gravity, it requires $\phi^{-1}(\rho_{\text{eff}} + P^r_{\text{eff}}) < 0$ to make wormholes flare outward, with $\rho_{\text{eff}} = \rho_m + \rho_\phi + a\rho_{\text{CP}} + \hat{b}\rho_{\text{GB}}$ and $P^r_{\text{eff}} = P^r_m + P^r_\phi + aP^r_{\text{CP}} + \hat{b}P^r_{\text{GB}}$; under the Morris-Thorne metric, we have $\rho_{\text{CP}} = 0 = P^r_{\text{CP}}$,

$$8\pi\rho_\phi = \left(1 - \frac{b}{r}\right)\left(\Phi'\phi' + \phi'' + \frac{2\phi'}{r} + \frac{\omega_{\text{L}}}{2}\frac{\phi'^2}{\phi}\right) + \frac{\phi'}{2r^2}(b - b'r) + V\,, \tag{7.27}$$

$$8\pi P^r_\phi = \left(1 - \frac{b}{r}\right)\left(\phi'' + \omega_{\text{L}}\frac{\phi'^2}{\phi}\right) - 8\pi\rho_\phi\,, \tag{7.28}$$

$$\begin{aligned} 8\pi\rho_{\text{GB}} = \frac{1}{r^5}\Big[& -4br\phi''(b-r) - 2\phi'(2r-3b)(b-b'r) + 4\Phi'^2\phi'r^2\left(bb'r + 2r^2 - b'r^2 + b^2 - 3br\right) \\ & + 2\Phi''\phi'r^2\left(bb'r - b'r^2 - b^2 + br\right) + 4\Phi'\Phi''\phi'r^3(b-r)^2 + \Phi'^3r^3\left(r^2 - 8br + 4b^2\right) \\ & + \Phi'\phi'r\left(8r^2 - 16br + 4b'r^2 + b'^2r^2 - 6bb'r + 9b^2\right)\Big], \quad \text{and} \end{aligned} \tag{7.29}$$

$$8\pi P^{r}_{\rm GB} = \frac{2}{r^5}\Big[\phi'\,(b-b'r)\,(3b-4r+b'r) + 2\phi'' br(r-b) + 4\Phi'\phi' r\,(\Phi' r+2)\,(b-r)^2\Big] - 8\pi\rho_{\rm GB}\,. \qquad (7.30)$$

7.5 Zero-tidal-force solution

In this section we will continue to work out an exact solution of Morris-Thorne wormholes in LBD gravity, so as to better analyze the flaring-out condition for the wormhole throat, and examine the states of the generalized and standard energy conditions.

There are two functions to be specified in the Morris-Thorne metric Eq.(7.22). To be more concentrative on the wormhole throat and the embedding geometry, we will consider a zero redshift function $\Phi(r) = 0$ or $e^{2\Phi(r)} = 1$, which corresponds to vanishing tidal force and stationary observers [3]. In this situation, the LBD curvature invariants and the Einstein tensor read

$$R = \frac{2b'}{r^2}\,, \quad {}^*RR = 0 = \mathcal{G}\,, \quad G^{\mu}{}_{\nu} = r^{-3}\cdot \mathrm{diag}\Big[-b'r,\ -b,\ b-b'r,\ b-b'r\Big]\,, \qquad (7.31)$$

and thus the componential field equations $G^{\mu}{}_{\nu} = 8\pi\phi^{-1}T^{\mu\,({\rm eff})}_{\ \nu}$ directly illustrate the influences of the flaring-out condition $(b-b'r)/b^2 > 0$ to $T^{\mu\,({\rm eff})}_{\ \nu} = \mathrm{diag}\left[-\rho_{\rm eff}, P^r_{\rm eff}, P^T_{\rm eff}, P^T_{\rm eff}\right]$.

To simplify the dynamical wave equation (7.8), we assume the potential $V(\phi)$ to satisfy the condition $V_\phi \phi = 2V$, which integrates to yield

$$V(\phi) = V_0\phi^2\,, \qquad (7.32)$$

where V_0 is an integration constant. Moreover, we adopt the following power-law ansatz for the static and spherically symmetric scalar field,

$$\phi(r) = \phi_0\left(\frac{r_0}{r}\right)^A\,, \qquad (7.33)$$

where ϕ_0 and the power index A are constants, and r_0 is the throat radius $r_0 = \min(r)$.

With these setups, the kinematical wave equation (7.7) leads to

$$(2+\omega_{\rm L}A)\,rb' - \omega_{\rm L}A(A-1)b + \omega_{\rm L}A(A-2)r - 4V_0\phi_0\left(\frac{r_0}{r}\right)^A r^3 = 0\,. \qquad (7.34)$$

Solving this equation for $b(r)$ with the boundary condition $b(r=r_0) = r_0$, we obtain the shape function

$$b(r) = \frac{2V_0\phi_0 r_0^3\left[\left(\frac{r_0}{r}\right)^{\frac{\omega_{\rm L}A(1-A)}{\omega_{\rm L}A+2}} - \left(\frac{r_0}{r}\right)^{A-3}\right]}{\omega_{\rm L}A^2 - 2\omega_{\rm L}A + A - 3} + \frac{\omega_{\rm L}A\,(A-2)\,r - 2r_0\left(\frac{r_0}{r}\right)^{\frac{\omega_{\rm L}A(1-A)}{\omega_{\rm L}A+2}}}{\omega_{\rm L}A^2 - 2\omega_{\rm L}A - 2}\,, \qquad (7.35)$$

and thus

$$b - b'r = \frac{2V_0\phi_0 r_0^3\left[\left(1+\frac{\omega_{\rm L}A(1-A)}{\omega_{\rm L}A+2}\right)\left(\frac{r_0}{r}\right)^{\frac{\omega_{\rm L}A(1-A)}{\omega_{\rm L}A+2}} - (A-2)\left(\frac{r_0}{r}\right)^{A-3}\right]}{\omega_{\rm L}A^2 - 2\omega_{\rm L}A + A - 3} + \frac{2r_0}{\omega_{\rm L}A+2}\left(\frac{r_0}{r}\right)^{\frac{\omega_{\rm L}A(1-A)}{\omega_{\rm L}A+2}}\,. \qquad (7.36)$$

At the throat $r = r_0$, the flaring-out constraint $(b - b'r)/b^2$ is evaluated as

$$b'(r_0) = \frac{4V_0\phi_0 r_0^2 + \omega_L A}{\omega_L A + 2} < 1\,. \tag{7.37}$$

There are five parameters in $b(r)$, among which $\{r_0, \phi_0, A, V_0\}$ attribute to our solution ansatz for the homogeneous scalar field $\phi(r)$ and the potential $V(\phi)$, while ω_L comes from LBD gravity. To illustrate the wormhole geometry, we will adopt the following setups for these parameters.

(1) Without any loss of generality, let $r_0 = 1$ for the throat radius, and $\phi_0 = 1$.

(2) According to Eq.(7.33), asymptotic flatness of the spacetime requires $A > 0$ so that the scalar field monotonically falls off as $r \to \infty$; moreover, $\phi(r)$ is positive definite and meets the expectation $G_{\text{eff}} = \phi^{-1} > 0$ for the effective gravitational coupling strength, so that the graviton of LBD gravity is non-ghost for the sake of quantum stability.

(3) A repulsive potential hill $V(\phi) > 0$ tends to open and maintain the wormhole tunnel, while a trapping potential well $V(\phi) < 0$ would collapse the wormhole tunnel. Thus, in our numerical modelings, let $V_0 = 1 > 0$ so that $V(\phi)$ serves as a potential hill.

(4) Furthermore, it follows from Eq.(7.37) that the Lovelock parameter satisfies

$$\omega_L < -\frac{2}{A} < 0 \quad \text{for} \;\; r_0 = \phi_0 = V_0 = 1 \;\; \text{and} \;\; A > 0\,. \tag{7.38}$$

This agrees with the indication of Eqs.(7.25) and (7.26) that a noncanonical ($\omega_L < 0$) scalar field could best help support the wormhole.

With the numerical setups in Eq.(7.38), only two parameters ω_L and A remain flexible in determining the behaviors of $b(r)$ and $(b - b'r)/b^2$, where A tunes the spatially decaying rate of the scalar field; appropriate values of ω_L and A should validate $b(r) < r$, $b - b'r > 0$, and $\omega_L < -\frac{2}{A} < 0$. In Fig. 7.1, $b(r)$ is plotted at the domain $r \geq r_0 = 1$, and the wormhole solution Eq.(7.35) is confirmed to be Lorentzian. In Fig. 7.2, we plot $b - b'r$ and equivalently verify the flaring-out condition $(b - b'r)/b^2 > 0$. In both figures, we fix $A = 2.3$ and illustrate the dependence on ω_L (note that inside Figs. 7.1 ∼ 7.4, ω_L is temporarily written as ω for the sake of greater clarity).

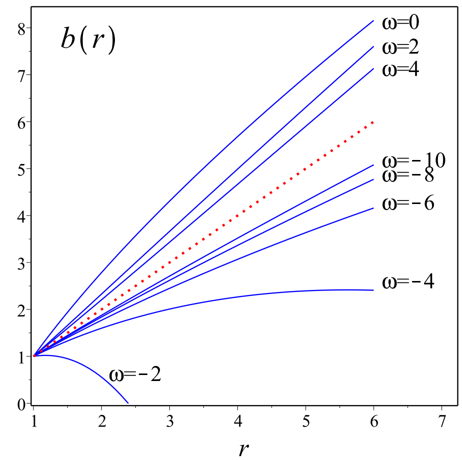


Figure 7.1: With $r_0 = \phi_0 = V_0 = 1$, $A = 2.3$ and in the domain $r \geq r_0 = 1$, $b(r)$ is plotted as the solid curves for various ω_L, along with the dotted diagonal for the auxiliary function $b(r) \equiv r$. For $\omega_L = \{-2, -4, -6, -8, -10 \cdots\} < -2/A = -2/2.3$ in light of the numerical setups in Eq.(7.38), $b(r)$ always falls below the auxiliary diagonal $b(r) \equiv r$. Thus, $1 - b(r)/r$ is positive definite and the wormhole solution Eq.(7.35) is Lorentzian. Moreover, the curve $b(r)$ approaches the dotted line when ω_L goes to $-\infty$, i.e. $\lim_{\omega_L \to -\infty} b(r)/r = 1$.

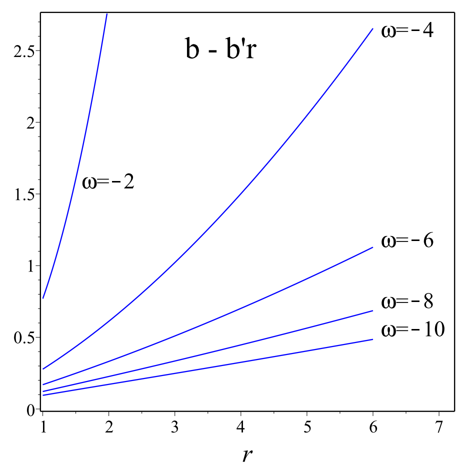


Figure 7.2: With $r_0 = \phi_0 = V_0 = 1$, $A = 2.3$ and in the domain $r \geq r_0 = 1$, $b - b'r$ is plotted for $\omega_L = \{-2, -4, -6, -8, -10 \cdots\} < -2/A = -2/2.3$ and manifests itself to be positive definite. This equivalently confirms the outward-flaring condition $(b - b'r)/b^2 > 0$ of the embedding geometry. Moreover, the curve $b - b'r$ tends to coincide with the horizontal r−axis when ω_L approaches $-\infty$, i.e. $\lim_{\omega_L \to -\infty} b - b'r = 0$, which is consistent with the tendency $\lim_{\omega_L \to -\infty} b(r)/r = 1$ in Fig. 7.1.

With the Einstein tensor $G^\mu{}_\nu$ given by Eq.(7.31) and $\phi^{-1} > 0$, adding up the componential field equations $G^t{}_t = -8\pi\phi^{-1}\rho_{\text{eff}}$ and $G^r{}_r = 8\pi\phi^{-1}P^r_{\text{eff}}$, one could obtain $b - b'r = -r^3 \cdot 8\pi\phi^{-1}(\rho_{\text{eff}} + P^r_{\text{eff}})$. Thus, for the numerical setups summarized by Eq.(7.38), Fig. 7.2 not only verifies the positive definiteness of $b - b'r$, but also implies the violation of the GNEC $\phi^{-1}(\rho_{\text{eff}} + P^r_{\text{eff}}) < 0$ – and consequently the GWEC, GSEC and GDEC in LBD gravity. On the other hand, can the standard energy conditions in Eq.(7.21) still hold along the radial direction for the matter threading the wormhole? The energy density ρ_m and the radial pressure P^r_m vary for different types of physical matter, and $\rho_m + P^r_m$ relies on the the equation of state $P^r_m = P^r_m(\rho_m)$. Thus, we choose to calculate $\rho_m + P^r_m$ from an indirect approach. Considering that $\frac{\phi}{8\pi}G^t{}_t = -(\rho_m + \rho_\phi + a\rho_{\text{CP}} + \hat{b}\rho_{\text{GB}})$

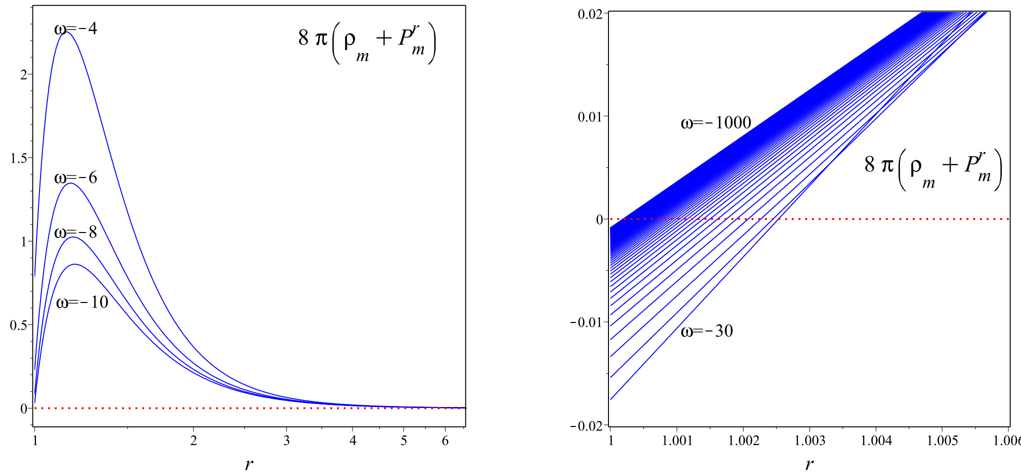


Figure 7.3: With $r_0 = \phi_0 = V_0 = 1$, $A = 2.3$, $\hat{b} = -1$ and in the domain $r \geq r_0 = 1$, $8\pi(\rho_m + P^r_m)$ is plotted as the solid curves, while the dotted horizontal depicts the zero reference level. The first subfigure shows that for $\omega_{\rm L} = \{-4, -6, -8, -10\}$, $8\pi(\rho_m + P^r_m)$ is positive definite with the expected asymptote $\lim_{r\to\infty} 8\pi(\rho_m + P^r_m) = 0^+$, so the standard NEC is respected. However, as $\omega_{\rm L}$ further decreases, $8\pi(\rho_m + P^r_m)$ gradually falls below the dotted horizontal near the throat $r \gtrapprox r_0 = 1$, which has been illustrated for $\omega_{\rm L} = \{-30, -40, -50, \cdots, -1000\}$ in the second subfigure by magnifying the region $r_0 = 1 \leq r \leq 1.0006$. Thus, large negative values of $\omega_{\rm L}$ (numerical analysis gives $\omega_{\rm L} \lesssim -12.9$) are unfavored in light of $8\pi(\rho_m + P^r_m) > 0$.

and $\frac{\phi}{8\pi} G^r{}_r = P^r_m + P^r_\phi + aP^r_{\rm CP} + \hat{b}P^r_{\rm GB}$, ρ_m and P^r_m can be recovered by

$$8\pi\rho_m = b' r\phi - 8\pi\rho_\phi - 8\pi\hat{b}\rho_{\rm GB} \quad , \quad 8\pi P^r_m = -b\phi - 8\pi P^r_\phi - 8\pi\hat{b}P^r_{\rm GB}\,, \tag{7.39}$$

where, according to Eqs.(7.27)-(7.30) with $\Phi(r) = 0$, we have

$$8\pi\rho_\phi = \left(1 - \frac{b}{r}\right)\left(\phi'' + \frac{2\phi'}{r} + \frac{\omega_{\rm L}}{2}\frac{\phi'^2}{\phi}\right) + \frac{\phi'}{2r^2}(b - b'r) + V \tag{7.40}$$

$$8\pi P^r_\phi = \left(1 - \frac{b}{r}\right)\left(\phi'' + \omega_{\rm L}\frac{\phi'^2}{\phi}\right) - 8\pi\rho_\phi \tag{7.41}$$

$$8\pi\rho_{\rm GB} = \frac{2}{r^5}\Big[\phi'(b - b'r)(3b - 2r) + 2br\phi''(r - b)\Big] \tag{7.42}$$

$$\text{and} \quad 8\pi P^r_{\rm GB} = \frac{2\phi'}{r^4}(b - b'r)(b' - 2)\,. \tag{7.43}$$

In Fig. 7.3, $8\pi(\rho_m + P^r_m)$ is plotted as the solid curves, where we let $\hat{b} = -1 < 0$ for the Gauss-Bonnet matter-topology coupling strength so that the Gauss-Bonnet part of LBD gravity could yield antigravitational effect to help maintain the wormhole tunnel. $\rho_m + P^r_m$ is positive definite for $\omega_{\rm L} = \{-4, -6, -8, -10\} < -2/A$ and thus the standard NEC $\rho_m + P^r_m \geq 0$ is respected by the physical matter, despite the violation of the GNEC due to $\phi^{-1}(\rho_{\rm eff} + P^r_{\rm eff}) < 0$; in fact, this has realized the null-energy supporting condition of Eq.(7.25) in an anisotropic perfect fluid form. However, large negative values of $\omega_{\rm L}$ is unfavored: careful numerical analysis finds that the standard NEC becomes slightly violated, i.e. $\rho_m + P^r_m < 0$ for $\omega_{\rm L} \lesssim -12.9$ in the very close vicinity of the wormhole throat.

Validity of the standard weak, strong and dominant energy conditions requires us to check the positivity of the physical matter density ρ_m. Plotting $8\pi\rho_m$ for $\omega_{\rm L} = \{-4, -6, -8, -10\cdots\}$ in Fig. 7.4, we find $\rho_m < 0$

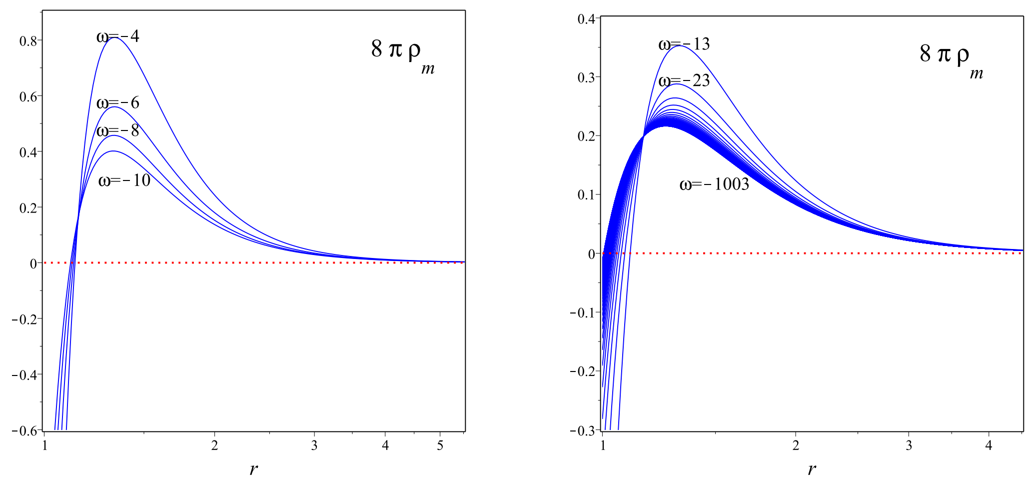


Figure 7.4: With $r_0 = \phi_0 = V_0 = 1$, $A = 2.3$, $\hat{b} = -1$ and in the domain $r \geq r_0 = 1$, $8\pi\rho_m$ is plotted as the solid curves for $\omega_{\rm L} = \{-4, -6, -8, -10\}$. Although $\rho_m > 0$ in the distance, one always observes $\rho_m < 0$ near the throat $r_0 = 1$, and thus the violation of the standard WEC, SEC and DEC. Moreover, as shown in the second subfigure for $\omega_{\rm L} = \{-13, -23, -33, \cdots, -1003\}$, the intersection point between $8\pi\rho_m$ and the dotted zero reference level moves leftwards when $\omega_{\rm L}$ decreases, so the violation of $\rho_m \geq 0$ gradually reduces.

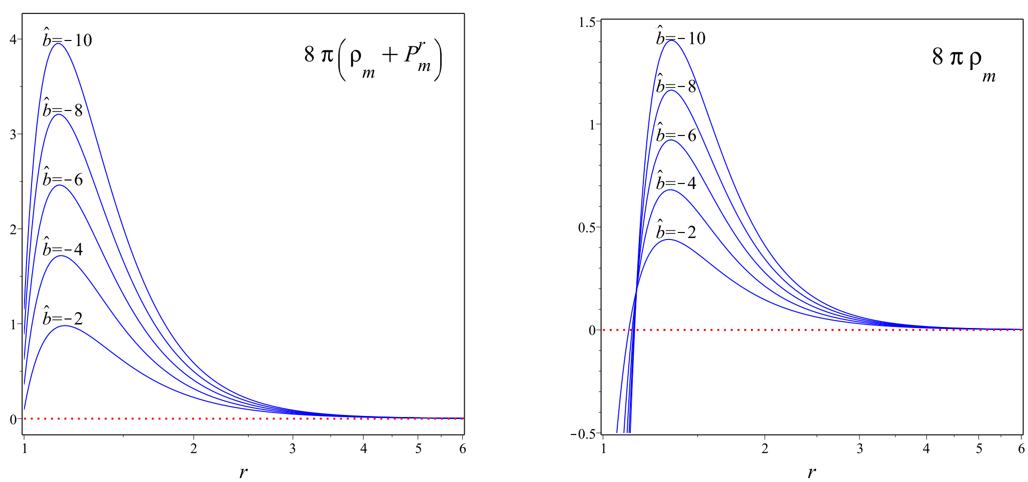


Figure 7.5: With $r_0 = \phi_0 = V_0 = 1$, $\omega_{\rm L} = -6$, $A = 2.3$ and in the domain $r \geq r_0 = 1$, we plot $8\pi(\rho_m + P_m^r)$ and $8\pi\rho_m$ for different Gauss-Bonnet topology-gravity coupling strength, as is given the decreasing series $\hat{b} = \{-2, -4, -6, -8, -10\}$. The standard NEC always holds with $\rho_m + P_m^r \geq 0$. Moreover, the intersection point between $8\pi\rho_m$ and the dotted reference level moves leftwards when $\hat{b} < 0$ increases from $\hat{b} = -10$ to -2,, so the violation of $\rho_m \geq 0$ gradually reduces.

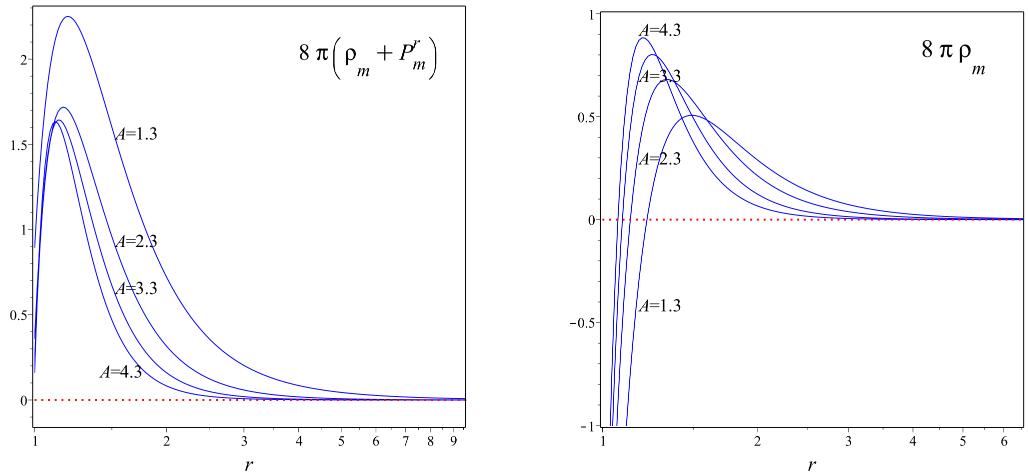


Figure 7.6: With $r_0 = \phi_0 = V_0 = 1$, $\omega_{\rm L} = -6$, $\hat{b} = -4$ and in the domain $r \geq r_0 = 1$, we plot $8\pi(\rho_m + P^r_m)$ and $8\pi\rho_m$ for different decaying rate of the scalar field, as is given by the increasing series $A = \{1.3, 2.3, 3.3, 4.3\}$. The standard NEC always holds with $\rho_m + P^r_m \geq 0$. Moreover, the intersection point between $8\pi\rho_m$ and the dotted reference level moves leftwards when $A > 0$ increases from $A = 1.3$ to 4.3, so the violation of $\rho_m \geq 0$ gradually reduces.

near the wormhole throat, and the violation of $\rho_m \geq 0$ can be reduced with the decrement of $\omega_{\rm L}$ in the domain $\omega_{\rm L} < -2/A$; actually, this has negated the weak-energy supporting condition of Eq.(7.26) in the anisotropic perfect fluid form, despite the validity of the null-energy Eq.(7.25). As expected, when one goes way from the wormhole throat, the normal behaviors $\rho_m \geq 0$ and $\lim_{r\to\infty} \rho_m = 0^+$ are recovered, and thus the standard WEC becomes valid as $\rho_m + P^r_m \geq 0$ for $r > r_0 = 1$ in light of Fig. 7.3.

Having seen from Fig. 7.4 that the decrement of the noncanonical $\omega_{\rm L}$ could reduce the violation of $\rho_m \geq 0$, we cannot help but ask are there any other factors that could help protect the standard WEC? The answer is yes. In Figs. 7.5 and 7.6, we respectively fix $\{\omega_{\rm L} = -6\,, A = 2.3\}$ and $\{\omega_{\rm L} = -6\,, \hat{b} = -4\}$ to plot $\{8\pi(\rho_m + P^r_m)\,, 8\pi\rho_m\}$. It turns out that when the standard NEC is obeyed, i.e. $\rho_m + P^r_m \geq 0$, the increment of $\hat{b}$ (Gauss-Bonnet topology-gravity coupling strength) in the repulsive domain $\hat{b} < 0$ and the increment of A (decaying-rate index of the scalar field) in the domain $A > 0$ could both help minimize the violation of $\rho_m \geq 0$ near the wormhole throat.

7.6 Implication: Wormholes in Brans-Dicke gravity

In the limits $a \to 0$ and $\hat{b} \to 0$ for the parity-gravity and the topology-gravity coupling coefficients in $\mathcal{S}_{\rm LBD}$, and in the absence of the potential $V(\phi)$, LBD gravity reduces to become Brans-Dicke gravity with the standard action [33]

$$\mathcal{S}_{\rm BD} = \frac{1}{16\pi} \int d^4x \sqrt{-g} \left(\phi R - \frac{\hat{\omega}}{\phi} \nabla_\alpha \phi \nabla^\alpha \phi \right) + \mathcal{S}_m \,, \tag{7.44}$$

where $\hat{\omega}$ refers to the Brans-Dicke parameter (in distinction with $\omega_{\rm L}$ for the Lovelock parameter). The gravitational field equation $\delta\mathcal{S}_{\rm BD}/\delta g^{\mu\nu} = 0$ and the kinematical wave equation $\delta\mathcal{S}_{\rm BD}/\delta\phi = 0$ are respectively

$$\phi \left(R_{\mu\nu} - \frac{1}{2} R g_{\mu\nu} \right) + \left(g_{\mu\nu} \Box - \nabla_\mu \nabla_\nu \right) \phi - \frac{\hat{\omega}}{\phi} \left(\nabla_\mu \phi \nabla_\nu \phi - \frac{1}{2} g_{\mu\nu} \nabla_\alpha \phi \nabla^\alpha \phi \right) = 8\pi T^{(\rm m)}_{\mu\nu} \,, \tag{7.45}$$

$$\text{and}\quad 2\hat{\omega}\cdot\Box\phi = -\phi R + \frac{\hat{\omega}}{\phi}\nabla_\alpha\phi\nabla^\alpha\phi\,. \tag{7.46}$$

With the trace of the field equation $-\phi R + \frac{\hat{\omega}}{\phi}\nabla_\alpha\phi\nabla^\alpha\phi + 3\Box\phi = 8\pi T^{(\mathrm{m})}$, Eq.(7.46) leads to the dynamical wave equation $(2\hat{\omega}+3)\Box\phi = 8\pi T^{(\mathrm{m})}$; however, the kinematical equation (7.46) is preferred so that temporarily we need not worry about $T^{(\mathrm{m})}$ for the physical matter.

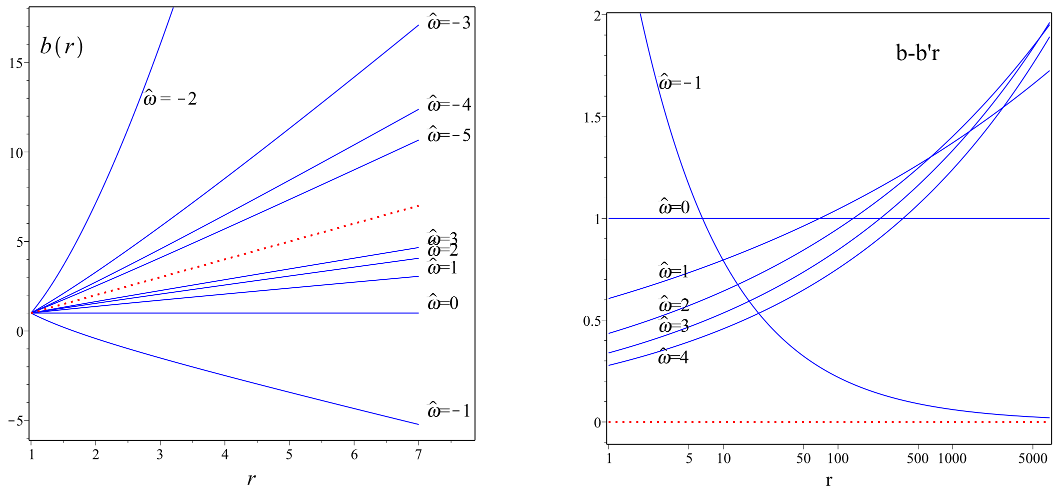


Figure 7.7: With $r_0 = \phi_0 = 1$ and $A = 1.3$, we plot $b(r)$ and $b - b'r$ as the solid curves. The first subfigure shows that for $\hat{\omega} = \{-1, 0, 1, 2, 3\cdots\} > -2/A = -2/1.3$, $b(r)$ always falls below the dotted diagonal of the auxiliary function $b(r) \equiv r$, and thus guarantees the Lorentzian signature as $1 - b(r)/r > 0$. Moreover, the second subfigure verifies $b - b'r > 0$ for $\hat{\omega} = \{-1, 0, 1, 2, 3, 4\cdots\} > -1/1.3$, so the flaring-out condition $(b - b'r)/b^2 > 0$ of the embedding geometry is satisfied.

For Morris-Thorne wormholes in Brans-Dicke gravity, consider a zero-tidal-force solution $\Phi(r) = 0$, and inherit the ansatz $\phi(r) = \phi_0\left(\frac{r_0}{r}\right)^A$ ($\phi_0 > 0$, $A =$ constant) of Eq.(7.33) for the scalar field. Directly solving Eq.(7.46) for $b(r)$ with the boundary condition $b(r_0) = r_0$, or just substituting $\{V_0 \equiv 0, \omega_{\mathrm{L}} \mapsto \hat{\omega}\}$ into Eqs.(7.35) and (7.36), we obtain

$$b(r) = r + \frac{2r - 2r_0\left(\frac{r_0}{r}\right)^{\frac{\hat{\omega}A(1-A)}{\hat{\omega}A+2}}}{\hat{\omega}A^2 - 2\hat{\omega}A - 2} \quad\text{and}\quad b - b'r = \frac{2r_0}{\hat{\omega}A+2}\left(\frac{r_0}{r}\right)^{\frac{\hat{\omega}A(1-A)}{\hat{\omega}A+2}}\,. \tag{7.47}$$

In light of the flaring-out condition at the wormhole throat, the parameters $\{A, \hat{\omega}\}$ have to meet the requirement

$$b'(r_0) = 1 - \frac{2}{\hat{\omega}A+2} < 1 \quad\Rightarrow\quad \hat{\omega}A > -2\,. \tag{7.48}$$

Note that this condition does not conflict with the $\omega_{\mathrm{L}}A < -2$ in Eq.(7.38): Eq.(7.48) comes from Eq.(7.37) with $\{V_0 \equiv 0, \omega_{\mathrm{L}} \mapsto \hat{\omega}\}$, while Eq.(7.38) specifies Eq.(7.37) by $r_0 = \phi_0 = V_0 = 1$; the choices $V_0 \equiv 0$ and $V_0 = 1$ (and also $V_0 = -1$, if one would like to check it), i.e. the potential being vanishing, repulsive or attractive, lead Eq.(7.37) to totally different situations.

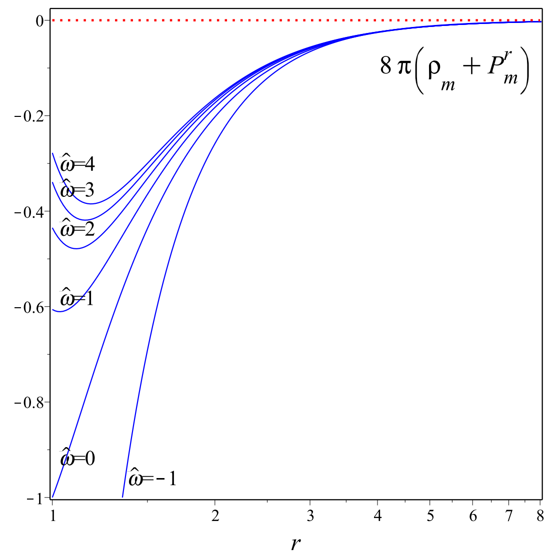


Figure 7.8: With $r_0 = \phi_0 = 1$ and $A = 1.3$, we plot $8\pi(\rho_m + P^r_m)$ for $\hat{\omega} = \{-1, 0, 1, 2, 3, 4\}$ as the solid curves, which always fall below the dotted horizontal for the zero reference level. Thus, the standard NEC is always violated. As $\hat{\omega}$ grows from -1 to 4, the curve of $8\pi(\rho_m + P^r_m)$ gradually moves upward, so in a sense the violation of $8\pi(\rho_m + P^r_m) \geq 0$ can be reduced for greater values of $\hat{\omega}$ in the domain $\hat{\omega} > -2/A$.

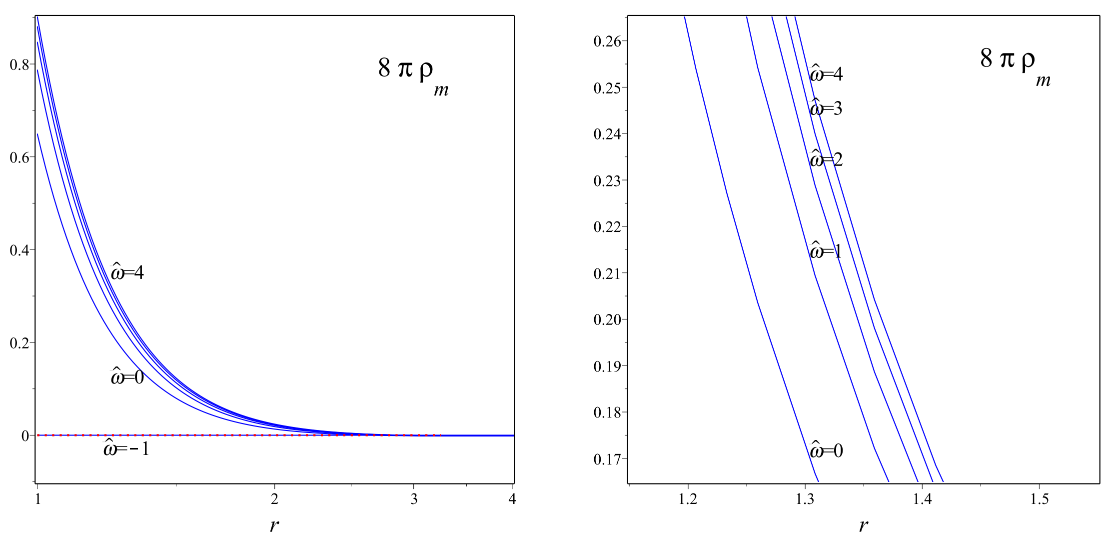


Figure 7.9: With $r_0 = \phi_0 = 1$ and $A = 1.3$, we plot $8\pi\rho_m$ for $\hat{\omega} = \{-1, 0, 1, 2, 3, 4\}$ as the solid curves. These curves stay above the zero reference level for $\hat{\omega} = \{0, 1, 2, 3, 4\}$ and coincide with it for $\hat{\omega} = -1$; since the curves for $\hat{\omega} = \{0, 1, 2, 3, 4\}$ are stickily close to each other in the first subfigure, we magnify them at $1.2 < r < 1.45$ for greater clarity in the second subfigure, which shows that from bottom to top or from left to right, the curves correspond to $\hat{\omega} = 0, ...4$ in sequence. Although the energy density is nonnegative for $\hat{\omega} \geq -1$, the standard WEC, SEC and DEC still fail as $8\rho_m + P^r_m < 0$ for all $\hat{\omega} > -2/A$ by Fig. 7.8.

Among the three parameters in $b(r)$, $\{\hat{\omega}, A\}$ jointly determine the wormhole structure, while r_0 acts as an auxiliary parameter; for the same reasons indicated in the proceeding section, we inherit the numerical setups $\{r_0 = \phi_0 = 1, A > 0\}$ to illustrate the Brans-Dicke wormhole Eq.(7.47), which implies $\hat{\omega} > -2/A$ from Eq.(7.48). To start with, the Lorentzian-signature condition $r > b(r)$ and the outward-flaring constraints

$b - b'r > 0$ are confirmed in Fig. 7.7.

Next, let's check the states of the standard energy conditions in Eq.(7.21). For the matter threading the wormhole, the energy density and radial pressure can be indirectly reconstructed from the field equations $8\pi\rho_m = b'r\phi - 8\pi\rho_\phi$ and $8\pi P^r_m = -b\phi - 8\pi P^r_\phi$, where

$$8\pi\rho_\phi = \left(1-\frac{b}{r}\right)\left(\phi'' + \frac{2\phi'}{r} + \frac{\hat{\omega}}{2}\frac{\phi'^2}{\phi}\right) + \frac{\phi'}{2r^2}\left(b - b'r\right) , \tag{7.49}$$

$$8\pi P^r_\phi = \left(1-\frac{b}{r}\right)\left(\phi'' + \hat{\omega}\frac{\phi'^2}{\phi}\right) - 8\pi\rho_\phi \, . \tag{7.50}$$

With $\phi_0 = 1 = r_0$ in $\phi(r) = \phi_0 \left(\frac{r_0}{r}\right)^A$ and the zero-tidal-force solution Eq.(7.47), it follows that

$$8\pi(\rho_m + P^r_m) = \frac{2\hat{\omega}A(\hat{\omega}A^2 + A^2 + 4A - 2) + 4(A^2 + A - 1)}{(\hat{\omega}A + 2)(\hat{\omega}A^2 - 2\hat{\omega}A - 2)} \frac{r^{\frac{\hat{\omega}A(A-1)}{\hat{\omega}A+2}}}{r^{A+3}} - \frac{2A(\hat{\omega}A + A + 1)}{(\hat{\omega}A^2 - 2\hat{\omega}A - 2)} \frac{r}{r^{A+3}} , \tag{7.51}$$

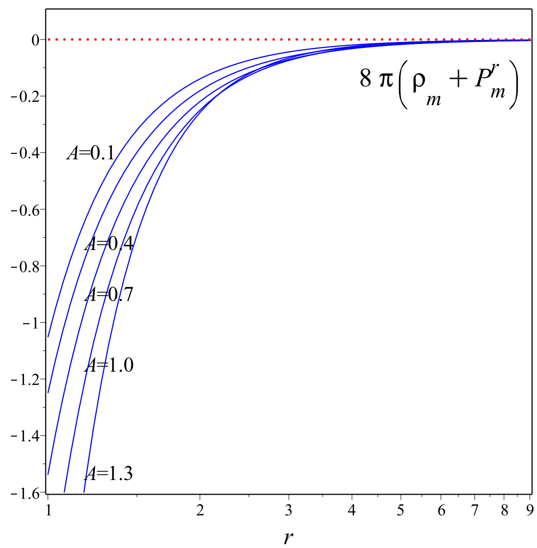
$$8\pi\rho_m = \frac{1}{r} + \frac{r(\hat{\omega}+6) - \left[\hat{\omega} + 3 + \frac{3\hat{\omega}A(A-1)}{\hat{\omega}A+2}\right] r^{\frac{\hat{\omega}A(A-1)}{\hat{\omega}A+2}}}{r^2(\hat{\omega}A^2 - 2\hat{\omega}A - 2)} \, . \tag{7.52}$$

Based on Eqs.(7.51) and (7.52), the behaviors of $8\pi(\rho_m + P^r_m)$ and $8\pi\rho_m$ are illustrated in Figs. 7.8 and 7.9 with the numerical setups $\{r_0 = \phi_0 = 1, A = 1.3 > 0, \hat{\omega} > -2/A\}$. Unfortunately, despite the nonnegative energy density, the standard null – and thus weak, strong and dominant energy conditions are always violated along the radial direction as $\rho_m + P^r_m < 0$ for $r \geq r_0$; to make matters slightly better, Fig. 7.8 indicates that in a sense such violation could be reduced for greater values of $\hat{\omega}$ in the domain $\hat{\omega} > -2/A$. Moreover, as shown in Fig. 7.10 which fixes $\hat{\omega} = 1$ and studies the influences of A instead, we notice that even $\rho_m \geq 0$ no longer holds throughout $r \geq r_0$ for a spatially quickly decaying ($A \gtrsim 2$) scalar field.

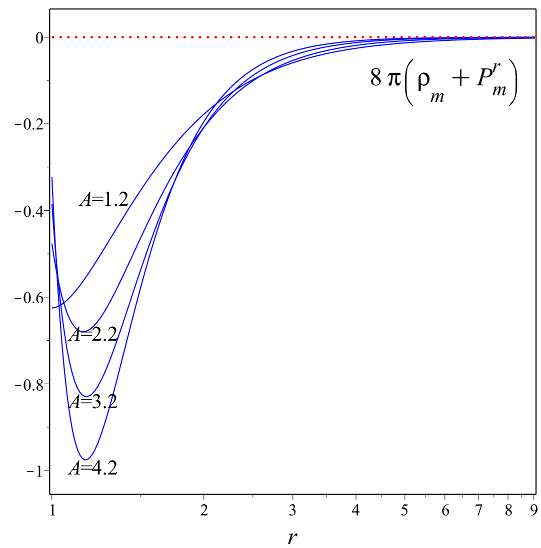
Comparing Figs. 7.8 ~ 7.10 of Brans-Dicke gravity with Fig. 7.3, one could find that due to the presence of the potential hill $V(\phi) > 0$ and the possibly antigravitational Gauss-Bonnet effect, LBD gravity could "better" protect the standard NEC when supporting wormholes. The results in this section supplement the earlier investigations in Ref.[19]. Moreover, recall that in scalar-tensor theory with the total Lagrangian density $\mathscr{L} = \frac{1}{16\pi G}\left[f(\phi)R - h(\phi)\cdot\nabla_\alpha\phi\nabla^\alpha\phi - 2U(\phi)\right] + \mathscr{L}_m$ in the Jordan frame, we have the following conditions for the sake of ghost-freeness and quantum stability [32]: the graviton is non-ghost if $f(\phi) > 0$ (as mentioned before in Sec. 7.4.1), while the scalar field $\phi(x^\alpha)$ itself is non-ghost if

$$\frac{3}{2}\left(\frac{df(\phi)}{d\phi}\right)^2 + f(\phi)h(\phi) > 0 \, . \tag{7.53}$$

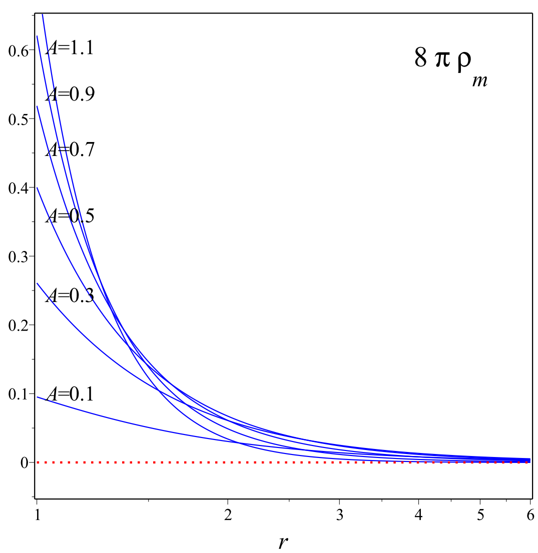
For Brans-Dicke gravity with $f(\phi) = \phi$ and $h(\phi) = \hat{\omega}/\phi$, it requires $\phi > 0$ and $\hat{\omega} > -3/2$ to be totally ghost-free. Thus, the lessons from Figs. 7.8 ~ 7.10 are consistent with the argument of Ref.[32] that in scalar-tensor gravity, there exists no static, spherically symmetric wormholes that are both ghost-free and obeying the standard NEC.



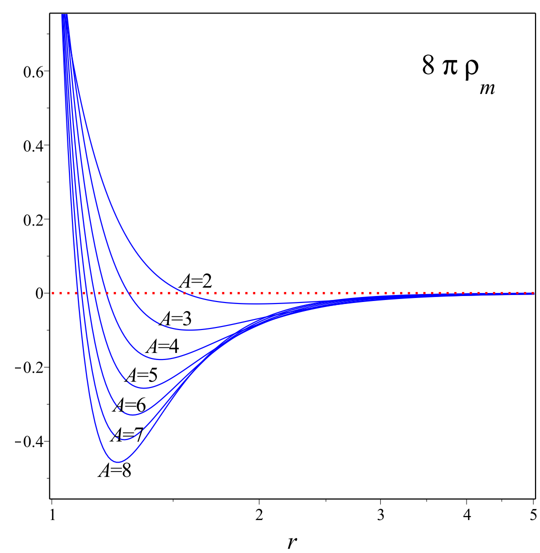
(a) From top to bottom, A =0.1, 0.4, $\cdots$, 1.3.



(b) From top to bottom, A =1.2, 2.2, 3.2, 4.2.



(c) From top to bottom, A =1.1, 0.9, $\cdots$, 0.1.



(d) From top to bottom, A =2, 3, $\cdots$, 8.

Figure 7.10: With $r_0 = \phi_0 = 1$ and $\hat{\omega} = 1$, we plot $8\pi(\rho_m + P^r_m)$ and $8\pi\rho_m$ for different values of A which governs the spatially decaying rate of the scalar field. Figs. 7.10a and 7.10b, with a similar appearance to Fig. 7.8, show $\rho_m + P^r_m < 0$ for $A > 0$ so that the standard NEC is violated; moreover, with Fig. 7.10c in an analogous pattern to Fig. 7.9, one finds $\rho_m > 0$ for slow decaying rate $A = \{0.1, 0.3, \cdots, 1.1\}$. As the most interesting observation, Fig. 7.10d shows that ρ_m is no longer positive definite throughout $r \geq r_0$ for high decaying rate $A \gtrsim 2$.

7.7 Discussion and conclusions

In Secs. 7.4 and 7.5, we have seen that $\rho_{\rm CP}$ and $P^r_{\rm CP}$ did not help in supporting Morris-Thorne wormholes; this is because $H^{\rm (CP)}_{\mu\nu}$ identically vanishes for all spherically symmetric spacetimes (no matter static or dynamical). In fact, it can be directly verified that the spacetime parity will come into effect via nonzero $H^{\rm (CP)}_{\mu\nu}$ in generic axially symmetric spacetimes, say the metric below that generalizes Morris-Thorne into rotating wormholes [7]:

$$ds^2 = -e^{2\Phi(r,\theta)}dt^2 + \left(1 - \frac{b(r,\theta)}{r}\right)^{-1} dr^2 + r^2\Big[d\theta^2 + \sin^2\theta\,(dt - \omega d\varphi)^2\Big], \tag{7.54}$$

where, as in the Kerr or Papapetrou metric, $\omega = \omega(r,\theta)$ is the angular velocity $d\varphi/dt$ acquired by a test particle falling to the point (r,θ) from infinity.

Also, the wormhole geometry is not only related to the energy-momentum distribution of the physical matter through the gravitational field equation, but also to the propagation of the scalar field through the kinematical wave equation. Hence, in Secs. 7.5 and 7.6, for the sake of simplicity, we have chosen to "recover" the shape function $b(r)$ and thus the wormhole geometry from the kinematics of $\phi(r)$, i.e. Eqs.(7.7) and (7.46), while the field equations were employed to analyze the energy conditions. When seeking for zero-tidal-force solutions with a vanishing redshift function $\Phi(r) = 0$, this provides a simpler method than that in Ref.[19] for Brans-Dicke gravity, or Ref.[21] for hybrid metric-Palatini $f(R)$ gravity which is equivalent to the mixture of GR and the $\hat{\omega} = -3/2$ Brans-Dicke gravity; they solve for $b(r)$ from the *dynamical* wave equation (i.e. Klein-Gordon equation) rather than the *kinematical* wave equation, and thus have to involve the trace of the matter tensor $T^{\rm (m)} = -\rho_m + P^r_m + 2P^T_m$ right from the beginning. However, when looking for more general solutions with $\Phi(r) \neq 0$, one should still turn to the method in Refs.[19] and [21], as it becomes insufficient to determine the two Morris-Thorne functions $\{\Phi(r)\,,b(r)\}$ from a single kinematical wave equation.

To sum up, in this paper we have investigated the conditions to support traversable wormholes in LBD gravity. The flaring-out condition, which arises from the wormholes' embedding geometry and thus applies to all metric gravities, requires the violation of the standard NEC in GR and the GNEC in modified gravities. Moreover, the breakdown of the null energy condition simultaneously violates the weak, strong and dominant energy conditions. With these considerations, we have derived the generalized energy conditions Eqs.(7.14), (7.15), (7.18) and (7.19) for LBD gravity in the form that explicitly contains the effective gravitational coupling strength $G_{\rm eff} = \phi^{-1}$. These energy conditions have been used to construct the conditions supporting Morris-Thorne-type wormholes, including the tensorial expressions Eqs.(7.25) and (7.26), and their anisotropic-perfect-fluid forms in Sec. 7.4.2. Moreover, in Sec. 7.5 we have obtained an exact solution of the Morris-Thorne wormhole with a vanishing redshift function and the shape function Eq.(7.35), which is supplemented by the homogeneous scalar field $\phi(x^\alpha) = \phi(r)$ in Eq.(7.33) and the potential $V(\phi) = V_0\phi^2$. With the flexible parameters in Eq.(7.35) for $b(r)$ specified by $\{\phi_0 = r_0 = V_0 = 1, A > 0, \omega_{\rm L} < -2/A\}$, we have further confirmed the Lorentzian signature, the flaring-out condition, breakdown of the GNEC, and validity of the standard NEC. Finally, we also investigated zero-tidal-force wormholes in Brans-Dicke gravity, and have shown that the condition $\rho_m + P^r_m \geq 0$ is not so well protected as in LBD gravity.

Note that natural existence of dark energy becomes effective only at scales greater than 1Mpc [35]. Similarly in modified gravties, the higher-order terms or extra degrees of freedom are astrophysically recognizable only at galactic and cosmic levels. Hence, supporting wormholes by dark energy requires to mine and condense dark energy, while supporting wormholes by modified gravity requires unusual distributions of ordinary matter. For example, in LBD gravity, the joint effects of $H_{\mu\nu}^{(\mathrm{CP})}$, $H_{\mu\nu}^{(\mathrm{GB})}$ and $T_{\mu\nu}^{(\phi)}$ have to become dominant over the physical matter source $T_{\mu\nu}^{(\mathrm{m})}$, and the scalar field is preferred to be noncanonical. As a closing remark, we have to admit that wormholes in existing studies are mainly theoretical exercises and hypothetical objects, and there seems a long way ahead before wormholes can be artificially constructed and put to astronomical use.

Acknowledgement

This work was supported by NSERC grant 261429-2013.

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Chapter 8. Local energy-momentum conservation in scalar-tensor-like gravity with generic curvature invariants

[*Gen. Relativ. Gravit.* (2016) **48**: 110]

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Abstract

For a large class of scalar-tensor-like gravity whose action contains nonminimal couplings between a scalar field $\phi(x^\alpha)$ and generic curvature invariants $\{\mathcal{R}\}$ beyond the Ricci scalar $R = R^\alpha{}_\alpha$, we prove the covariant invariance of its field equation and confirm/prove the local energy-momentum conservation. These $\phi(x^\alpha) - \mathcal{R}$ coupling terms break the symmetry of diffeomorphism invariance under a particle transformation, which implies that the solutions to the field equation should satisfy the consistency condition $\mathcal{R} \equiv 0$ when $\phi(x^\alpha)$ is nondynamical and massless. Following this fact and based on the accelerated expansion of the observable Universe, we propose a primary test to check the viability of the modified gravity to be an effective dark energy, and a simplest example passing the test is the "Weyl/conformal dark energy".

PACS numbers: 04.20.Cv , 04.20.Fy , 04.50.Kd
Key words: energy-momentum conservation, diffeomorphism invariance, effective dark energy

8.1 Introduction

An important problem in relativistic theories of gravity is the divergence-freeness of the field equation and the covariant conservation of the energy-momentum tensor. In general relativity (GR), Einstein's equation $G_{\mu\nu} \equiv R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} = 8\pi G T^{(m)}_{\mu\nu}$ has a vanishing covariant divergence due to the contracted Bianchi identities $\nabla^\mu G_{\mu\nu} \equiv 0$, which guarantees the local energy-momentum conservation $\nabla^\mu T^{(m)}_{\mu\nu} = 0$ or $\partial^\mu(\sqrt{-g}\, T^{(m)}_{\mu\nu}) = 0$ for the matter tensor $T^{(m)}_{\mu\nu}$. In modified gravities beyond GR and its Hilbert-Einstein action, the conservation problem becomes more complicated and has attracted a lot of interest.

In Ref.[1], the generalized Bianchi identities were derived for the Palatini formulation of the nonlinear $f(R)$ gravity, and its local energy-momentum conservation was further confirmed in Ref.[2] by the equivalence between Palatini $f(R)$ and the $\omega = -3/2$ Brans-Dicke gravity. Ref.[3] investigated a mixture of $f(R)$ and the generalized Brans-Dicke gravity, and proved the covariant conservation from both the metric and the Palatini variational approaches. For Einstein-Cartan gravity which allows for spacetime torsion, both the energy-momentum and the angular momentum conservation were studied in Ref.[4] by decomposing the

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Bianchi identities in Riemann-Cartan spacetimes. In Refs.[3, 5–7], the nontrivial divergences $\nabla^\mu T^{(m)}_{\mu\nu}$ were analyzed for the situations where the matter Lagrangian density is multiplied by different types of curvature invariants in the action. Also, interestingly in Ref.[8], the possible consequences after dropping the energy-momentum conservation in GR, such as the modified evolution equation for the Hubble parameter, were investigated.

Besides the covariant invariance $\nabla^\mu T^{(m)}_{\mu\nu} = 0$ for the matter tensor $T^{(m)}_{\mu\nu}$ that has been standardly defined in GR and modified gravities (cf. Eq.(8.20) below), the conservation problem has also been studied for more fundamental definitions of energy-momentum tensors from a wider perspective, i.e. from a first-principle approach making use of Noether's theorem and the classical field theory. For example, the Noether-induced canonical energy-momentum conservation for the translational invariance of the Lagrangian was studied in Ref.[9] for general spacetimes with torsion and nonmetricity. The conservation equations and the Noether currents for the Poincaré-transformation invariance were studied in Ref.[10] for the 3+1 and 2+1 dimensional Einstein gravity and the 1+1 dimensional string-inspired gravity. Also, Refs.[11] and [12] extensively discussed the diffeomorphically invariant metric-torsion gravity whose action contains first- and second-order derives of the torsion tensor, and derived the full set of Klein-Noether differential identities and various types of conserved currents.

In this paper, our interest is the covariant invariance of such modified gravities whose actions involve nonminimal couplings between arbitrary curvature invariants $\{\mathcal{R}\}$ and a background scalar field $\phi(x^\alpha)$. For example, $\phi(x^\alpha)$ is coupled to the Ricci scalar $R = R^\alpha{}_\alpha$ in Brans-Dicke and scalar-tensor gravity in the Jordan frame [13], to the Chern-Pontryagin topological density in the Chern-Simons modification of GR [14], and to the Gauss-Bonnet invariant $\mathcal{G} = R^2 - 4R_{\alpha\beta}R^{\alpha\beta} + R_{\alpha\mu\beta\nu}R^{\alpha\mu\beta\nu}$ in the Gauss-Bonnet effective dark energy [15]. In theory, one could consider the nonminimal coupling of $\phi(x^\alpha)$ to an arbitrarily complicated curvature invariant beyond the Ricci scalar. In such situations, however, the covariant invariance of the field equation has not been well understood, so we aim to carefully look into this problem by this work. Note that it might sound more complete to analyze the global conservation $\partial^\mu[\sqrt{-g}(T^{(m)}_{\mu\nu} + t_{\mu\nu})] = 0$, where $t_{\mu\nu}$ refers to the energy-momentum pseudotensor for the gravitational field, but to make this paper more clear and readable, we choose to concentrate on the local conservation $\nabla^\mu T^{(m)}_{\mu\nu} = 0$, while the incorporation of $t_{\mu\nu}$ will be discussed separately.

This paper is organized as follows. In Sec. 8.2, we introduce the generic class of modified gravity with the nonminimal $\phi(x^\alpha)$−couplings to arbitrary Riemannian invariants $\{\mathcal{R}\}$, calculate the divergence for different parts of the total action, prove the covariant invariance of the field equation, and confirm the local energy-momentum conservation. Section 8.3 investigates the reduced situations that the scalar field is non-dynamical and massless, and derives the consistency constraint $\mathcal{R} \equiv 0$ which suppresses the breakdown of diffeomorphism invariance. Finally, applications of the theories in Secs. 8.2 and 8.3 are considered in Sec. 8.4. Throughout this paper, we adopt the geometric conventions $\Gamma^\alpha_{\beta\gamma} = \Gamma^\alpha{}_{\beta\gamma}$, $R^\alpha{}_{\beta\gamma\delta} = \partial_\gamma\Gamma^\alpha_{\delta\beta} - \partial_\delta\Gamma^\alpha_{\gamma\beta}\cdots$ and $R_{\mu\nu} = R^\alpha{}_{\mu\alpha\nu}$ with the metric signature $(-, +++)$.

8.2 General theory

8.2.1 Scalar-tensor-like gravity

Consider a theory of modified gravity or effective dark energy given by the following action,

$$\mathcal{S} = \int d^4x \sqrt{-g} \left(\mathscr{L}_{\text{HE}} + \mathscr{L}_{\text{G}} + \mathscr{L}_{\text{NC}} + \mathscr{L}_{\phi}\right) + \mathcal{S}_m \,, \tag{8.1}$$

where $\mathscr{L}_{\text{HE}}$ refers to the customary Hilbert-Einstein Lagrangian density as in GR,

$$\mathscr{L}_{\text{HE}} = R \,, \tag{8.2}$$

while $\mathscr{L}_{\text{G}}$ denotes the extended dependence on generic curvature invariants $\mathcal{R}$,

$$\mathscr{L}_{\text{G}} = f\left(R, \cdots, \mathcal{R}\right) \,. \tag{8.3}$$

Here $\mathcal{R} = \mathcal{R}\left(g_{\alpha\beta}\,, R_{\mu\alpha\nu\beta}\,, \nabla_\gamma R_{\mu\alpha\nu\beta}\,, \dots\right)$ is an arbitrary invariant function of the metric as well as the Riemann tensor and its derivatives up to any order. For example, $\mathcal{R}$ can come from the fourteen[1] algebraically independent real invariants of the Riemann tensor [16] and their combinations, say $R_{\alpha\beta}R^{\alpha\beta} + R_{\alpha\mu\beta\nu}R^{\alpha\mu\beta\nu} + R_{\alpha\mu\beta\nu}R^{\alpha\beta}R^{\mu\nu}$, which will yield fourth–order field equations; or differential Riemannian invariants that will lead to sixth– or even higher–order field equations, like $R\nabla^\alpha\nabla_\alpha R + R^\alpha{}_\mu R^\beta{}_\nu \nabla_\alpha\nabla_\beta R^{\mu\nu}$.

In the total Lagrangian density, $\mathscr{L}_{\text{NC}}$ represents the nonminimal coupling effects,

$$\mathscr{L}_{\text{NC}} = h(\phi) \cdot \widehat{f}\left(R, \cdots, \mathcal{R}\right) \,, \tag{8.4}$$

where $h(\phi)$ is an arbitrary function of the scalar field $\phi = \phi(x^\alpha)$, and $\widehat{f}\left(R, \cdots, \mathcal{R}\right)$ has generic dependence on curvature invariants, with the dots "$\cdots$" in $\widehat{f}\left(R, \cdots, \mathcal{R}\right)$ and the $f\left(R, \cdots, \mathcal{R}\right)$ above denoting different choices of $\mathcal{R}$. Moreover, the kinetics of $\phi(x^\alpha)$ is governed by

$$\mathscr{L}_{\phi} = -\lambda(\phi) \cdot \nabla_\alpha\phi\nabla^\alpha\phi - V(\phi) \,. \tag{8.5}$$

In the $(-, +\,+\,+)$ system of conventions, $\phi(x^\alpha)$ is canonical if $\lambda(\phi) > 0$, noncanonical if $\lambda(\phi) < 0$, and nondynamical if $\lambda(\phi) = 0$.

Finally, as usual, the matter action $\mathcal{S}_m$ in Eq.(8.1) is given by the matter Lagrangian density via

$$\mathcal{S}_m = 16\pi G \int d^4x \sqrt{-g}\, \mathscr{L}_m\left(g_{\mu\nu}, \psi_m, \partial_\mu\psi_m\right) \,, \tag{8.6}$$

where the variable ψ_m collectively describes the matter fields, and ψ_m is minimally coupled to the metric tensor $g_{\mu\nu}$. Unlike the usual dependence on $\partial_\mu\psi_m$ in its standard form, $\mathscr{L}_m = \mathscr{L}_m\left(g_{\mu\nu}, \psi_m, \partial_\mu\psi_m\right)$ does not contain derivatives of the metric tensor – such as Christoffel symbols or curvature invariants, in light of the minimal gravity-matter coupling and Einstein's equivalence principle; physically, this means $\mathscr{L}_m$ reduces to the matter Lagrangian density for the flat spacetime in a freely falling local reference frame (i.e. a locally

[1] When one combines the spacetime geometry with matter fields in the framework of GR, the amount of independent algebraic invariants will be extended to sixteen in the presence of electromagnetic or perfect-fluid fields [17].

geodesic coordinate system).

To sum up, we are considering the modifications of GR into the total Lagrangian density $\mathscr{L} = R + f(R, \cdots, \mathcal{R}) + h(\phi) \cdot \widehat{f}(R, \cdots, \mathcal{R}) - \lambda(\phi) \cdot \nabla_\alpha\phi\nabla^\alpha\phi - V(\phi) + 16\pi G\mathscr{L}_m$, which has been rescaled so that the numerical coefficient $16\pi G$ is associated to $\mathscr{L}_m$. It can be regarded as a mixture of the nonlinear higher-order gravity $\mathscr{L} = R + f(R, \cdots, \mathcal{R}) + 16\pi G\mathscr{L}_m$ in the metric formulation for the curvature invariants, and the generalized scalar-tensor gravity $\mathscr{L} = h(\phi) \cdot \widehat{f}(R, \cdots, \mathcal{R}) - \lambda(\phi) \cdot \nabla_\alpha\phi\nabla^\alpha\phi - V(\phi) + 16\pi G\mathscr{L}_m$ in the Jordan frame for the scalar field. Hereafter we will mainly work with actions, and for simplicity we will sometimes adopt the total Lagrangian density in place of the corresponding action in full integral form.

8.2.2 Divergence-freeness of gravitational field equation

Pure curvature parts

For the Hilbert-Einstein part of the total action, i.e. $\mathcal{S}_{\text{HE}} = \int d^4x\sqrt{-g}\,\mathscr{L}_{\text{HE}}$, its variation with respect to the inverse metric yields the well-known result $\delta\mathcal{S}_{\text{HE}} \cong \int d^4x\sqrt{-g}\,G_{\mu\nu}\delta g^{\mu\nu}$. By the symbol $\cong$ we mean the equality after neglecting all total derivatives in the integrand or equivalently boundary terms of the action when integrating by parts, and the Einstein tensor $G_{\mu\nu} = R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu}$ respects the twice-contracted Bianchi identity $\nabla^\mu G_{\mu\nu} = 0$.

For the gravitational action $\mathcal{S}_{\text{G}} = \int d^4x\sqrt{-g}\,\mathscr{L}_{\text{G}}$ for the extended dependence on generic Riemannian invariants, formally we write down the variation as $\delta\mathcal{S}_{\text{G}} \cong \int d^4x\sqrt{-g}\,H^{(\text{G})}_{\mu\nu}\delta g^{\mu\nu}$, where $H^{(\text{G})}_{\mu\nu}$ resembles and generalizes the Einstein tensor by

$$H^{(\text{G})}_{\mu\nu} \;\cong\; \frac{1}{\sqrt{-g}}\,\frac{\delta\left[\sqrt{-g}\,f(R, \cdots, \mathcal{R})\right]}{\delta g^{\mu\nu}}\,. \tag{8.7}$$

Due to the coordinate invariance of $\mathcal{S}_{\text{G}}$, $H^{(\text{G})}_{\mu\nu}$ satisfies the generalized contracted Bianchi identities [18, 19]

$$\nabla^\mu\left(\frac{1}{\sqrt{-g}}\,\frac{\delta\left[\sqrt{-g}\,f(R, \cdots, \mathcal{R})\right]}{\delta g^{\mu\nu}}\right) = \;0\,, \tag{8.8}$$

or just $\nabla^\mu H^{(\text{G})}_{\mu\nu} = 0$ by the definition of $H^{(\text{G})}_{\mu\nu}$. Similar to the relation $G_{\mu\nu} = R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu}$, one can further expand $H^{(\text{G})}_{\mu\nu}$ to rewrite Eq.(8.8) into

$$\nabla^\mu\left(f_R R_{\mu\nu} + \sum f_{\mathcal{R}}\mathcal{R}_{\mu\nu} - \frac{1}{2}f(R, \cdots, \mathcal{R})\,g_{\mu\nu}\right) = 0\,, \tag{8.9}$$

where $f_R \coloneqq \partial f(R, \cdots, \mathcal{R})/\partial R$, $f_{\mathcal{R}} \coloneqq \partial f(R, \cdots, \mathcal{R})/\partial\mathcal{R}$, and $\mathcal{R}_{\mu\nu} \cong (f_{\mathcal{R}}\delta\mathcal{R})\,/\delta g^{\mu\nu}$ – note that in the calculation of $\mathcal{R}_{\mu\nu}$, $f_{\mathcal{R}}$ will serve as a nontrivial coefficient if $f_{\mathcal{R}} \neq$ constant and should be absorbed into the variation $\delta\mathcal{R}$ when integrated by parts.

Nonminimal $\phi(x^\alpha)$-curvature coupling part

For the componential action $\mathcal{S}_{\rm NC} = \int d^4x \sqrt{-g}\, \mathscr{L}_{\rm NC}$ for the nonminimal coupling effect, formally we have the variation $\delta\mathcal{S}_{\rm NC} \cong \int d^4x \sqrt{-g}\, H^{(\rm NC)}_{\mu\nu} \delta g^{\mu\nu}$, where

$$H^{(\rm NC)}_{\mu\nu} \cong \frac{1}{\sqrt{-g}} \frac{\delta\left[\sqrt{-g}\,\phi\,\widehat{f}(R,\cdots,\mathcal{R})\right]}{\delta g^{\mu\nu}} \,. \tag{8.10}$$

Unlike $H^{(\rm G)}_{\mu\nu}$ with Eq.(8.8), $H^{(\rm NC)}_{\mu\nu}$ does not respect some straightforward generalized Bianchi identities; this is because $\mathcal{S}_{\rm NC}$ involves the coupling with the background scalar field $\phi(x^\alpha)$ and is no longer purely tensorial gravity. Thus, we will analyze the divergence of $H^{(\rm NC)}_{\mu\nu}$ by the diffeomorphism of $\mathcal{S}_{\rm NC}$.

Consider an arbitrary infinitesimal coordinate transformation $x^\mu \mapsto x^\mu + \delta x^\mu$, where $\delta x^\mu = k^\mu$ is an infinitesimal vector field that vanishes on the boundary, $k^\mu = 0\,|_{\partial\Omega}$, so that the spacetime manifold is mapped onto itself. $\mathcal{S}_{\rm NC}$ responds to this transformation by

$$\delta\mathcal{S}_{\rm NC} = \int d^4x\, h(\phi)\cdot\partial_\mu\left[k^\mu\sqrt{-g}\,\widehat{f}(R,\cdots,\mathcal{R})\right] \tag{8.11}$$

$$\cong -\int d^4x\sqrt{-g}\,\widehat{f}(R,\cdots,\mathcal{R})\cdot\left(h_\phi\partial_\mu\phi\right)k^\mu, \tag{8.12}$$

where $h_\phi \coloneqq dh(\phi)/d\phi$. For Eq.(8.11), one should note that $\phi(x^\alpha)$ acts as a fixed background, as it only relies on the coordinates (i.e. spatial location and time) and is independent of the spacetime metric; moreover, the coordinate shift $x^\mu \mapsto x^\mu + k^\mu$ is an active transformation, under which the dynamical tensor field $g_{\mu\nu}$ and thus $\sqrt{-g}\,\widehat{f}(R,\cdots,\mathcal{R})$ transform, while the background field $\phi(x^\alpha)$ and the coordinate system parameterizing the spacetime remain unaffected [20].

Under the active transformation $x^\mu \mapsto x^\mu + k^\mu$, the metric tensor varies by $g_{\mu\nu} \mapsto g_{\mu\nu} + \delta g_{\mu\nu}$ with $\delta g_{\mu\nu} = \pounds_{\vec{k}} g_{\mu\nu} = \nabla_\mu k_\nu + \nabla_\nu k_\mu$, and therefore $g^{\mu\nu} \mapsto g^{\mu\nu} + \delta g^{\mu\nu}$ with $\delta g^{\mu\nu} = -\pounds_{\vec{k}} g^{\mu\nu} = -\nabla^\mu k^\nu - \nabla^\nu k^\mu$. Recalling the definition of $H^{(\rm NC)}_{\mu\nu}$ with $H^{(\rm NC)}_{\mu\nu}$ being symmetric for the index switch $\mu \leftrightarrow \nu$, one has

$$\delta\mathcal{S}_{\rm NC} = -2\int d^4x\sqrt{-g}\,H^{(\rm NC)}_{\mu\nu}\nabla^\mu k^\nu \cong 2\int d^4x\sqrt{-g}\left(\nabla^\mu H^{(\rm NC)}_{\mu\nu}\right)k^\nu, \tag{8.13}$$

Comparing Eq.(8.12) with Eq.(8.13), we conclude that $H^{(\rm NC)}_{\mu\nu}$ has a nontrivial divergence for $\phi(x^\alpha) \neq$ constant, and

$$\nabla^\mu H^{(\rm NC)}_{\mu\nu} = -\frac{1}{2}\widehat{f}(R,\cdots,\mathcal{R})\cdot h_\phi\partial_\nu\phi\,. \tag{8.14}$$

In fact, Eq.(8.14) reflects the breakdown of diffeomorphism invariance in the presence of a fixed background scalar field. As a comparison, it is worthwhile to mention that under an observer/passive transformation where the observer or equivalently the coordinate system transforms, both the tensor fields and the background scalar field will be left unchanged, so the symmetry of observer-transformation invariance continues to hold [20].

Purely scalar-field part

Next, for the purely scalar-field part $\mathcal{S}_\phi = \int d^4x \sqrt{-g}\, \mathscr{L}_\phi$ with the variation $\delta \mathcal{S}_\phi \cong \int d^4x \sqrt{-g}\, H^{(\phi)}_{\mu\nu} \delta g^{\mu\nu}$, explicit calculations find

$$H^{(\phi)}_{\mu\nu} = -\lambda(\phi) \cdot \nabla_\mu \phi \nabla_\nu \phi + \frac{1}{2}\Big(\lambda(\phi) \cdot \nabla_\alpha \phi \nabla^\alpha \phi + V(\phi)\Big) g_{\mu\nu} \,. \tag{8.15}$$

Taking its contravariant derivative, we immediately obtain the nontrivial divergence

$$\nabla^\mu H^{(\phi)}_{\mu\nu} = -\frac{1}{2}\left(\lambda_\phi \cdot \nabla_\alpha \phi \nabla^\alpha \phi + 2\lambda(\phi) \cdot \Box \phi - V_\phi\right) \cdot \nabla_\nu \phi \,, \tag{8.16}$$

where $\lambda_\phi := d\lambda(\phi)/d\phi$, $V_\phi := dV(\phi)/d\phi$, and $\Box$ denotes the covariant d'Alembertian with $\Box\phi = g^{\alpha\beta}\nabla_\alpha \nabla_\beta \phi = \frac{1}{\sqrt{-g}}\partial_\alpha(\sqrt{-g}\, g^{\alpha\beta}\partial_\beta \phi)$. On the other hand, extremizing the entire action Eq.(8.1) with respect to the scalar field, i.e. $\delta S/\delta\phi = 0$, one could obtain the kinematical wave equation

$$2\lambda(\phi) \cdot \Box\phi = -\widehat{f}\,(R, \cdots, \mathcal{R}) \cdot h_\phi - \lambda_\phi \cdot \nabla_\alpha \phi \nabla^\alpha \phi + V_\phi \,. \tag{8.17}$$

We regard it as "kinematical" because it does not explicitly relate the propagation of $\phi(x^\alpha)$ to $T^{(\mathrm{m})} = g^{\mu\nu} T^{(\mathrm{m})}_{\mu\nu}$ for the matter distribution, while the "dynamical" wave equation can be obtained after combing Eq.(8.17) with the trace of the gravitational field equation. Substitute Eq.(8.17) into the right hand side of Eq.(8.16), and it follows that

$$\nabla^\mu H^{(\phi)}_{\mu\nu} = \frac{1}{2}\widehat{f}\,(R, \cdots, \mathcal{R}) \cdot h_\phi \nabla_\nu \phi \,, \tag{8.18}$$

which exactly cancels out the divergence of $H^{(\mathrm{NC})}_{\mu\nu}$ in Eq.(8.14) for the nonminimal-coupling part $\mathcal{S}_{\mathrm{NC}}$.

Covariant invariance of field equation and local energy-momentum conservation

To sum up, for the modified gravity or effective dark energy given by Eq.(8.1), its field equation reads

$$G_{\mu\nu} + H^{(\mathrm{G})}_{\mu\nu} + H^{(\mathrm{NC})}_{\mu\nu} + H^{(\phi)}_{\mu\nu} = 8\pi G T^{(m)}_{\mu\nu} \,, \tag{8.19}$$

where, unlike $G_{\mu\nu}$ and $H^{(\phi)}_{\mu\nu}$, the exact forms of $\left\{H^{(\mathrm{G})}_{\mu\nu},\ H^{(\mathrm{NC})}_{\mu\nu}\right\}$ will not be determined until the concrete expressions of $\{\mathscr{L}_{\mathrm{G}},\ \mathscr{L}_{\mathrm{NC}}\}$ or $\left\{f(R, \cdots, \mathcal{R}), \widehat{f}(R, \cdots, \mathcal{R})\right\}$ are set up. In Eq.(8.19), the energy-momentum tensor $T^{(\mathrm{m})}_{\mu\nu}$ is defined as in GR via [21]

$$\delta \mathcal{S}_m = -\frac{1}{2} \times 16\pi G \int d^4x \sqrt{-g}\, T^{(\mathrm{m})}_{\mu\nu} \delta g^{\mu\nu} \quad \text{with} \quad T^{(\mathrm{m})}_{\mu\nu} := \frac{-2}{\sqrt{-g}} \frac{\delta\left(\sqrt{-g}\, \mathscr{L}_m\right)}{\delta g^{\mu\nu}} \,, \tag{8.20}$$

with $\mathcal{S}_m$ rescaled by $16\pi G$ in Eq.(8.6). Instead of the variational definition Eq.(8.20), it had been suggested that $T^{(\mathrm{m})}_{\mu\nu}$ could be derived solely from the equations of motion $\dfrac{\partial \mathscr{L}_m}{\partial \psi_m} - \nabla_\mu \dfrac{\partial \mathscr{L}_m}{\partial(\partial_\mu \psi_m)} = 0$ for the ψ_m field in $\mathscr{L}_m\left(g_{\mu\nu}, \psi_m, \partial_\mu \psi_m\right)$ [22]; however, further analyses have shown that this method does not hold a general validity, and Eq.(8.20) remains as the most reliable approach to $T^{(\mathrm{m})}_{\mu\nu}$ [23].

Adding up the (generalized) contracted Bianchi identities $\nabla^\mu G_{\mu\nu} = 0$ and Eq.(8.8), and the nontrivial divergences Eqs.(8.14) and (8.18), eventually we conclude that the left hand side of the field equation (8.19) is divergence free, the local energy-momentum conservation $\nabla^\mu T^{(m)}_{\mu\nu} = 0$ holds, and the tensorial equations of motion for test particles remain the same as in GR.

In fact, the matter Lagrangian density $\mathscr{L}_m = \mathscr{L}_m\left(g_{\mu\nu}, \psi_m, \partial_\mu\psi_m\right)$ is a scalar invariant that respects the diffeomorphism invariance under the active transformation $x^\mu \mapsto x^\mu + k^\mu$, and Noether's conservation law directly yields

$$\nabla^\mu\left(\frac{1}{\sqrt{-g}}\,\frac{\delta\left(\sqrt{-g}\,\mathscr{L}_m\right)}{\delta g^{\mu\nu}}\right) = 0\,, \tag{8.21}$$

which can be recast into $-\frac{1}{2}\nabla^\mu T^{(m)}_{\mu\nu} = 0$. That is to say, under minimal geometry-matter coupling with an isolated $\mathscr{L}_m$ in the total Lagrangian density, the matter tensor $T^{(\mathrm{m})}_{\mu\nu}$ in Eq.(8.20) has been defined in a *practical* way so that $T^{(\mathrm{m})}_{\mu\nu}$ is automatically symmetric, Noether compatible, and covariant invariant, which naturally guarantees the local conservation $\nabla^\mu T^{(m)}_{\mu\nu} = 0$. In this sense, one can regard the vanishing divergence $\nabla^\mu\left(G_{\mu\nu} + H^{(\mathrm{G})}_{\mu\nu} + H^{(\mathrm{NC})}_{\mu\nu} + H^{(\phi)}_{\mu\nu}\right) = 0$ for Eq.(8.19) to either *imply* or *confirm* the conservation $\nabla^\mu T^{(m)}_{\mu\nu} = 0$.

One should be aware that in the presence of nonminimal gravity-matter couplings, like $\mathcal{R}\cdot\mathscr{L}_m$ or more generally $F(R,\cdots,\mathcal{R})\cdot\mathscr{L}_m$ in the total Lagrangian density, the divergence $\nabla^\mu T^{(m)}_{\mu\nu}$ becomes nonzero as well and obeys the relation $\nabla^\mu T^{(m)}_{\mu\nu} = F(R,\cdots,\mathcal{R})^{-1}\cdot\left(\mathscr{L}_m\, g_{\mu\nu} - T^{(m)}_{\mu\nu}\right)\cdot\nabla^\mu F(R,\cdots,\mathcal{R})$ instead [5–7], which recovers the local conservation $\nabla^\mu T^{(m)}_{\mu\nu} = 0$ for $F(R,\cdots,\mathcal{R}) = $ constant.

Also, at a more fundamental level, the $T^{(\mathrm{m})}_{\mu\nu}$ in Eq.(8.20) for GR and modified gravities, though practical with all desired properties, is not defined from the first-principle approach, i.e. directly from symmetry and Noether's theorem in the classical field theory. In this larger framework, the $T^{(\mathrm{m})}_{\mu\nu}$ in Eq.(8.20) is often referred to as the Hilbert energy-momentum tensor: it symmetrizes the canonical energy-momentum tensor of translational invariance by adding a superpotential term, and it is a special case of the Belinfante energy-momentum tensor that minimally couples to gravity [24].

8.3 Nondynamical massless scalar field

8.3.1 Nondynamical massive scalar field

Due to the $\lambda(\phi)$-dependence in $\mathcal{S}_\phi$, its Lagrangian density becomes $\mathscr{L}_\phi = -V(\phi)$ when $\lambda(\phi) \equiv 0$; considering that $V(\phi)$ is usually related to the mass of the scalar field in cosmology and high energy physics, we will call $\phi(x^\alpha)$ nondynamical and massive for the situation $\lambda(\phi) \equiv 0$ and $V(\phi) \neq 0$. As such, instead of producing a propagation equation $\Box\phi$, the extremization $\delta S/\delta\phi = 0$ leads to the following constraint for the potential $V(\phi)$:

$$V_\phi = \widehat{f}\,(R,\cdots,\mathcal{R})\cdot h_\phi\,. \tag{8.22}$$

In the meantime, Eqs.(8.15), (8.16), and (8.17) reduce to become

$$H^{(\phi)}_{\mu\nu} = \frac{1}{2}V(\phi)\,g_{\mu\nu} \qquad \text{and} \qquad \nabla^\mu H^{(\phi)}_{\mu\nu} = \frac{1}{2}V_\phi\nabla_\nu\phi = \frac{1}{2}\widehat{f}\,(R,\cdots,\mathcal{R})\cdot h_\phi\nabla_\nu\phi\,. \tag{8.23}$$

Thus, for a nondynamical yet massive scalar field, $\nabla^\mu H^{(\phi)}_{\mu\nu}$ can still balance the nontrivial divergence $\nabla^\mu H^{(\mathrm{NC})}_{\mu\nu}$ of the nonminimal $\phi(x^\alpha)$-curvature coupling effect, while the potential or the mass of the scalar field is restricted by the condition Eq.(8.22).

8.3.2 Nondynamical massless scalar field

Within the situation $\lambda(\phi) \equiv 0$, it becomes even more interesting when the potential vanishes as well in Eqs.(8.5), (8.15), (8.16), and (8.17); we will call the scalar field *nondynamical and massless*[2] for $\lambda(\phi) = 0 = V(\phi)$. With $\mathscr{L}_\phi = 0$, the total action simplifies into

$$\mathcal{S} = \int d^4x \sqrt{-g} \Big(R + \mathscr{L}_{\mathrm{G}} + \mathscr{L}_{\mathrm{NC}} + 16\pi G \mathscr{L}_m \Big) . \tag{8.24}$$

Since $H^{(\phi)}_{\mu\nu} = 0$ and $\nabla^\mu H^{(\phi)}_{\mu\nu} = 0$, the divergence $\nabla^\mu H^{(\mathrm{NC})}_{\mu\nu}$ for the nonminimal coupling part as in Eq.(8.14) can no longer be neutralized. Instead, with $\nabla^\mu G_{\mu\nu} = 0$, the generalized contracted Bianchi identities Eq.(8.8), and the covariant conservation $\nabla^\mu T^{(m)}_{\mu\nu} = 0$ under minimal geometry-mater coupling, the contravariant derivative of the field equation $G_{\mu\nu} + H^{(\mathrm{G})}_{\mu\nu} + H^{(\mathrm{NC})}_{\mu\nu} = 8\pi G T^{(m)}_{\mu\nu}$ forces $\nabla^\mu H^{(\mathrm{NC})}_{\mu\nu}$ to vanish. Together with Eq.(8.14), this implies that to be a solution to the gravity of Eq.(8.24), the metric tensor $g_{\mu\nu}$ must satisfy the constraint

$$\widehat{f}(R, \cdots, \mathcal{R}) \equiv 0 \quad \text{for} \quad \phi(x^\alpha) \neq \text{constant} . \tag{8.25}$$

Since the nonzero divergence $\nabla^\mu H^{(\mathrm{NC})}_{\mu\nu} = -\frac{1}{2}\widehat{f}(R, \cdots, \mathcal{R}) \cdot h_\phi \partial_\nu \phi$ measures the failure of diffeomorphism invariance in the componential action $\mathcal{S}_{\mathrm{NC}}$, the consistency condition Eq.(8.25) indicates that the symmetry breaking of diffeomorphism invariance is suppressed in gravitational dynamics of Eq.(8.24).

Here one should note that the variation $\delta\mathcal{S}/\delta\phi = 0$ yields the condition $\widehat{f}(R, \cdots, \mathcal{R}) \cdot h_\phi = 0$, which also leads to $\widehat{f}(R, \cdots, \mathcal{R}) \equiv 0$ if the scalar field is nonconstant. In addition, the constraint $\widehat{f}(R, \cdots, \mathcal{R}) \equiv 0$ does not mean $H^{(\mathrm{NC})}_{\mu\nu} = 0$ or the removal of $\mathscr{L}_{\mathrm{NC}}$ from the action Eq.(8.24). This can be seen by an analogous situation in GR: all vacuum solutions of Einstein's equation have to satisfy the condition $R \equiv 0$, but the GR action $\mathcal{S} = \int d^4x \sqrt{-g}\, (R + 16\pi G \mathscr{L}_m)$ still holds in its standard form.

After $\mathscr{L}_{\mathrm{G}}$ and $\mathscr{L}_{\mathrm{NC}}$ get specified in Eq.(8.24), how can we know whether it yields a viable theory or not? In accordance with Eq.(8.25), we adopt the following basic assessment.

Primary test: For the action Eq.(8.24) to be a viable modified gravity or effective dark energy carrying a nondynamical and massless scalar field, an elementary requirement is that the function $\widehat{f}(R, \cdots, \mathcal{R})$ in $\mathscr{L}_{\mathrm{NC}}$ vanishes identically for the flat and accelerating Friedmann-Robertson-Walker (FRW) Universe with the metric

$$ds^2 = -dt^2 + a(t)^2 \sum_{i=1}^{3} \left(dx^i\right)^2 \quad \text{and} \quad \ddot{a}(t) > 0 , \tag{8.26}$$

where $a(t)$ is the cosmic scale factor and the overdot means derivative with respect to the comoving time.

This primary test is inspired by the fact that the observable Universe is homogeneous and isotropic at

[2] We simply use "massive" and "massless" to distinguish the situation $V(\phi) \neq 0$ from $V(\phi) = 0$ when the scalar field is nondynamical. However, we do not follow this usage to call $\phi(x^\alpha)$ "dynamical and massless" when $\{\lambda(\phi) \neq 0, V(\phi) = 0\}$, as it sounds inappropriate to from the spirit of relativity.

the largest cosmological scale, and the discovery that the Universe is nearly perfectly flat and currently undergoing accelerated spatial expansion. These features have been extensively examined and received strong support from the surveys on the large scale structures, the expansion history, and the structure-growth rate of the Universe, such as the measurements of the distance modulus of Type Ia supernovae, peaks of the baryon acoustic oscillation, and temperature polarizations of the cosmic microwave background. Clearly, the primary test is updatable and subject to the progress in observational cosmology.

8.3.3 Weyl dark energy

Following the primary test above, one can start to explore possible modifications of GR into the total Lagrangian density $\mathscr{L} = R + f(R, \cdots, \mathcal{R}) + h(\phi)\widehat{f}(R, \cdots, \mathcal{R}) + 16\pi G\mathscr{L}_m$ and then check the consistency condition $\widehat{f}(R, \cdots, \mathcal{R}) \equiv 0$ under the flat FRW metric Eq.(8.26). In the integrand of the Hilbert-Einstein action for GR, the Ricci scalar R is the simplest curvature invariant formed by second-order derivatives of the metric; similarly, we can start with the simplest situation that $\widehat{f}(R, \cdots, \mathcal{R})$ is some quadratic Riemannian scalar. One possible example is the square of the conformal Weyl tensor $C_{\alpha\beta\gamma\delta} = R_{\alpha\beta\gamma\delta} + \frac{1}{2}\Big(g_{\alpha\delta}R_{\beta\gamma} - g_{\alpha\gamma}R_{\beta\delta} + g_{\beta\gamma}R_{\alpha\delta} - g_{\beta\delta}R_{\alpha\gamma}\Big) + \frac{1}{6}\left(g_{\alpha\gamma}g_{\beta\delta} - g_{\alpha\delta}g_{\beta\gamma}\right)R$, which is the totally traceless part in the Ricci decomposition of the Riemann tensor. In this case, we consider the action

$$\mathcal{S}_{C^2} = \int d^4x\,\sqrt{-g}\,\left(R + \gamma\phi\, C^2 + 16\pi G\mathscr{L}_m\right), \tag{8.27}$$

where $\gamma \neq 0$ is a coupling constant, and

$$C^2 := C_{\alpha\mu\beta\nu}C^{\alpha\mu\beta\nu} \equiv \frac{1}{3}R^2 - 2R_{\mu\nu}R^{\mu\nu} + R_{\mu\alpha\nu\beta}R^{\mu\alpha\nu\beta}. \tag{8.28}$$

It is straightforward to verify that $C^2 \equiv 0$ for arbitrary forms of the scale factor $a(t)$ in the flat FRW metric. We would like to dub Eq.(8.27) as the "Weyl dark energy" or "conformal dark energy". The field equation is $R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} + \gamma H^{(C^2)}_{\mu\nu} = 8\pi G T^{(m)}_{\mu\nu}$, where

$$\begin{aligned} H^{(C^2)}_{\mu\nu} =& -\frac{1}{2}\phi C^2 g_{\mu\nu} + 2\phi\left(\frac{1}{3}RR_{\mu\nu} - 2R_{\mu}{}^{\alpha}R_{\alpha\nu} + R_{\mu\alpha\beta\gamma}R_{\nu}{}^{\alpha\beta\gamma}\right) + \frac{2}{3}\left(g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu\right)(\phi R) - 2\Box\left(\phi R_{\mu\nu}\right) \\ &+ 2\nabla_\alpha\nabla_\nu\left(\phi R_\mu{}^\alpha\right) + 2\nabla_\alpha\nabla_\mu\left(\phi R_\nu{}^\alpha\right) - 2g_{\mu\nu}\nabla_\alpha\nabla_\beta\left(\phi R^{\alpha\beta}\right) + 4\nabla^\beta\nabla^\alpha\left(\phi R_{\alpha\mu\beta\nu}\right), \end{aligned} \tag{8.29}$$

and according to Eq.(8.14), its covariant divergence is

$$\nabla^\mu H^{(C^2)}_{\mu\nu} = -\frac{\gamma}{2}C^2\,\nabla_\nu\phi\,. \tag{8.30}$$

The Weyl dark energy $\mathcal{S}_{C^2}$, where the scalar field is nondynamical and massless, can be generalized into the dynamical case

$$\mathcal{S} = \int d^4x\,\sqrt{-g}\Big(R + h(\phi)C^2 - \lambda(\phi)\cdot\nabla_\alpha\phi\nabla^\alpha\phi - V(\phi) + 16\pi G\mathscr{L}_m\Big), \tag{8.31}$$

for which the constraint $C^2 \equiv 0$ is no longer necessary and should be removed.

The complete validity of the Weyl dark energy $\mathcal{S}_{C^2}$ or its extension Eq.(8.31), including the value of the coupling strength γ in $\mathcal{S}_{C^2}$, should be carefully constrained by the observational data from astronomical surveys. Following the field equation of $\mathcal{S}_{C^2}$, consider a C^2CDM model (i.e. C^2 cold dark matter) for the Universe instead of ΛCDM. Then the first Friedmann equation under the flat FRW metric reads

$$H^2 = \frac{8}{3}\pi G\left[\rho_{M0}\left(\frac{a_0}{a}\right)^3 + \rho_{r0}\left(\frac{a_0}{a}\right)^4 + \rho_{C^2}\right], \tag{8.32}$$

where the densities of nonrelativistic matter $\rho_M(t)$ and relativistic matter $\rho_r(t)$ have been related to their present-day values ρ_{M0} and ρ_{r0} via by the continuity equation $\dot\rho + 3H\rho(1+w) = 0$, with the equation of state parameters being $w_M = 0$ and $w_r = 1/3$, respectively. Also, $H := \dot a/a$ is the evolutionary Hubble parameter, and ρ_{C^2} denotes the effective energy density of the Weyl dark energy,

$$\begin{aligned}\rho_{C^2} = \gamma\,[5\dot\phi\frac{\ddot a}{a}\frac{\dot a}{a} - 2\dot\phi\frac{\ddot a^2}{a^2}\frac{\dot a}{a} - \dot\phi\frac{\dot a^3}{a^3} - 2\dot\phi\frac{\dot a^5}{a^5} + 5\phi\frac{\dddot a}{a}\frac{\dot a}{a} + 2\phi\frac{\ddot a^3}{a^3}\\ -4\phi\frac{\ddot a}{a}\frac{\dot a^2}{a^2} - 4\phi\frac{\dddot a}{a}\frac{\ddot a}{a}\frac{\dot a}{a} + 4\phi\frac{\ddot a^2}{a^2}\frac{\dot a^2}{a^2} - 6\phi\frac{\ddot a}{a}\frac{\dot a^4}{a^4} + 8\phi\frac{\dot a^6}{a^6}].\end{aligned} \tag{8.33}$$

Employing the cosmological redshift $z := a_0/a - 1$ as well as the replacements $\ddot a/a = \dot H + H^2$ and $\dddot a/a = \ddot H + 3\dot H H + H^3$, Eq.(8.32) can be parameterized into

$$H(z; H_0, \boldsymbol{p}) = H_0\sqrt{\Omega_{M0}(1+z)^3 + \Omega_{r0}(1+z)^4 + \Omega_{C^2}}\,, \tag{8.34}$$

where H_0 represents the Hubble constant $H(z=0)$, $\Omega_{M0} = 8\pi G\rho_{M0}/(3H_0^2)$, $\Omega_{r0} = 8\pi G\rho_{r0}/(3H_0^2)$, and

$$\begin{aligned}\Omega_{C^2} = \frac{32\pi G}{H_0^2}\gamma\Big\{\dot\phi H\Big[5\left(\dot H + H^2\right) - 2\left(\dot H + H^2\right)^2 - H^2 - 2H^4\Big] + \phi H\left(5 - 4\dot H - 4H^2\right)\left(\ddot H + 3\dot H H + H^3\right)\\ + 8\phi H^6 + \phi\left(\dot H + H^2\right)\Big[\left(2\dot H + 2H^2 + 4H^2\right)\left(\dot H + H^2\right) - 4H^2 - 6H^4\Big]\Big\}.\end{aligned} \tag{8.35}$$

Typically, we can use the Markov-Chain Monte-Carlo engine CosmoMC [25] to explore the parameter space $\boldsymbol{p} = (\Omega_{M0}, \Omega_{r0}, \gamma)$ for the Weyl dark energy $\mathcal{S}_{C^2}$, and find out how well it matches the various sets of observational data. This goes beyond the scope of this paper and will be analyzed separately.

8.4 Applications

8.4.1 Chern-Simons gravity

The four-dimensional Chern-Simons modification of GR was proposed by the action [14] (note that not to confuse with the traditional gauge gravity carrying a three-dimensional Chern-Simons term [26])

$$\mathcal{S}_{\text{CS}} = \int d^4x\sqrt{-g}\left(R + \gamma\phi\frac{{}^*RR}{\sqrt{-g}} + 16\pi G\mathscr{L}_m\right). \tag{8.36}$$

The scalar field $\phi = \phi(x^\alpha)$ is nonminimally coupled to the Chern-Pontryagin density ${}^*RR := {}^*R_{\alpha\beta\gamma\delta}R^{\alpha\beta\gamma\delta} = \frac{1}{2}\epsilon_{\alpha\beta\mu\nu}R^{\mu\nu}{}_{\gamma\delta}R^{\alpha\beta\gamma\delta}$, where ${}^*R_{\alpha\beta\gamma\delta} := \frac{1}{2}\epsilon_{\alpha\beta\mu\nu}R^{\mu\nu}{}_{\gamma\delta}$ is the left dual of the Riemann tensor, and $\epsilon_{\alpha\beta\mu\nu}$ represents the totally antisymmetric Levi-Civita pseudotensor with $\epsilon_{0123} = \sqrt{-g}$ and $\epsilon^{0123} = 1/\sqrt{-g}$. The field equation reads $R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} + \gamma H^{(\mathrm{CP})}_{\mu\nu} = 8\pi G T^{(\mathrm{m})}_{\mu\nu}$, where $H^{(\mathrm{CP})}_{\mu\nu} \cong \frac{1}{\sqrt{-g}} \frac{\delta(\phi^* RR)}{\delta g^{\mu\nu}}$ collects the contributions from the $\phi(x^\alpha)$-coupled Chern-Pontryagin density,

$$\sqrt{-g}\, H^{(\mathrm{CP})}_{\mu\nu} = 2\partial^\xi \phi \cdot \left(\epsilon_{\xi\mu\alpha\beta} \nabla^\alpha R^\beta{}_\nu + \epsilon_{\xi\nu\alpha\beta} \nabla^\alpha R^\beta{}_\mu\right) + 2\partial_\alpha \partial_\beta \phi \cdot \left({}^*R^\alpha{}_\mu{}^\beta{}_\nu + {}^*R^\alpha{}_\nu{}^\beta{}_\mu\right). \tag{8.37}$$

According to the general theory in Secs. 8.2.2 and 8.3.2, the Chern-Simons gravity Eq.(8.36) involves a nondynamical and massless scalar field. Identifying $\widehat{f}(R, \cdots, \mathcal{R})$ as ${}^*RR/\sqrt{-g}$ and with $h(\phi) = \gamma\phi$ in Eqs.(8.14) and (8.25), we obtain the divergence

$$\nabla^\mu H^{(\mathrm{CP})}_{\mu\nu} = -\frac{\gamma^* RR}{2\sqrt{-g}} \cdot \partial_\nu \phi\,, \tag{8.38}$$

as well as the constraint ${}^*RR \equiv 0$ for nontrivial $\phi(x^\alpha)$. It can be easily verified that ${}^*RR$ vanishes for the flat and accelerating FRW Universe, and thus passes the primary test in Sec. 8.3.2. Also the condition ${}^*RR \equiv 0$ only applies to the action Eq.(8.36), and is invalid for the massive Chern-Simons gravity $\mathscr{L} = R + \gamma\phi \frac{{}^*RR}{\sqrt{-g}} - V(\phi) + 16\pi G \mathscr{L}_m$ or the dynamical case $\mathscr{L} = R + \gamma\phi \frac{{}^*RR}{\sqrt{-g}} - \lambda(\phi) \cdot \nabla_\alpha \phi \nabla^\alpha \phi + 16\pi G \mathscr{L}_m$.

8.4.2 Reduced Gauss-Bonnet dark energy

The Gauss-Bonnet dark energy was introduced by the action $\mathcal{S}^{(1)}_{\mathrm{GB}} = \int d^4x \sqrt{-g}\Big(R + h(\phi)\mathcal{G} - \bar{\lambda}\nabla_\alpha\phi\nabla^\alpha\phi - V(\phi) + 16\pi G\mathscr{L}_m\Big)$ [15], where $\bar{\lambda} \in \{\pm 1, 0\}$, and the scalar field is nonminimally coupled to the Gauss-Bonnet invariant $\mathcal{G} := \left(\frac{1}{2}\epsilon_{\alpha\beta\gamma\zeta} R^{\gamma\zeta\eta\xi}\right) \cdot \left(\frac{1}{2}\epsilon_{\eta\xi\rho\sigma} R^{\rho\sigma\alpha\beta}\right) \equiv R^2 - 4R_{\alpha\beta}R^{\alpha\beta} + R_{\alpha\mu\beta\nu}R^{\alpha\mu\beta\nu}$. If $\phi(x^\alpha)$ is nondynamical with $\bar{\lambda} = 0$, the action $\mathcal{S}^{(1)}_{\mathrm{GB}}$ reduces to become $\mathcal{S}^{(2)}_{\mathrm{GB}} = \int d^4x \sqrt{-g}\Big(R + h(\phi)\mathcal{G} - V(\phi) + 16\pi G\mathscr{L}_m\Big)$, and according to Eq.(8.22) with $\widehat{f}(R, \cdots, \mathcal{R})$ identified as the Gauss-Bonnet invariant, $V(\phi)$ has to satisfy the constraint $V_\phi = \mathcal{G}\, h_\phi$. Moreover, the nonminimally coupled $h(\phi)\mathcal{G}$ part in $\mathcal{S}^{(1)}_{\mathrm{GB}}$ and $\mathcal{S}^{(2)}_{\mathrm{GB}}$ contributes to the field equation by

$$\begin{aligned} H^{(\mathrm{GB})}_{\mu\nu} =& \,2R\left(g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu\right)h + 4R_\mu{}^\alpha\nabla_\alpha\nabla_\nu h + 4R_\nu{}^\alpha\nabla_\alpha\nabla_\mu h \\ & - 4R_{\mu\nu}\Box h - 4g_{\mu\nu}\cdot R^{\alpha\beta}\nabla_\alpha\nabla_\beta h + 4R_{\alpha\mu\beta\nu}\nabla^\beta\nabla^\alpha h\,, \end{aligned} \tag{8.39}$$

where, compared with the original field equation in Ref.[15], we have removed the algebraic terms in $H^{(\mathrm{GB})}_{\mu\nu}$ by the Bach-Lanczos identity $\frac{1}{2}\mathcal{G}g_{\mu\nu} \equiv 2RR_{\mu\nu} - 4R_\mu{}^\alpha R_{\alpha\nu} - 4R_{\alpha\mu\beta\nu}R^{\alpha\beta} + 2R_{\mu\alpha\beta\gamma}R_\nu{}^{\alpha\beta\gamma}$ [27]. The divergence of $H^{(\mathrm{GB})}_{\mu\nu}$, in accordance with Eq.(8.14), reads

$$\nabla^\mu H^{(\mathrm{GB})}_{\mu\nu} = -\frac{1}{2}\mathcal{G}\cdot h_\phi \partial_\nu\phi\,. \tag{8.40}$$

However, it would be problematic if one further reduces $\mathcal{S}^{(2)}_{\mathrm{GB}}$ into

$$\mathcal{S}^{(3)}_{\mathrm{GB}} = \int d^4x \sqrt{-g}\Big(R + h(\phi)\mathcal{G} + 16\pi G\mathscr{L}_m\Big), \tag{8.41}$$

where $\phi(x^\alpha)$ is both nondynamical and massless. The metric tensor has to satisfy $\mathcal{G} \equiv 0$ to be a solution to the field equation $R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} + H^{(\mathrm{GB})}_{\mu\nu} = 8\pi G T^{(\mathrm{m})}_{\mu\nu}$ for the reduced Gauss-Bonnet dark energy $S^{(3)}_{\mathrm{GB}}$. For the flat FRW Universe with the metric Eq.(8.26), the Gauss-Bonnet invariant is

$$\mathcal{G} = 24\frac{\dot{a}^2\ddot{a}}{a^3}\,, \tag{8.42}$$

and thus $\mathcal{G}$ vanishes only if the Universe were of static state ($\dot{a}=0$) or constant acceleration ($\ddot{a}=0$). Hence, the constraint $\mathcal{G}\equiv 0$ for $S^{(3)}_{\text{GB}}$ is inconsistent with the cosmic acceleration, which indicates that unlike $S^{(1)}_{\text{GB}}$ and $S^{(2)}_{\text{GB}}$, $S^{(3)}_{\text{GB}}$ is oversimplified and can not be a viable candidate of effective dark energy.

8.4.3 Generalized scalar-tensor theory

Since $\mathcal{S}_{\text{HE}}$ and $\mathcal{S}_{\text{G}}$ in Eq.(8.1) respect the diffeomorphism invariance and the (generalized) contracted Bianchi identities, in this subsection we will ignore them and focus on the following scalar-tensor-type gravity in the Jordan frame:

$$\begin{aligned}\mathcal{S}_{\text{ST}} &= \int d^4x\sqrt{-g}\Big(f(R,\phi)+\mathscr{L}_{\text{NC}}+\mathscr{L}_{\phi}+16\pi G\mathscr{L}_m\Big)\\ &= \int d^4x\sqrt{-g}\Big(f(R,\phi)+h(\phi)\cdot\widehat{f}(R,\cdots,\mathcal{R})-\lambda(\phi)\cdot\nabla_\alpha\phi\nabla^\alpha\phi-V(\phi)+16\pi G\mathscr{L}_m\Big),\end{aligned} \tag{8.43}$$

where $f(R,\phi)$ is a hybrid function of the Ricci scalar and the scalar field. $f(R,\phi)$ contributes to the field equation by

$$H^{f(R,\phi)}_{\mu\nu} \cong \frac{1}{\sqrt{-g}}\frac{\delta\left(\sqrt{-g}\,f(R,\phi)\right)}{\delta g^{\mu\nu}} = -\frac{1}{2}f(R,\phi)\cdot g_{\mu\nu}+f_R R_{\mu\nu}+\left(g_{\mu\nu}\Box-\nabla_\mu\nabla_\nu\right)f_R\,, \tag{8.44}$$

where $f_R = f_R(R,\phi) = \partial f(R,\phi)/\partial R$. With the Bianchi identity $\nabla^\mu\left(R_{\mu\nu}-\frac{1}{2}Rg_{\mu\nu}\right)=0$ and the third-order-derivative commutator $(\nabla_\nu\Box-\Box\nabla_\nu)\,f_R = -R_{\mu\nu}\nabla^\mu f_R$, explicit calculations yield

$$\nabla^\mu H^{f(R,\phi)}_{\mu\nu} = -\frac{1}{2}f_\phi\cdot\nabla_\nu\phi\,, \tag{8.45}$$

where $f_\phi = f_\phi(R,\phi) = \partial f(R,\phi)/\partial\phi$. On the other hand, the kinematical wave equation $\delta\mathcal{S}_{\text{ST}}/\delta\phi = 0$ reads $2\lambda(\phi)\cdot\Box\phi = -f_\phi-\widehat{f}\cdot h_\phi-\lambda_\phi\cdot\nabla_\alpha\phi\nabla^\alpha\phi+V_\phi$, which recasts the divergence $\nabla^\mu H^{(\phi)}_{\mu\nu} = -\frac{1}{2}\Big(\lambda_\phi\cdot\nabla_\alpha\phi\nabla^\alpha\phi+2\lambda(\phi)\cdot\Box\phi$ $-V_\phi\Big)\cdot\nabla_\nu\phi$ as in Eq.(8.16) into

$$\nabla^\mu H^{(\phi)}_{\mu\nu} = \frac{1}{2}\Big(f_\phi+\widehat{f}(R,\cdots,\mathcal{R})\cdot h_\phi\Big)\cdot\nabla_\nu\phi\,. \tag{8.46}$$

Hence, with Eqs.(8.14), (8.45) and(8.46), we immediately learn that the field equation $H^{f(R,\phi)}_{\mu\nu}+H^{(\text{NC})}_{\mu\nu}+H^{(\phi)}_{\mu\nu} = 8\pi G T^{(m)}_{\mu\nu}$ for the scalar-tensor-type gravity $\mathcal{S}_{\text{ST}}$ is divergence free. By the total Lagrangian density for the sake of simplicity, the concretization of Eq.(8.43) includes, for example, standard Brans-Dicke gravity $\mathscr{L} = \phi R-\frac{\omega_{\text{BD}}}{\phi}\nabla_\alpha\phi\nabla^\alpha\phi+16\pi\mathscr{L}_m$ (where Newton's constant G is encoded into ϕ^{-1} in the spirit of Mach's principle) [13], generalized Brans-Dicke gravity $\mathscr{L} = \phi R-\frac{\omega(\phi)}{\phi}\nabla_\alpha\phi\nabla^\alpha\phi-V(\phi)+16\pi G\mathscr{L}_m$ with a self-interaction potential, Lovelock-Brans-Dicke gravity $\mathscr{L} = \phi\left(R+\frac{a}{\sqrt{-g}}{}^*RR+b\mathcal{G}\right)-\frac{\omega_{\text{L}}}{\phi}\nabla_\alpha\phi\nabla^\alpha\phi-V(\phi)+16\pi G\mathscr{L}_m$ [27], Lovelock-scalar-tensor gravity $\mathscr{L} = f_1(\phi)R+\frac{f_2(\phi)}{\sqrt{-g}}{}^*RR+f_3(\phi)\mathcal{G}-\omega(\phi)\cdot\nabla_\alpha\phi\nabla^\alpha\phi-V(\phi)+16\pi G\mathscr{L}_m$ [27], minimal dilatonic gravity $\mathscr{L} = \phi R-2\Lambda U(\phi)$ [28], Gauss-Bonnet dilatonic gravity $\mathscr{L} = R-\nabla_\alpha\phi\nabla^\alpha\phi+e^{-\gamma\phi}\mathcal{G}$

or $\mathscr{L} = e^{-\gamma\phi}(R - \nabla_\alpha\phi\nabla^\alpha\phi + \mathcal{G})$ motivated by the low-energy heterotic string theory [29], and the standard scalar-tensor gravity $\mathscr{L} = F(\phi)R - Z(\phi)\cdot\nabla_\alpha\phi\nabla^\alpha - V(\phi) + 16\pi G\mathscr{L}_m$ [30]; all these examples satisfy the local energy-momentum conservation $\nabla^\mu T^{(m)}_{\mu\nu} = 0$ and have divergence-free field equations.

8.4.4 Hybrid metric-Palatini $f(R)$ gravity

So far we have been using the metric formulation for the curvature invariants; however, the local conservation can be proved for the Palatini or hybrid metric-Palatini $f(R)$ gravity without referring to the Palatini formulation of the (generalized) Bianchi identities. Consider the following hybrid metric-Palatini $f(R)$ action

$$\mathcal{S}^{(1)}_{\mathrm{H}f} = \int d^4x\,\sqrt{-g}\Big(R + f(\hat{R}) + 16\pi G\mathscr{L}_m\Big), \tag{8.47}$$

where R is the usual Ricci scalar for the metric $g_{\mu\nu}$, while $\hat{R} = \hat{R}(\boldsymbol{g},\hat{\boldsymbol{\Gamma}}) = g^{\mu\nu}\hat{R}_{\mu\nu}(\hat{\boldsymbol{\Gamma}})$ denotes the Palatini Ricci scalar, with the Palatini Ricci tensor given by $\hat{R}_{\mu\nu}(\hat{\boldsymbol{\Gamma}}) = \hat{R}^\alpha{}_{\mu\alpha\nu}(\hat{\boldsymbol{\Gamma}}) = \partial_\alpha\hat{\Gamma}^\alpha_{\nu\mu} - \partial_\nu\hat{\Gamma}^\alpha_{\alpha\mu} + \hat{\Gamma}^\alpha_{\alpha\zeta}\hat{\Gamma}^\zeta_{\mu\nu} - \hat{\Gamma}^\alpha_{\mu\zeta}\hat{\Gamma}^\zeta_{\alpha\nu}$. Variation of $\mathcal{S}_{\mathrm{H}f}$ with respect to the independent connection $\hat{\Gamma}^\alpha_{\mu\nu}$ yields $\hat{\nabla}_\alpha(\sqrt{-g}\,f_{\hat{R}}g^{\mu\nu}) = 0$, where $\hat{\nabla}$ is the covariant derivative of the connection and $f_{\hat{R}} \coloneqq df(\hat{R})/d\hat{R}$. Thus, $\hat{\nabla}$ is compatible with the auxiliary metric $f_{\hat{R}}g_{\mu\nu} \eqqcolon \hat{g}_{\mu\nu}$, as $\sqrt{-\hat{g}}\,\hat{g}^{\mu\nu} = \sqrt{-g}\,f_{\hat{R}}g^{\mu\nu}$. Relating $\hat{g}_{\mu\nu}$ to $g_{\mu\nu}$ by the conformal transformation $g_{\mu\nu} \mapsto \hat{g}_{\mu\nu}$, and accordingly rewriting $\hat{R}_{\mu\nu}$ and $\hat{R}$ in the metric formulation, one could find that $\mathcal{S}^{(1)}_{\mathrm{H}f}$ is equivalent to [31]

$$\mathcal{S}^{(2)}_{\mathrm{H}f} = \int d^4x\,\sqrt{-g}\Big(R + \phi R + \frac{3}{2\phi}\nabla_\alpha\phi\nabla^\alpha\phi - V(\phi) + 16\pi G\mathscr{L}_m\Big), \tag{8.48}$$

where $\phi(x^\alpha) = f_{\hat{R}}(\hat{R})$ and $V(\phi) = f_{\hat{R}}\hat{R} - f(\hat{R})$. $\mathcal{S}^{(2)}_{\mathrm{H}f}$ is just the mixture of GR and the $\omega_{\mathrm{BD}} = -3/2$ Brans-Dicke gravity. Recall that Eq.(8.43) has employed the generic function $f(R,\phi)$ for $\mathcal{S}_{\mathrm{ST}}$, which includes the hybrid situations like $f(R,\phi) = R + \phi R$. Hence, following Sec. 8.4.3, it is clear that the hybrid scalar-tensor gravity $\mathcal{S}^{(2)}_{\mathrm{H}f}$ and thus the hybrid metric-Palatini $f(R)$ gravity $\mathcal{S}^{(1)}_{\mathrm{H}f}$ have divergence-free field equations and respect the local energy-mentum conservation.

8.5 Conclusions

In this paper, we have investigated the covariant invariance of the field equation for a large class of hybrid modified gravity $\mathscr{L} = R + f(R,\cdots,\mathcal{R}) + h(\phi)\cdot\widehat{f}(R,\cdots,\mathcal{R}) - \lambda(\phi)\cdot\nabla_\alpha\phi\nabla^\alpha\phi - V(\phi) + 16\pi G\mathscr{L}_m$. For the four components $\mathscr{L}_{\mathrm{HE}} = R$, $\mathscr{L}_{\mathrm{G}} = f(R,\cdots,\mathcal{R})$, $\mathscr{L}_{\mathrm{NC}} = h(\phi)\cdot\widehat{f}(R,\cdots,\mathcal{R})$, and $\mathscr{L}_\phi = -\lambda(\phi)\cdot\nabla_\alpha\phi\nabla^\alpha\phi - V(\phi)$, we have calculated their contributions $\Big\{G_{\mu\nu}, H^{(\mathrm{G})}_{\mu\nu}, H^{(\mathrm{NC})}_{\mu\nu}, H^{(\phi)}_{\mu\nu}\Big\}$ to the gravitational field equation along with the respective divergences, which proves the divergence-freeness of the field equation (8.19) and confirms/proves the local energy-momentum conservation under minimal gravity-matter coupling.

$H^{(\mathrm{NC})}_{\mu\nu}$ and $H^{(\phi)}_{\mu\nu}$ fail to obey the generalized contracted Bianchi identities due to the presence of the background scalar field $\phi(x^\alpha)$, but fortunately, the two nontrivial divergences $\nabla^\mu H^{(\mathrm{NC})}_{\mu\nu}$ and $\nabla^\mu H^{(\phi)}_{\mu\nu}$ exactly cancel out each other. When $\phi(x^\alpha)$ is nondynamical and massless, i.e. $\lambda(\phi) = 0 = V(\phi)$, the divergence $\nabla^\mu H^{(\mathrm{NC})}_{\mu\nu} = -\frac{1}{2}\widehat{f}(R,\cdots,\mathcal{R})\cdot h_\phi\partial_\nu\phi$ is forced to vanish, which implies the constraint $\widehat{f}(R,\cdots,\mathcal{R}) \equiv 0$ for nonconstant $\phi(x^\alpha)$. We have suggested a primary viability test for the gravity $\mathscr{L} = R + f(R,\cdots,\mathcal{R}) + h(\phi)\cdot\widehat{f}(R,\cdots,\mathcal{R}) + 16\pi G\mathscr{L}_m$ by requiring that $\widehat{f}(R,\cdots,\mathcal{R})$ vanishes identically for the flat and accelerating FRW

Universe, and a simplest example is the Weyl dark energy $\mathscr{L} = R + \gamma\phi C^2 + 16\pi G\mathscr{L}_m$.

With the general theory developed in Secs. 8.2.2 and 8.3.2, we have considered the applications to the Chern-Simons gravity, Gauss-Bonnet dark energy, and various (generalized) scalar-tensor gravities. In fact, the theory $\mathscr{L}_{\text{ST}} = f(R,\phi) + h(\phi)\cdot\widehat{f}(R,\cdots,\mathcal{R}) - \lambda(\phi)\cdot\nabla_\alpha\phi\nabla^\alpha\phi - V(\phi) + 16\pi G\mathscr{L}_m$ in Sec. 8.4.3 can be further extended into $\mathscr{L}_{\text{EST}} = f(R,\cdots,\mathcal{R},\phi) - \lambda(\phi)\cdot\nabla_\alpha\phi\nabla^\alpha\phi - V(\phi) + 16\pi G\mathscr{L}_m$, for which we conjecture that the covariant conservation still holds, with

$$H_{\mu\nu}^{(f)} \cong \frac{1}{\sqrt{-g}}\frac{\delta\left[\sqrt{-g}\,f(R,\cdots,\mathcal{R},\phi)\right]}{\delta g^{\mu\nu}} \quad \text{and} \quad \nabla^\mu H_{\mu\nu}^{(f)} = -\frac{1}{2}f_\phi(R,\cdots,\mathcal{R},\phi)\cdot\nabla_\nu\phi\,. \tag{8.49}$$

However, this divergence relation has not yet been proved in this paper, and we hope it could be solved in future.

In prospective studies, we will take into account the existent candidates of the energy-momentum pseudotensor $t_{\mu\nu}$ for the gravitation field (cf. Ref.[32] for a review), and discuss the global conservation $\partial^\mu[\sqrt{-g}(T_{\mu\nu}^{(m)} + t_{\mu\nu})] = 0$. Also, we will make use of more fundamental definitions of the energy-momentum tensor, and look deeper into the conservation problem in modified gravities from the perspective of Noether's theorem and the classical field theory.

Acknowledgement

This work was supported by NSERC grant 261429-2013.

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Chapter 9. Big Bang nucleosynthesis in power-law $f(R)$ gravity: Corrected constraints from the semianalytical approach [arXiv:1511.03258]

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Abstract

In this paper we investigate the primordial nucleosynthesis in $\mathscr{L} = \varepsilon^{2-2\beta}R^{\beta} + 16\pi m_{\text{Pl}}^{-2}\mathscr{L}_m$ gravity, where ε is a constant balancing the dimension of the field equation, and $1 < \beta < (4+\sqrt{6})/5$ for the positivity of energy density and temperature. From the semianalytical approach, the influences of β to the decoupling of neutrinos, the freeze-out temperature and concentration of nucleons, the opening of deuterium bottleneck, and the ^{4}He abundance are all extensively analyzed; then β is constrained to $1 < \beta < 1.05$ for $\varepsilon = 1$ [s^{-1}] and $1 < \beta < 1.001$ for $\varepsilon = m_{\text{Pl}}$ (Planck mass), which correspond to the extra number of neutrino species $0 < \Delta N_\nu^{\text{eff}} \leq 0.6296$ and $0 < \Delta N_\nu^{\text{eff}} \leq 0.0123$, respectively. Supplementarily from the empirical approach, abundances of the lightest elements (D, ^{4}He, ^{7}Li) are computed by the model-independent best-fit formulae for nonstandard primordial nucleosynthesis, and we find the constraint $1 < \beta \leq 1.0505$ and equivalently $0 < \Delta N_\nu^{\text{eff}} \leq 0.6365$; also, the ^{7}Li abundance problem cannot be solved by $\mathscr{L} = \varepsilon^{2-2\beta}R^{\beta} + 16\pi m_{\text{Pl}}^{-2}\mathscr{L}_m$ gravity within this domain of β.

PACS numbers 26.35.+c, 98.80.Ft, 04.50.Kd
Key words Big Bang nucleosynthesis, power-law $f(R)$ gravity, thermal history

9.1 Introduction

In the past few decades, the increasingly precise measurements for the cosmic abundances of the lightest elements have imposed stringent constraints to the thermal history of the very early Universe. The observed protium, deuterium (D) and ^{4}He abundances prove to agree well with those predicted by the standard Big Bang nucleosynthesis (BBN) in general relativity (GR).

As is well known, any modification to the Hubble expansion rate and the time-temperature correspondence would affect the decoupling of neutrinos, the freeze-out of nucleons, the time elapsed to open the deuterium bottleneck, and the abundances of ^{4}He along with other lightest elements. To better meet the observations regarding the very early Universe, nonstandard BBN beyond the $SU(3)_C\times SU(2)_W\times U(1)_Y$ minimal standard model [1] or beyond the standard gravitational framework of GR have received a lot of attention, such as nonstandard BBN in scalar-tensor gravity [2–5], Brans-Dicke gravity with a varying energy term related to the cosmic radiation background [6], $f(R)$ gravity [7–9], and $f(\mathcal{G})$ generalized Gauss-Bonnet gravity [10]. Also, Ref.[11] tried to recover the standard BBN within Brans-Dicke gravity under the unusual assumption that the BBN era were dominated by the Brans-Dicke scalar field rather than the standard-model

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radiation. Nonstandard BBN helps constrain these modified gravities from the properties of the very early Universe, which supplements the more popular constraints from the accelerated expansion of the late-time Universe.

To our interest, nonstandard BBN in $\mathscr{L} = m_{\rm Pl}^{2-2\beta} R^\beta + 16\pi m_{\rm Pl}^{-2}\mathscr{L}_m$ gravity has been involved in Ref.[7] and studied in Refs.[8, 9], where $m_{\rm Pl}$ refers to the Planck mass. Ref.[7] proposed the power-law $f(R)$ gravity $\mathscr{L} = m_{\rm Pl}^{2-2\beta} R^\beta + 16\pi m_{\rm Pl}^{-2}\mathscr{L}_m$ with the dimension of R^β balanced by $m_{\rm Pl}^{2-2\beta}$, and checked the decoupling temperature of nucleons; however, the BBN energy scale was extended to $T \leq 100$ MeV, and in the "interaction rate = expansion rate" criterion, the interconversion rate Γ_{np} between neutrons and protons was inappropriately approximated by that at the high-temperature domain $T \gg m_n - m_p \simeq 1.2933$ MeV. Ref.[8] endeavored to complete the BBN research of Ref.[7], and calculated the primordial ^{4}He synthesis in $\mathscr{L} = m_{\rm Pl}^{2-2\beta} R^\beta + 16\pi m_{\rm Pl}^{-2}\mathscr{L}_m$ gravity from the semianalytical approach; however, we noticed that it still faces the following problems:

(1) The decoupling of neutrinos, which is the initial event towards BBN, was not analyzed.

(2) For the concentration of free neutrons, its evolution was numerically calculated using the standard Hubble expansion rate of GR rather than the generalized $f(R)$ Hubble rate.

(3) The temperature at the opening of the deuterium bottleneck relies on the time-temperature relation and varies for different value of β, but it was manually fixed at 1/25 of the deuteron binding energy.

(4) Due to the inconsistent setups of the geometric conventions, the domain of β was incorrectly set to be $(4-\sqrt{6})/5 < \beta < 1$, which had led to quite abnormal behaviors for $\beta \approx (4-\sqrt{6})/5$ (this is a common mistake in Refs.[7, 8]).

(5) With the dimension of R^β balanced by $m_{\rm Pl}^{2-2\beta}$, $\mathscr{L} = m_{\rm Pl}^{2-2\beta} R^\beta + 16\pi m_{\rm Pl}^{-2}\mathscr{L}_m$ gravity is mathematically and gravitationally equivalent to

$$\mathcal{I} = \int d^4x\sqrt{-g}\left(R^\beta + 16\pi m_{\rm Pl}^{2\beta-4}\mathscr{L}_m\right) = \int d^4x\sqrt{-g}\left(R^\beta + 16\pi G^{2-\beta}\mathscr{L}_m\right), \tag{9.1}$$

and thus the deviation between $f(R) = R$ and R^β (i.e. the non-unity of β) would indicate a change of the matter-gravity coupling strength from Newton's contant G to $G^{2-\beta}$. Consequently, if aiming to constrain the parameter β for $\mathscr{L} = m_{\rm Pl}^{2-2\beta} R^\beta + 16\pi m_{\rm Pl}^{-2}\mathscr{L}_m$ gravity, one just needs to examine the measurements of Newton's constant rather than recalculate testable processes like BBN.

Ref.[9] solved the problem (4) by correcting the domain of β into $1 < \beta < (4+\sqrt{6})/5$, and re-constrained the parameter β by the abundances of both deuterium and ^{4}He. However, the computations were carried out using the public BBN code, and the details regarding the influences of β to the BBN procedures were not brought to light. In addition, the problem (5) still exists in Ref.[9].

In this work, we aim to overcome the problems (1)-(5) above, and reveal every detail of the BBN process in $f(R) \propto R^\beta$ gravity. This paper is analyzed as follows. Section 9.2 introduces the generalized Friedmann equations for the radiation-dominated Universe in generic $f(R)$ gravity, sets up the power-law $f(R)$ gravity with the total Lagrangian density $\mathscr{L} = \varepsilon^{2-2\beta} R^\beta + 16\pi m_{\rm Pl}^{-2}\mathscr{L}_m$ (ε being some constant balancing the dimensions of the field equation), with the nonstandard Hubble expansion and the generalized time-temperature relation derived. The decoupling of neutrinos is studied in Sec. 9.3, while the freeze-out temperature T_n^f

and concentration X_n^f for free neutrons are computed in Sec. 9.4. In Sec. 9.5, the opening of the deuterium bottleneck and the primordial ^{4}He abundance are found out, which exerts constraints to the parameter β compared with the ^{4}He abundance in astronomical measurement. The semianalytical discussion in Secs. 9.3~9.5 for $\mathscr{L} = \varepsilon^{2-2\beta}R^\beta + 16\pi m_{\rm Pl}^{-2}\mathscr{L}_m$ gravity is taken the GR limit $\beta \to 1^+$ in Sec. 9.7 to recover the standard BBN. Moreover, the primordial abundances of deuterium, ^{4}He and ^{7}Li are calculated in Sec. 9.8 from the empirical approach using the model-independent best-fit formulae, which supplements the results from the semianalytical approach.

Throughout this paper, for the physical quantities involved in the thermal history of the early Universe, we use the natural unit system of particle physics which sets $c = \hbar = k_B = 1$ and is related to le système international d'unités by 1 MeV = 1.1604×10^{10} kelvin = 1.7827×10^{-30} kg = $(1.9732 \times 10^{-13}$ meters$)^{-1}$ = $(6.5820 \times 10^{-22}$ seconds$)^{-1}$. On the other hand, for the spacetime geometry, we adopt the conventions $\Gamma^\alpha_{\beta\gamma} = \Gamma^\alpha{}_{\beta\gamma}$, $R^\alpha{}_{\beta\gamma\delta} = \partial_\gamma\Gamma^\alpha_{\delta\beta} - \partial_\delta\Gamma^\alpha_{\gamma\beta}\cdots$ and $R_{\mu\nu} = R^\alpha{}_{\mu\alpha\nu}$ with the metric signature $(-,+++)$.

9.2 Gravitational framework: from generic to power-law $f(R)$ gravity

As a straightforward generalization of GR with the Hilbert-Einstein action $I_{\rm HE} = \int \sqrt{-g}\, d^4x\, (R + 16\pi m_{\rm Pl}^{-2}\mathscr{L}_m)$, $f(R)$ gravity is given by the action $\mathcal{I} = \int d^4x\sqrt{-g}\left[f(R,\varepsilon) + 16\pi m_{\rm Pl}^{-2}\mathscr{L}_m\right]$, where ε is some constant (not an independent variable) balancing the dimensions of the field equation (see Ref.[12] for comprehensive reviews of $f(R)$ gravity in mathematical relativity without the ε term), and the Planck mass $m_{\rm Pl}$ takes the value $m_{\rm Pl} := 1/\sqrt{G} \simeq 1.2209 \times 10^{22}$ MeV. Variation of the $f(R)$ action with respect to the inverse metric, i.e. $\delta\mathcal{I}/\delta g^{\mu\nu} = 0$ yields the field equation

$$f_R R_{\mu\nu} - \frac{1}{2}f + \left(g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu\right) f_R = 8\pi m_{\rm Pl}^{-2}\mathcal{T}^{(m)}_{\mu\nu}\,, \tag{9.2}$$

where $f_R := df(R,\varepsilon)/dR$, $\Box := g^{\alpha\beta}\nabla_\alpha\nabla_\beta$ denotes the covariant d'Alembertian, and the stress-energy-momentum tensor $\mathcal{T}^{(m)}_{\mu\nu}$ of the physical matter is defined by the matter Lagrangian density $\mathscr{L}_m$ via $\mathcal{T}^{(m)}_{\mu\nu} := \frac{-2}{\sqrt{-g}}\frac{\delta\left(\sqrt{-g}\mathscr{L}_m\right)}{\delta g^{\mu\nu}}$.

This paper considers the spatially flat, homogeneous and isotropic Universe, which, in the (t, r, θ, φ) comoving coordinates, is depicted by the Friedmann-Robertson-Walker (FRW) line element $ds^2 = -dt^2 + a(t)^2dr^2 + a(t)^2r^2(d\theta^2 + \sin^2\theta d\varphi^2)$, where $a(t)$ denotes the cosmic scale factor. Assume a perfect-fluid content $\mathcal{T}^{\mu(m)}_{\nu} = \text{diag}[-\rho, P, P, P]$, where the energy density ρ and the pressure P satisfy the equation of state $\rho = 3P$ around BBN that is absolutely radiation-dominated (with negligible contaminations from baryons). Then Eq.(9.2) under the flat FRW metric yields the modified Friedmann equations

$$3\frac{\ddot{a}}{a}f_R - \frac{1}{2}f - 3\frac{\dot{a}}{a}f_{RR}\dot{R} = -8\pi m_{\rm Pl}^{-2}\rho\,, \tag{9.3}$$

$$\left(\frac{\ddot{a}}{a} + 2\frac{\dot{a}^2}{a^2}\right)f_R - \frac{1}{2}f - f_{RR}\ddot{R} - f_{RRR}(\dot{R})^2 - 3\frac{\dot{a}}{a}f_{RR}\dot{R} = 8\pi m_{\rm Pl}^{-2}P\,, \tag{9.4}$$

where overdot denotes the time derivative, $f_{RR} := d^2f(R,\varepsilon)/dR^2$, and $f_{RRR} := d^3f(R,\varepsilon)/dR^3$. Moreover, the equation of covariant conservation $\nabla^\mu \mathcal{T}^{(m)}_{\mu\nu} = 0$ leads to

$$\dot{\rho} + 3\frac{\dot{a}}{a}(\rho + P) = 0\,, \tag{9.5}$$

which integrates to yield $\rho = \rho_0 \left(\frac{a_0}{a}\right)^4 \propto a^{-4}$ under radiation dominance, with $\{\rho_0, a_0\}$ being the present-day values of $\{\rho, a\}$. Near the BBN era, ρ attributes to the energy densities of all relativistic species, $\rho = \sum \rho_i(\text{boson}) + \frac{7}{8}\sum \rho_j(\text{fermion}) = \sum \frac{\pi^2}{30} g_i^{(b)} T_i^4(\text{boson}) + \frac{7}{8}\sum \frac{\pi^2}{30} g_j^{(f)} T_j^4(\text{fermion})$, where $\{g_i^{(b)}, g_j^{(f)}\}$ are the numbers of intrinsic degrees of freedom (mainly spin and color) for bosons and fermions, respectively. Thus, one has the generalized Stefan-Boltzmann law

$$\rho = \frac{\pi^2}{30} g_* T^4 \qquad \text{with} \qquad g_* := \sum_{\text{boson}} g_i^{(b)} \left(\frac{T_i}{T}\right)^4 + \frac{7}{8} \sum_{\text{fermion}} g_j^{(f)} \left(\frac{T_j}{T}\right)^4, \tag{9.6}$$

where, $T \equiv T_\gamma$ refers to photons' temperature, which is the common temperature of all relativistic species in thermal equilibrium.

This paper works with the specific power-law $f(R)$ gravity

$$\mathcal{I} = \int d^4x\sqrt{-g}\left(\varepsilon^{2-2\beta} R^\beta + 16\pi m_{\text{Pl}}^{-2} \mathscr{L}_m\right), \tag{9.7}$$

where β = constant > 0, and ε has the unit of [s^{-1}] or [MeV]. Among Eqs.(9.3), (9.4) and (9.5), only two equations are independent, and we choose to work with Eqs.(9.3) and (9.5). With $\rho = \rho_0 \left(\frac{a_0}{a}\right)^4$ and $f(R) = \varepsilon^{2-2\beta} R^\beta$, the generalized first Friedmann equation (9.3) yields

$$a = a_0 t^{\beta/2} \propto t^{\beta/2}\,, \quad H := \frac{\dot{a}}{a} = \frac{\beta}{2t}\,, \quad \text{and} \tag{9.8}$$

$$\left[\frac{12(\beta-1)}{\beta} H^2\right]^\beta \frac{(-5\beta^2 + 8\beta - 2)}{\beta - 1} = 32\pi\varepsilon^{2\beta-2} m_{\text{Pl}}^{-2} \rho\,, \tag{9.9}$$

where H refers to the cosmic Hubble parameter. Note that unlike the approximated power-law ansatz $a = a_0 t^\alpha$ (α = constant > 0) for generic $f(R)$ gravity, $a = a_0 t^{\beta/2}$ is an *exact solution* to $\mathscr{L} = \varepsilon^{2-2\beta} R^\beta + 16\pi m_{\text{Pl}}^{-2} \mathscr{L}_m$ gravity for the radiation-dominated Universe; for GR with $\beta \to 1^+$, Eq.(9.8) recovers the behavior $a \propto t^{1/2}$ which respects the GR Friedmann equation $3\dot{a}^2/a^2 = -8\pi m_{\text{Pl}}^{-2} \rho_0 \left(\frac{a_0}{a}\right)^4$.

Moreover, the weak, strong and dominant energy conditions for classical matter fields require the energy density ρ to be positive definite. As a consequence, the positivity of the left hand side of Eq.(9.9) limits β to the domain

$$1 < \beta < \frac{4 + \sqrt{6}}{5} \lesssim 1.2899\,; \tag{9.10}$$

note that the Ricci scalar for the flat FRW metric with $a = a_0 t^{\beta/2}$ reads[1] $R = 6\left(\frac{\ddot{a}}{a} + \frac{\dot{a}^2}{a^2}\right) = \frac{3\beta(\beta-1)}{t^2}$, so $R > 0$ and R^β is always well defined in the domain Eq.(9.10).

Eqs.(9.6) and (9.9) imply that the expansion rate of the Universe is related to the radiation temperature

[1] With $\ddot{a}/a = \dot{H} + H^2$, $\ddot{a}/a = R/6 - H^2$ and $\ddot{a}/a + 2\dot{a}^2/a^2 = R/2 - 2\dot{H} - 3H^2$, the Friedmann equations (9.3) and (9.4) can also be written into

$$H^2 = \frac{1}{3f_R}\left(8\pi m_{\text{Pl}}^{-2}\rho + \frac{Rf_R - f}{2} - 3Hf_{RR}\dot{R}\right), \tag{9.11}$$

by

$$
\begin{aligned}
H &= \sqrt{\frac{\beta}{12(\beta-1)}} \times \left(\sqrt{\frac{(\beta-1)\, g_*}{-5\beta^2+8\beta-2}}\right)^{1/\beta} \left(\sqrt{\frac{32\pi^3}{30}}\, \frac{T^2}{m_{\rm Pl}}\right)^{1/\beta} \varepsilon^{1-\frac{1}{\beta}} \\
&= \sqrt{\frac{\beta}{12(\beta-1)}} \times \left(\sqrt{\frac{(\beta-1)\, g_*}{-5\beta^2+8\beta-2}}\right)^{1/\beta} \left(0.7164 \cdot T_{\rm MeV}^2\right)^{1/\beta} \varepsilon_s^{1-\frac{1}{\beta}}\ [{\rm s}^{-1}]\,,
\end{aligned}
\tag{9.13}
$$

where $T_{\rm MeV}$ refers to the pure value of temperature in the unit of MeV, $T = T_{\rm MeV} \times$ [1 MeV], ε_s is the value of ε in the unit of [s^{-1}], and numerically $T^2/m_{\rm Pl} = T_{\rm MeV}^2/8.0276$ [s^{-1}].

Moreover, as time elapses after the Big Bang, the space expands and the Universe cools. Eq.(9.13) along with $H = \beta/(2t)$ leads to the time-temperature relation

$$
\begin{aligned}
t &= \sqrt{3\beta(\beta-1)} \left(\sqrt{\frac{-5\beta^2+8\beta-2}{(\beta-1)\, g_*}}\right)^{1/\beta} \left(\sqrt{\frac{30}{32\pi^3}}\, \frac{m_{\rm Pl}}{T^2}\right)^{1/\beta} \varepsilon^{\frac{1}{\beta}-1} \\
&= \sqrt{3\beta(\beta-1)} \left(\sqrt{\frac{-5\beta^2+8\beta-2}{(\beta-1)\, g_*}}\right)^{1/\beta} \left(\frac{1.3959}{T_{\rm MeV}^2}\right)^{1/\beta} \varepsilon_s^{\frac{1}{\beta}-1}\ [{\rm s}]\,.
\end{aligned}
\tag{9.14}
$$

Eqs.(9.13) and (9.14) play important roles in studying the primordial nucleosynthesis and the gravitational baryogenesis. The candidate of ε is not unique, and for the calculations in the subsequent sections, we will utilize two choices of ε to balance the dimensions:

(i) $\varepsilon^2 = m_{\rm Pl} H_0 \Omega_{M0}$. $m_{\rm Pl}$ is the energy scale of the Planck era, the Hubble constant H_0 represents the present-day energy scale, while the fractional density Ω_{M0} emphasizes the effect of physical matter in modified gravity. Numerically, following the 2015 PDG and Planck data [23, 24], one has $m_{\rm Pl}$ [MeV$\rightarrow$ 1/s] $\simeq 0.1854 \times 10^{44}$ [s^{-1}], $\Omega_{M0} = 0.3089$, and $H_0 = 67.74$ km/s/Mpc $= 2.1954 \times 10^{-18}$ s^{-1} (with 1 Mpc$= 3.0856 \times 10^{19}$ km), so

$$
\varepsilon = \sqrt{m_{\rm Pl} H_0 \Omega_{M0}} = 3.5459 \times 10^{12}\ [{\rm s}^{-1}] = 2.3344 \times 10^{-9}\ {\rm MeV}\,. \tag{9.15}
$$

(ii) $\varepsilon = 1$ [s^{-1}] $= 6.5820 \times 10^{-22}$ MeV. This choice can best respect and preserve existent investigations in mathematical relativity for the $f(R)$ class of modified gravity, which have been analyzed for $\widetilde{\mathscr{L}} = f(R) + 16\pi m_{\rm Pl}^{-2} \mathscr{L}_m$ without caring the physical dimensions. Supplementarily, we have $\varepsilon_s = 1$.

9.3 Weak freeze-out of neutrinos

According to the SU(3)$_C$×SU(2)$_W$×U(1)$_Y$ minimal standard model, primordial nucleosynthesis is prepared after the temperature drops below $T \sim 10$ MeV, when all mesons have decayed into more stable stable nucleons. The electron-positron annihilation has not occurred at $T \lesssim 10$ MeV, and $e^{\pm}$ are far more abundant than

---

$$
2\dot{H} + 3H^2 = -\frac{1}{f_R}\left(8\pi m_{\rm Pl}^{-2} P + \frac{f - R f_R}{2} + f_{RR}\ddot{R} + f_{RRR}(\dot{R})^2 + 3H f_{RR}\dot{R}\right). \tag{9.12}
$$

which are often used in the construction of effective dark energy for the late-time Universe.

nucleons; $e^{\pm}$, photons, neutrinos and nucleons are kept in thermal equilibrium by electromagnetic reactions like the elastic scattering $e^{\pm} + \nu_e \to e^{\pm} + \nu_e$ and $e^{\pm} + p \to e^{\pm} + p$, and by the prototype weak interactions for the neutron-proton transition. To the interest of BBN, neutrons and protons are interconverted by the two-body reactions

$$n + \nu_e \rightleftharpoons p + e^- \,, \quad n + e^+ \rightleftharpoons p + \bar{\nu}_e \,, \tag{9.16}$$

as well as the neutron decay/fusion

$$n \rightleftharpoons p + e^- + \bar{\nu}_e \,. \tag{9.17}$$

When the reaction rate $\Gamma(n \rightleftharpoons p)$ is faster than the Hubble expansion rate H, the interconversions in Eqs.(9.16) and (9.17) are fast enough to maintain neutrons and protons in weak-interaction and thermal equilibrium, until neutrinos decouple when the temperature drops to T_ν^f.

Let X_n (X_p) be the number concentration of free neutrons (protons) among all nucleons, including those possibly entering unstable baryons or complex nuclei. Initially in equilibrium for $T \geq T_\nu^f$, we have $X_n = X_n^{\rm eq} = n_n/(n_n + n_p)$ and thus $X_p = X_p^{\rm eq} = n_p/(n_n + n_p)$. Regarding neutrons and protons as the two energy states of nucleons, and approximating the Fermi-Dirac and the Bose-Einstein energy distribution functions by the Maxwell-Boltzmann function, one has

$$\frac{X_n^{\rm eq}}{X_p^{\rm eq}} = \exp\left(-\frac{Q}{T} + \frac{\mu_e - \mu_{\nu_e}}{T}\right) \simeq \exp\left(-\frac{Q}{T}\right) , \tag{9.18}$$

or

$$X_n^{\rm eq} = \frac{1}{1 + \exp\left(\frac{Q}{T}\right)} , \tag{9.19}$$

where $Q := m_n - m_p = 1.2933$ MeV denotes the neutron-proton mass difference (with $m_n = 939.5654$ MeV, $m_p = 938.2721$ MeV), μ_e / μ_{ν_e} is the chemical potential (i.e. energy associated to particle number) of electrons/neutrinos, and we have applied the standard-model assumption $\mu_{\nu_e} = 0$ and the fact that $\mu_e \ll T$ for $T \gtrsim 0.03$ MeV. Eq.(9.19) implies that $X_n^{\rm eq} \to 1/2 = X_p^{\rm eq}$ for $T \gg 1.2933$ MeV, and as the temperature drops along the cosmic spatial expansion, $X_n^{\rm eq}$ gradually decreases in favor of the lower-energy proton state.

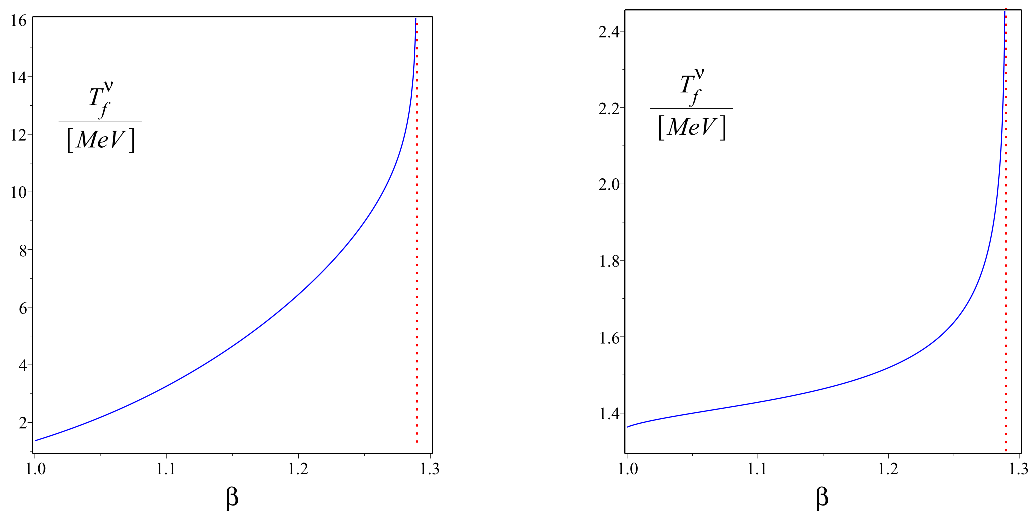
Neutrinos are in equilibrium with photons, nucleons and electrons via weak interactions and elastic scattering. The dominant reaction that keeps the neutrino numbers in equilibrium at this pre-BBN era is $\nu_e + \bar{\nu}_e \leftrightarrow e^- + e^+$, for which the interaction rate is [13]

$$\Gamma_{\nu_e} \simeq 1.3 G_F^2 T^5 \simeq 0.2688\, T_{\rm MeV}^5\ [{\rm s}^{-1}] , \tag{9.20}$$

where $G_F = 1.1664{\times}10^{-11}{\rm MeV}^{-2}$ is Fermi's constant in beta decay and generic weak interactions. Neutrinos decouple when $\Gamma_{\nu_e} = H$, and according to Eqs.(9.13) and (9.20), the weak freeze-out temperature T_ν^f is the solution to

$$T_{\rm MeV}^{5-2/\beta} = 1.0741 \times \sqrt{\frac{\beta}{\beta - 1}} \times \left(2.3577 \cdot \sqrt{\frac{\beta - 1}{-5\beta^2 + 8\beta - 2}}\right)^{1/\beta} \times \left(\sqrt{\frac{g_*}{10.8305}}\right)^{1/\beta} \varepsilon_s^{1-1/\beta} . \tag{9.21}$$

After the weak freeze-out,neutrinos effectively stopped interacting, and the two-body reactions $\{n + \nu_e \to$



(a) **(b)**

Figure 9.1: Decoupling temperature T_ν^f (in MeV) for neutrinos. Fig.(9.1a) is for $\varepsilon = \sqrt{m_{\text{Pl}} H_0 \Omega_{M0}} = 6.58 \times 10^{-22}$ MeV, Fig.(9.1a) is for $\varepsilon = 1\ \text{sec}^{-1} = 6.58 \times 10^{-22}$ MeV, and the dotted vertical line represents the asymptote $\beta = (4 + \sqrt{6})/5$.

$p + e^-$, $p + \bar{\nu}_e \to n + e^+\}$ in Eq.(9.16) and the three-body fusion $p + e^- + \bar{\nu}_e \to n$ in Eq.(9.17) cease; the reactions following T_ν^f are

$$p + e^- \to n + \nu_e\,, \quad n + e^+ \to p + \bar{\nu}_e\,, \tag{9.22}$$

as well as the beta decay of neutrons

$$n \to p + e^- + \bar{\nu}_e\,. \tag{9.23}$$

Figs. (9.1a) and (9.1b) illustrate the dependence of T_ν^f on β for both choices of ε, and some typical values of T_ν^f for a discrete set of β have been collected in Tables 9.1 and 9.2. In the calculation of T_ν^f, we have used $g_* = g_*(T \geq T_\nu^f)$, $g_b = 2$ (photon), $g_f = 2 \times 2\,(e^\pm) + 2 \times 3.046$ (neutrino) $= 10.092$, and thus the effective number of degree of freedom $g_* = g_b + \frac{7}{8} g_f = 10.8305$, with all these relativistic species in thermal equilibrium at the same temperature. Here for the effective number of species for massless/light neutrinos during BBN, we adopt $N_{\text{eff}} = 3.046$ rather than $N_{\text{eff}} = 3$; this correction attributes to the fact that the neutrino decoupling during BBN is a thermal process of finite time rather than an instantaneous event [25], and in other processes like baryogenesis, decoupling of dark matter and hydrogen recombination, one should return to $N_{\text{eff}} = 3$. Also, although the detected oscillation phenomenon requires neutrinos to carry nonzero mass [15–17], the mass is negligible during BBN and neutrinos remain relativistic. For example, the latest cosmological data on the large scale structure and the anisotropies of the cosmic microwave background imply $\sum m_\nu = 0.320 \pm 0.081$ eV for the summed mass of three known neutrino flavors [26], while the Planck data has placed an tighter constraint $\sum m_\nu < 0.194$ eV in the 95 % limit [24].

From Figs. (9.1a), (9.1b) and the "T_ν^f [MeV]" columns in Tables 9.1 and 9.2, one can clearly observe that T_ν^f goes higher when β increases, and T_ν^f is minimized in the GR limit $\beta \to 1$, with $\min(T_\nu^f) = \lim_{\beta \to 1} T_\nu^f$=1.3630 MeV. Thus, as expected, neutrinos still decouple before the electron-positron annihilation in $\mathscr{L} = \varepsilon^{2-2\beta} R^\beta + 16\pi m_{\text{Pl}}^{-2} \mathscr{L}_m$ gravity. Since $t \propto T^{-2/\beta}$ in light of Eq.(9.14), the time t_ν^f elapsed from Big

Bang to the weak freeze-out shortens when β increases, and t_ν^f is maximized in the GR limit $\beta \to 1$, with $\max(t_\nu^f) = \lim_{\beta\to 1} t_\nu^f = 0.3955$ s.

9.4 Freeze-out of free neutrons

9.4.1 Temperature at the freeze-out of neutrons

After the decoupling of neutrinos, the neutron concentration X_n deviates from the equilibrium value X_n^{eq} in Eq.(9.19), and the evolution of X_n satisfies

$$\frac{dX_n}{dt} = -\Gamma_{n\to p} X_n + \Gamma_{p\to n}(1 - X_n) = -\Gamma_{n\to p}\left(1 + e^{-\frac{Q}{T}}\right)\left(X_n - X_n^{\text{eq}}\right), \tag{9.24}$$

where $\Gamma_{n\to p}$ ($/\Gamma_{p\to n}$) denotes the reaction rate to convert neutrons (/protons) into protons (/neutrons). When nucleons and leptons are carried apart by the Hubble expansion faster than their collisions, the reactions in Eq.(9.22) cease, and the only reaction alive is the beta decay of free neutrons in Eq.(9.23).

To find out the resultant reaction rate $\Gamma_{n\to p}$ for the two-body reactions in Eq.(9.22), one can apply the Bernstein-Brown-Feinberg approximations in the early BBN era [20]: (i) Neglect the recoil energy of nucleons; this way, let $\{p_e\,, p_{\nu_e}\}$ be the momenta of electrons and electron neutrinos, with the corresponding energies $\{E_e = \sqrt{p_e^2 + m_e^2}, E_{\nu_e} = p_{\nu_e}\}$, and then the energy conservation yields $E_e = E_{\nu_e} + Q$. (ii) Nucleons freeze out before the $e^- - e^+$ annihilation, so that photons are not yet reheated and $T = T_\gamma = T_{\nu_e} = T_{e^\pm}$; as will be verified *a posteriori* in the "T_n^f [MeV]" columns of Tables 9.1 and 9.2, this assumption holds in both GR and $\mathscr{L} = \varepsilon^{2-2\beta} R^\beta + 16\pi m_{\text{Pl}}^{-2}\mathscr{L}_m$ gravity. (iii) Approximate the Fermi-Dirac energy distribution function by the Boltzmann function, and neglect the blocking effect due to Pauli's exclusion principle. As a result, the reaction rates can be computed by $\Gamma(n\nu_e \to pe^-) = A\int_0^\infty dp_{\nu_e} p_{\nu_e}^2 p_e E_e \exp\left(-\frac{E_{\nu_e}}{T}\right)$, $\Gamma(ne^+ \to p\bar{\nu}_e) = A\int_0^\infty dp_e p_e^2 p_{\nu_e} E_{\nu_e} \exp\left(-\frac{E_e}{T}\right)$, and thus

$$\Gamma_{n\to p} = 2\Gamma(n\nu_e \to pe^-) = 4AT^3\left(12T^2 + 6TQ + Q^2\right), \tag{9.25}$$

while the decaying rate of free neutrons is

$$\begin{aligned}
\Gamma(n \to pe^-\bar{\nu}_e) &= A\int_0^{\sqrt{Q^2-m_e^2}} dp_e p_e^2 p_{\nu_e} E_{\nu_e} \\
&= \frac{A}{5}\sqrt{Q^2 - m_e^2}\left(\frac{1}{6}Q^2 - \frac{3}{4}Q^2 m_e^2 - \frac{2}{3}m_e^4\right) + \frac{A}{4}m_e^4 Q \cdot \text{arcosh}\left(\frac{Q}{m_e}\right) \\
&= 1.5752\times 10^{-2} AQ^5 = \frac{1}{\tau_n}\,,
\end{aligned} \tag{9.26}$$

where $m_e = 0.5110$ MeV$= 0.3951Q$, p_e takes the upper limit $\sqrt{Q^2 - m_e^2}$ in accordance with the energy conservation $E_{\nu_e} = Q - E_e$, and τ_n denotes the mean lifetime of free neutrons. Eq.(9.26) implies that the effective coupling constant A satisfies

$$4A = \frac{253.9332}{\tau_n Q^5}\,, \tag{9.27}$$

which, along with Eq.(9.25), leads to

$$\Gamma_{n\to p} \simeq \frac{253.9332}{\tau_n\, x^5}\left(x^2 + 6x + 12\right)\ [\mathrm{s}^{-1}] \quad \text{with} \quad x := \frac{Q}{T}\,. \tag{9.28}$$

Here the dimensionless variable x has been employed, which will considerably facilitate the subsequent calculations.

We will adopt Eq.(9.28) as the neutron-proton reaction rates, which neglects the beta-decay rate of free neutrons. This approximation is acceptable: the free-out of neutrons closely follows the weak freeze-out of neutrinos, whose decoupling time satisfies $\max(t_\nu^f) = \lim_{\beta\to 1} t_\nu^f = 0.3955$ s $<< \tau_n = 880.0 \pm 0.9$ [s], where we adopt the PDG recommended value for the mean time of neutron decay [23]; this will become more clear after the computation of t_n^f (the time elapsed from Big Bang to neutrons' decoupling) below, as will be collected in the "t_n^f [s]" columns of Tables 9.1 and 9.2. Also, for the sake of higher precision, we have updated the original formula $\Gamma_{n\to p} \simeq \frac{255}{\tau_n\, x^5}\left(x^2 + 6x + 12\right)$ [s^{-1}] by Bernstein *et al.* [20] into Eq.(9.28).

The concentration X_n freezes out at $\Gamma_{n\to p}(x) = H(x)$, where the Hubble parameter is recast into

$$H(x) = \sqrt{\frac{\beta}{12(\beta-1)}} \times \left(\sqrt{\frac{(\beta-1)\, g_*}{-5\beta^2 + 8\beta - 2}}\right)^{1/\beta} \left(\frac{1.1983}{x^2}\right)^{1/\beta} \varepsilon_s^{1-1/\beta}\ [\mathrm{s}^{-1}] = \frac{H(Q)}{x^{2/\beta}}\ [\mathrm{s}^{-1}]\,, \tag{9.29}$$

with the constant $H(Q) := H(T = Q) = H(x = 1)$ being β-dependent. Hence, $\Gamma_{n\to p}(x) = H(x)$ yields

$$\frac{253.9332}{\tau_n}\frac{x^2 + 6x + 12}{x^5} = \sqrt{\frac{\beta}{12(\beta-1)}} \times \left(\sqrt{\frac{(\beta-1)\, g_*}{-5\beta^2 + 8\beta - 2}}\right)^{1/\beta} \left(\frac{1.1983}{x^2}\right)^{1/\beta} \varepsilon_s^{1-1/\beta}\,, \tag{9.30}$$

so the freeze-out temperature $T_n^f = \frac{1.2933}{x_n^f}$ [MeV] can be found out by solving $x = x_n^f$ from

$$\frac{x^2 + 6x + 12}{x^{5-2/\beta}} = 1.0004 \times \frac{\tau_n}{880.0} \times \sqrt{\frac{\beta}{\beta-1}} \times \left(3.8613 \cdot \sqrt{\frac{\beta-1}{-5\beta^2 + 8\beta - 2}}\right)^{1/\beta} \left(\sqrt{\frac{g_*}{10.3835}}\right)^{1/\beta} \varepsilon_s^{1-1/\beta}\,. \tag{9.31}$$

An exact and generic solution to Eq.(9.31) with $1 < \beta < (4 + \sqrt{6})/5$ is difficult (if not impossible) to work out, so we numerically solve Eq.(9.31) for a series of β, as shown in the "T_n^f [MeV]" columns of Tables 9.1 and 9.2, where x_n^f has been transformed back into T_n^f. One can clearly observe that T_n^f increases along with the increment of β.

9.4.2 Freeze-out concentration of free neutrons

To figure out the concentration of free neutrons at the freeze-out temperature T_n^f, firstly rewrite Eq.(9.24) into

$$\frac{dX_n}{dt} = \frac{dX_n}{dx}\frac{dx}{dT}\frac{dT}{dt} = -\frac{dX_n}{dx} \cdot x \cdot \frac{\dot{T}}{T} = -\Gamma_{n\to p}\left(1 + e^{-x}\right)\left(X_n - X_n^{\mathrm{eq}}\right)\,. \tag{9.32}$$

Eqs.(9.6) and (9.13) imply that

$$T = \left(\frac{30}{\pi^2 g_*}\rho\right)^{1/4} = \left\{ \frac{30\varepsilon^{2-2\beta} m_{\rm Pl}^2(-5\beta^2+8\beta-2)}{32\pi^3 g_*(\beta-1)} \left[3\beta(\beta-1)\right]^{\beta} \right\}^{1/4} t^{-\beta/2} \propto t^{-\beta/2}\,, \tag{9.33}$$

so Ta = constant and $\dot{T}/T = -\dot{a}/a = -\beta/(2t) = -H(Q)x^{-2/\beta}$, which recast Eq.(9.32) into

$$\frac{dX_n}{dx} = -\Gamma_{n\to p}\frac{x^{\frac{2}{\beta}-1}}{H(Q)}\left(1+e^{-x}\right)\left(X_n - X_n^{\rm eq}\right)\,. \tag{9.34}$$

Define a new function $F(x) \coloneqq X_n(x) - X_n^{\rm eq}(x)$ to measure the departure of X_n from the ideal equilibrium concentration $X_n^{\rm eq} = 1/(1+e^x)$, and transform dX_n/dx into the evolution equation of $F(x)$:

$$\frac{dF(x)}{dx} + \Gamma_{n\to p}\frac{x^{\frac{2}{\beta}-1}}{H(Q)}\left(1+e^{-x}\right)F(x) = \frac{e^x}{(1+e^x)^2}\,. \tag{9.35}$$

Its general solution can be written as $F(x) = \widetilde{F}(x)E(x)$, where

$$\widetilde{F}(x) = \exp\left[-\int^x \Gamma_{n\to p}\frac{y^{\frac{2}{\beta}-1}}{H(Q)}\left(1+e^{-y}\right)dy\right]\,, \tag{9.36}$$

and $E(x)$ satisfies

$$\frac{dE(x)}{dx} = \frac{1}{\widetilde{F}(x)}\frac{e^x}{(1+e^x)^2}\,. \tag{9.37}$$

Integrating $\widetilde{F}(x)E(x)$, we obtain

$$F(x) = \int^x d\tilde{x}\frac{e^{\tilde{x}}}{(1+e^{\tilde{x}})^2}\exp\left[-\int_{\tilde{x}}^x \Gamma_{n\to p}\frac{y^{\frac{2}{\beta}-1}}{H(Q)}\left(1+e^{-y}\right)dy\right]\,, \tag{9.38}$$

and the reverse of $F(x) = X_n(x) - X_n^{\rm eq}(x)$ leads to

$$X_n(x) = X_n^{\rm eq}(x) + \int^x d\tilde{x}\frac{e^{\tilde{x}}}{(1+e^{\tilde{x}})^2}\exp\left[-\int_{\tilde{x}}^x \Gamma_{n\to p}\frac{y^{\frac{2}{\beta}-1}}{H(Q)}\left(1+e^{-y}\right)dy\right]\,, \tag{9.39}$$

which satisfies the initial condition $X_n(T \gg Q) = X_n(x\to 0) = X_n^{\rm eq}$. Without beta decay of free neutrons, X_n would eventually freeze out to some fixed value after T_f^n or x_n^f. Effectively setting $x=\infty$ in Eq.(9.39), we obtain the freeze-out concentration $X_n^f \coloneqq X_n(x=\infty)$

$$\begin{aligned} X_n^f &= \int_0^\infty d\tilde{x}\frac{e^{\tilde{x}}}{(1+e^{\tilde{x}})^2}\exp\left[-\int_{\tilde{x}}^\infty \Gamma_{n\to p}\frac{y^{\frac{2}{\beta}-1}}{H(Q)}\left(1+e^{-y}\right)dy\right] \\ &= \int_0^\infty d\tilde{x}\frac{e^{\tilde{x}}}{(1+e^{\tilde{x}})^2}\exp\left[-\frac{253.9332}{H(Q)\,\tau_n}\int_{\tilde{x}}^\infty\left(\frac{y^2+16y+12}{y^{6-\frac{2}{\beta}}}\right)\left(1+e^{-y}\right)dy\right]\,, \end{aligned} \tag{9.40}$$

where $X_n^{\rm eq}(x=\infty)=0$. Similar to the treatment to Eq.(9.31), we have numerically integrated X_n^f for the same set of β, as collected in the "X_n^f" columns of Tables 9.1 and 9.2, which show that X_n^f considerably grows with the increment of β.

9.5 Opening of deuterium bottleneck and helium synthesis

The number densities of neutrons, protons and deuterons (D), which are very nonrelativistic particles at the energy scale $T \lesssim T_n^f \lesssim 10$ MeV, are separately [13, 19]

$$n_n = 2\left(\frac{m_n T}{2\pi}\right)^{3/2} e^{\frac{\mu_n - m_n}{T}}\,, \quad n_p = 2\left(\frac{m_p T}{2\pi}\right)^{3/2} e^{\frac{\mu_p - m_p}{T}}\,, \quad n_D = 3\left(\frac{m_D T}{2\pi}\right)^{3/2} e^{\frac{\mu_D - m_D}{T}}\,, \tag{9.41}$$

so the equilibrium of chemical potentials $\mu_D = \mu_n + \mu_p$ leads to

$$\begin{aligned} X_D &:= \frac{2n_D}{n_n + n_p} = \frac{3}{2}\frac{n_n n_p}{n_n + n_p}\left(\frac{2\pi}{T}\frac{m_D}{m_n m_p}\right)^{3/2} e^{(m_n + m_p - m_D)/T} \\ &= \frac{3}{2} X_n X_p n_b \left(\frac{2\pi}{T}\frac{m_D}{m_n m_p}\right)^{3/2} e^{B_D/T}\,, \end{aligned} \tag{9.42}$$

where $n_b = n_n + n_p$, and $B_D = m_n + m_p - m_D = 2.2246$ MeV refers to the deuteron binding energy (with $m_D = 1875.6129$ MeV, $m_n = 939.5654$ MeV, and $m_p = 938.2721$ MeV [23]). Moreover, n_b is related to the photon number density by $n_b = \eta_{10} \times 10^{-10} \times n_\gamma = \eta_{10} \times 10^{-10} \times \frac{2\zeta(3)}{\pi^2} T^3$, where $\eta_{10} := 10^{10} \times n_b / n_\gamma$ rescales the photon-to-baryon ratio. Then Eq.(9.42) becomes

$$\begin{aligned} X_D &= 10^{-10} \times \frac{3\zeta(3)}{\pi^2}\eta_{10} X_n X_p \left(\frac{2\pi}{T}\frac{m_D}{m_n m_p}\right)^{3/2} e^{B_D/T} T^3 \\ &\simeq 5.6474 \times 10^{-14} \times \eta_{10} X_n X_p e^{B_D/T_{\rm MeV}} T_{\rm MeV}^{3/2}\,. \end{aligned} \tag{9.43}$$

Note that the value of η_{10} can be determined through

$$\eta_{10} \simeq 10^{10} \times \frac{\rho_{\rm crit}\Omega_{b0}/m_p}{n_\gamma} = 273.4604\,\Omega_b h^2 = 6.0982\,, \tag{9.44}$$

where we have h for the normalized Hubble constant in the unit of 100 km/s/Mpc, $n_\gamma = 410.7/\text{cm}^3$ for the cosmic background photons, $\rho_{\rm crit} = 1.8785\,h^2 \times 10^{-29}$ g/cm^3 for the critical density of the Universe, $m_p = 1.6726 \times 10^{-24}$g for the proton mass, and $\Omega_{b0} h^2 = 0.02230 \pm 0.00014$ [23, 24].

After the freeze-out of free neutrons, the Universe further expands and cools. Finally the high-energy photons at the Planck distribution tail are no longer energetic enough to photodissociate a deuteron, and the deuterium bottleneck opens. Taking the logarithm of Eq.(9.43), one obtains

$$\begin{aligned} \frac{B_D}{T_{\rm MeV}} - \frac{3}{2}\ln\frac{B_D}{T_{\rm MeV}} &= \ln\frac{X_D}{5.6474 \times 10^{-14} \times \eta_{10} X_n^f \left(1 - X_n^f\right) B_D^{3/2}} \\ &= 27.4976 - \ln\left[X_n^f\left(1 - X_n^f\right)\right] + \ln\frac{X_D}{\eta_{10}/6.0982}\,. \end{aligned} \tag{9.45}$$

Table 9.1: $\varepsilon = \sqrt{m_{\rm Pl} H_0 \Omega_{M0}} = 3.5459 \times 10^{12}$ [s^{-1}] = 2.3344×10^{-9} MeV for $H(Q)$

β	T_ν^f [MeV]	t_ν^f [s]	$X_n^{\rm eq}(T_\nu^f)$	T_n^f [MeV]	t_n^f [s]	$H(Q)$ [s^{-1}]	X_n^f	$t_{\rm BBN}$ [s]	$Y_p = 2X_n^{\rm BBN}$
1.289	16.1208	2.2025×10^{-6}	0.4780	10.9672	4.0040×10^{-6}	5837.9072	0.4683	0.0133	0.9366
1.25	8.9635	4.0191×10^{-5}	0.4640	5.9799	7.6803×10^{-5}	702.3051	0.4425	0.1242	0.8848
1.2	6.4418	2.0125×10^{-4}	0.4500	4.2076	4.0928×10^{-4}	205.2347	0.4189	0.5011	0.8373
1.15	4.6496	0.0010	0.4309	2.9523	0.0022	63.0969	0.3863	1.9534	0.7710
1.1	3.2612	0.0055	0.4021	1.9860	0.0137	18.4481	0.3372	8.1565	0.6682
1.09	3.0226	0.0146	0.3561	1.8207	0.0204	14.2832	0.3245	10.9907	0.6409
1.07	2.5807	0.0473	0.2981	1.5153	0.0470	8.4580	0.2955	20.2540	0.5775
1.05	2.1833	0.0946	0.2812	1.2416	0.1154	4.9179	0.2609	38.1526	0.4998
1.03	1.8275	0.1658	0.2793	0.9977	0.3045	2.7998	0.2203	73.6899	0.4054
1.01	1.5101	0.2392	0.2791	0.7811	0.8827	1.5530	0.1737	146.6845	0.2944
1.001	1.3778	0.3832	0.2791	0.6912	1.4882	1.1770	0.1580	202.8328	0.2514
$\beta \to 1^+$	1.3630	0.3955	0.2791	0.6800	1.5889	1.1385	0.1480	210.6044	0.2334

Table 9.2: $\varepsilon = 1$ [s^{-1}] or $\varepsilon_s = 1$ for $H(Q)$

β	T_ν^f [MeV]	t_ν^f [s]	$X_n^{eq}(T_\nu^f)$	T_n^f [MeV]	t_n^f [s]	$H(Q)$ [s^{-1}]	X_n^f	t_{BBN} [s]	$Y_p = 2X_n^{BBN}$
1.289	2.4629	0.0265	0.3717	1.5172	0.0561	8.9650	0.3030	8.6383	0.6001
1.25	1.6378	0.1973	0.3122	0.9403	0.4795	2.1706	0.2183	40.1737	0.4174
1.2	1.5189	0.2762	0.2991	0.8473	0.7306	1.6620	0.1974	61.8763	0.3683
1.15	1.4636	0.3185	0.2924	0.7969	0.9170	1.4558	0.1843	84.6670	0.3351
1.1	1.4283	0.3443	0.2879	0.7586	1.0879	1.3337	0.1732	112.8207	0.3051
1.09	1.4223	0.3484	0.2871	0.7527	1.1199	1.3140	0.1711	119.4649	0.2991
1.07	1.4109	0.3560	0.2856	0.7386	1.1937	1.2772	0.1667	134.1281	0.2866
1.05	1.3997	0.3636	0.2841	0.7230	1.2795	1.2423	0.1621	151.0530	0.2735
1.03	1.3878	0.3722	0.2825	0.7092	1.3707	1.2067	0.1572	170.9754	0.2594
1.01	1.3736	0.3842	0.2806	0.6909	1.4989	1.1666	0.1517	195.2714	0.2434
1.001	1.3646	0.3936	0.2793	0.6814	1.5760	1.1425	0.1496	208.7735	0.2350
$\beta \to 1^+$	1.3630	0.3955	0.2791	0.6800	1.5889	1.1385	0.1480	210.6044	0.2334

Solve it by iteration, and the deuteron concentration at the temperature T_{MeV} can be approximated by

$$\begin{aligned}\frac{B_D}{T_{\text{MeV}}} \simeq 27.4976 - \ln\left[X_n^f\left(1-X_n^f\right)\right] + \ln\frac{X_D}{\eta_{10}/6.0982} + \\ \frac{3}{2}\ln\left\{27.4976 - \ln\left[X_n^f\left(1-X_n^f\right)\right] + \ln\frac{X_D}{\eta_{10}/6.0982}\right\},\end{aligned} \tag{9.46}$$

so

$$\begin{aligned}T_{\text{MeV}}^{-1} \simeq 12.3607 - 0.4495\ln\left[X_n^f\left(1-X_n^f\right)\right] + 0.4495\ln\frac{X_D}{\eta_{10}/6.0982} \\ + 0.6743\ln\left\{27.4976 - \ln\left[X_n^f\left(1-X_n^f\right)\right] + \ln\frac{X_D}{\eta_{10}/6.0982}\right\}.\end{aligned} \tag{9.47}$$

On the other hand, the evolution of X_D satisfies the Boltzmann equation

$$\frac{dX_D}{dt} = -\frac{1}{2}\langle\sigma v\rangle X_D^2 n_b\,. \tag{9.48}$$

dX_D/dt becomes visible when it is comparable to X_D, and $|dX_D/dt| \simeq X_D$ yields $X_D \simeq \frac{2}{\langle\sigma v\rangle n_b t}\frac{1}{2}\langle\sigma v\rangle X_D^2 n_b \simeq X_D$, which can be regarded as the opening of the deuterium bottleneck. Recall that

$$n_b = \eta_{10}\times 10^{-10}\times\frac{2\zeta(3)}{\pi^2}T^3 = 0.2346\times 10^{-10}\,\eta_{10}T^3 = 3.0536\times 10^{21}\,\eta_{10}T_{\text{MeV}}^3\ [\text{cm}^{-3}]\,, \tag{9.49}$$

and

$$\frac{1}{t} = \frac{1}{\sqrt{3\beta(\beta-1)}}\left(\sqrt{\frac{\beta-1}{-5\beta^2+8\beta-2}}\right)^{1/\beta}\left(\sqrt{\frac{g_*}{3.3835}}\right)^{1/\beta}\left(1.3177\,T_{\text{MeV}}^2\right)^{1/\beta}\varepsilon_s^{1-\frac{1}{\beta}}\ [\text{s}]\,, \tag{9.50}$$

so $X_D^{(\text{open})} \simeq \frac{2}{\langle\sigma v\rangle n_b t}$ expands into

$$\begin{aligned}X_D^{(\text{open})} =& \frac{6.2009\times 10^{-23}}{\langle\sigma v\rangle}\left(\frac{6.0982}{\eta_{10}}\right)\left(\sqrt{\frac{g_*}{3.3835}}\right)^{1/\beta}\frac{\varepsilon_s^{1-\frac{1}{\beta}}}{\sqrt{\beta(\beta-1)}}\left(1.3178\cdot\sqrt{\frac{\beta-1}{-5\beta^2+8\beta-2}}\right)^{1/\beta} \\ &\times\left\{12.3607 - 0.4495\ln\left[X_n^f\left(1-X_n^f\right)\right] + 0.4495\ln\frac{X_D}{\eta_{10}/6.0982}\right\}^{3-\frac{2}{\beta}}.\end{aligned} \tag{9.51}$$

Solving this equation by iteration, one obtains

$$\begin{aligned}X_D^{(\text{open})} =& \frac{6.2009\times 10^{-23}}{\langle\sigma v\rangle}\left(\frac{6.0982}{\eta_{10}}\right)\left(\sqrt{\frac{g_*}{3.3835}}\right)^{1/\beta}\frac{\varepsilon_s^{1-\frac{1}{\beta}}}{\sqrt{\beta(\beta-1)}}\left(1.3178\cdot\sqrt{\frac{\beta-1}{-5\beta^2+8\beta-2}}\right)^{1/\beta} \\ &\times\left\{12.3607 - 0.4495\ln\left[X_n^f\left(1-X_n^f\right)\right]\right\}^{3-\frac{2}{\beta}} + 0.4495\ln\frac{\cdots}{\eta_{10}/6.0982}\,,\end{aligned} \tag{9.52}$$

where $\cdots$ denotes the repeating iteration terms. Here $g_* \simeq 3.3835$; this because around the temperature $T_D^{(\text{open})} \ll m_e = 0.5110$ MeV after the electron-positron annihilation, only photons and neutrinos remain as relativistic species with $T_\nu/T_\gamma = T_\nu/T = (4/11)^{1/3}$ (this ratio is independent of the number of neutrino species), hence $g_*(T \lesssim m_e) = 2 + \frac{7}{8} \times 3.046 \times 2 \times \left(\frac{4}{11}\right)^{4/3} \simeq 3.3835$.

At $T_{\rm BBN}$, X_D peaks and X_n drops below the concentration predicted by beta decay. The deuterium bottleneck has broken and the remaining free neutrons are quickly fused into ^{4}He via the strong interaction through the sequence of reactions [13]

$$\begin{aligned} n + p &\to {\rm D}\,, \\ {\rm D} + n \to {}^3{\rm H}\ &+ p \to {}^4{\rm He}\,, \\ {\rm D} + p \to {}^3{\rm He} &+ n \to {}^4{\rm He}\,. \end{aligned} \tag{9.53}$$

Following the time-temperature relation Eq.(9.14) with $T_{\rm MeV} = T_{\rm BBN}$, nucleosynthesis occurs at

$$t_{\rm BBN} = \sqrt{3\beta(\beta-1)}\left(0.7589 \cdot \sqrt{\frac{-5\beta^2+8\beta-2}{\beta-1}}\right)^{1/\beta}\left(\sqrt{\frac{3.3835}{g_*}}\right)^{1/\beta}\left(T_{\rm MeV}^{\rm (BBN)}\right)^{-2/\beta}\varepsilon_s^{\frac{1}{\beta}-1}\ [{\rm s}]\,. \tag{9.54}$$

while the neutron concentration at BBN is

$$X_n^{\rm BBN} = X_n^f \exp\left(\frac{t_n^f - t_{\rm BBN}}{\tau_n}\right), \tag{9.55}$$

and the primordial ^{4}He abundance is $Y_p \simeq 2X_n^{\rm BBN}$. For different values of β, $t_{\rm BBN}$, $X_n^{\rm BBN}$ and Y_p have been numerically calculated, and the results have been collected in Tables 9.1 and 9.2.

9.6 Comparison with $\varepsilon = m_{\rm Pl}$

To facilitate the comparison with Refs.[7–9], we will also consider the situation of $\varepsilon = m_{\rm Pl} = 1.2209 \times 10^{-22}$ MeV 0.1854×10^{44} [s^{-1}], or $1/\ell_{\rm Pl}$ where $\ell_{\rm Pl} = \sqrt{G}$ refers to Planck length. As emphasized in problem (5) of the Introduction, this choice of ε suffers from the ambiguity with the change of Newton's constant. To make matters worse, the weak freeze-out temperature of neutrinos is depicted in Fig. 9.2, and the relevant energy scales have been collected in Table 9.3; they clearly show that the process of nucleosynthesis breaks down for $1.06 \lesssim \beta < (4+\sqrt{6})/5$, as the interactions of muons, tauons, their associated neutrinos, and unstable hadrons beyond nucleons are all involved, which make it impossible to examine the full domain $1 \leq \beta < (4+\sqrt{6})/5$. For completeness, we calculate the full set of nucleosynthesis parameters in Table 9.4.

Table 9.3: g_* for the T_f^ν in Fig. 9.2, based on the data of Particle Data Group. where $m_e = m(\text{electron}) = 0.5110$ MeV, $m_\mu = m(\text{muon}) = 105.6584$ MeV, $m_\pi = m(\text{pion}^\pm) = 139.5702$ MeV, $T_c = T(\text{quark-hadron phase transition}) \approx 150$ MeV, $m_c = m(\text{charm quark}) = 1275$ MeV, $m_\tau = m(\text{tauon}) = 1776.82$ MeV, and we have taken $m_{\pi^\pm} = 139.5702 > m_{\pi^0} = 134.9766$ MeV. Note that between 100~200 MeV, g_{*s} is also subject to the phase transition of quantum chromodynamics for strange quarks.

Temperature	Temperature	new particles	$g_* - 0.0805$	g_*
$m_e < T < m_\mu$	$0.5110 < T < 105.6584$	–	10.75	10.8305
$m_\mu < T < m_\pi$	$105.6584 < T < 139.5702$	$\mu^\pm$	14.25	14.3305
$m_\pi < T < T_c$	$139.5702 < T < T_c$	$\pi^0, \pi^\pm$	17.25	17.3305
$T_c < T < m_c$	$T_c < T < 1275$	$u, \bar{u}, d, \bar{d}$, $s, \bar{s}$, gluon	61.75	61.8305
$m_c < T < m_\tau$	$1275 < T < 1776.82$	$c, \bar{c}$	72.25	72.3305
$m_\tau < T < m_b$	$1776.82 < T < 4180$	$\tau^\pm$	75.75	75.8305

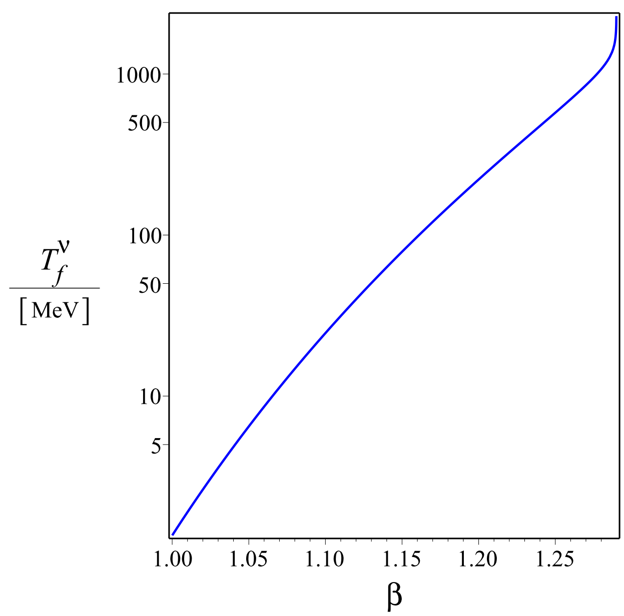


Figure 9.2: T_ν^f (in MeV) for $\varepsilon = m_{\rm Pl} = 1.2209 \times 10^{-22}$ MeV, with g_* fixed to 10.8305.

9.7 GR limit

When $f(R,\epsilon) = R$ in Eqs.(9.2), (9.3) and (9.4), one recovers Einstein's equation $R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} = 8\pi m_{\rm Pl}^{-2}\mathcal{T}_{\mu\nu}^{(m)}$, as well as the standard Friedmann equations $3\frac{\dot{a}^2}{a^2} = -8\pi m_{\rm Pl}^{-2}\rho$ and $3\frac{\ddot{a}}{a} = -4\pi m_{\rm Pl}^{-2}(\rho + 3P)$. For the specific power-law $f(R)$ gravity under discussion, it reduces from $\mathscr{L} = \varepsilon^{2-2\beta}R^\beta + 16\pi m_{\rm Pl}^{-2}\mathscr{L}_m$ to GR in the limit

Table 9.4: $\varepsilon = m_{\text{Pl}} = 0.1854 \times 10^{44}$ [s^{-1}] for $H(Q)$, with $1.06 \lesssim \beta < (4+\sqrt{6})/5$ invalid for nucleosynthesis.

β	T_ν^f [MeV]	t_ν^f [s]	X_n^ν	T_n^f [MeV]	t_n^f [s]	$H(Q)$ [s^{-1}]	X_n^f	t_{BBN} [s]	$Y_p = 2X_n^{\text{BBN}}$
1.05	6.4819	0.1707×10^{-3}	0.4503	4.0862	0.0004	142.758	0.4135	1.3145	0.8258
1.01	1.9043	0.0750	0.3365	1.0369	0.2500	3.1286	0.2262	72.8185	0.4164
1.009	1.8428	0.0883	0.3314	0.9980	0.2979	2.8313	0.2191	80.8654	0.3998
1.007	1.7252	0.1226	0.3209	0.9201	0.4272	2.3175	0.2039	99.8026	0.3642
1.005	1.6142	0.1706	0.3098	0.8468	0.6160	1.8950	0.1883	123.3100	0.3277
1.003	1.5095	0.2381	0.2980	0.7777	0.8935	1.5476	0.1725	152.5414	0.2904
1.001	1.4106	0.3334	0.2856	0.7113	1.3096	1.2622	0.1630	188.9951	0.2630
$\beta \to 1^+$	1.3630	0.3955	0.2791	0.6800	1.5889	1.1385	0.1480	210.6044	0.2334

$\beta \to 1^+$, with

$$\lim_{\beta\to 1^+} \sqrt{\frac{\beta}{\beta-1}} \times \left(\sqrt{\frac{\beta-1}{-5\beta^2+8\beta-2}}\right)^{1/\beta} = 1\,, \tag{9.56}$$

and

$$\lim_{\beta\to 1^+} \sqrt{\beta(\beta-1)}\left(\frac{-5\beta^2+8\beta-2}{\beta-1}\right)^{\frac{1}{2\beta}} = 1 = \lim_{\beta\to 1^+}\left[\beta(\beta-1)\right]^{\beta}\left(\frac{-5\beta^2+8\beta-2}{\beta-1}\right), \tag{9.57}$$

so from Eqs.(9.13), (9.14) and (9.33) one recovers the standard Hubble expansion [note: by "standard" we mean the standard Big Bang cosmology of GR]

$$\mathcal{H} = \frac{1}{2t} = \left(\frac{8\pi^3}{90}g_*\right)^{1/2}\frac{T^2}{m_{\rm Pl}} \simeq 1.6602\sqrt{g_*}\,\frac{T^2}{m_{\rm Pl}} \simeq 0.2068\sqrt{g_*}\,T^2_{\rm MeV}\ [{\rm s}^{-1}]\,. \tag{9.58}$$

as well as the the standard time-temperature relation

$$t = \sqrt{\frac{90}{32\pi^3}}\,g_*^{-1/2}\frac{m_{\rm Pl}}{T^2} \simeq \frac{2.4177}{\sqrt{g_*}\,T^2_{\rm MeV}}\ [{\rm s}] \quad \text{or} \quad tT^2_{\rm MeV} \simeq \frac{2.4177}{\sqrt{g_*}}\,. \tag{9.59}$$

Equating $\mathcal{H}$ to the neutrino reaction rate Γ_{ν_e} in Eq.(9.20), i.e. $0.2688\,T^5_{\rm MeV} = 0.2068\sqrt{g_*}\,T^2_{\rm MeV}$, one can find that neutrinos decouple at $T = 1.3630$ MeV and $t = 0.3955$ [s]. Furthermore, equating $\mathcal{H}$ to the combined two-body reaction rate $\Gamma_{n\to p}$ in Eq.(9.28),

$$\mathcal{H}(x) = \frac{\mathcal{H}(Q)}{x^2} = \frac{253.9332}{\tau_n}\frac{x^2+6x+12}{x^5}\,, \tag{9.60}$$

where $\mathcal{H}(Q) = 0.3459\sqrt{g_*}$, it turns out that nucleons freeze out at $x = 1.9020$, $T_n^f = 0.6800$ MeV, and $t_n^f = 1.5889$ [s]. According to Eq.(9.39) with $\beta \to 1^+$, the neutron concentration after the weak freeze-out of neutrinos is determined by

$$\begin{aligned} X_n(x) &= X_n^{\rm eq} + \int^x d\tilde{x}\frac{e^{\tilde{x}}}{(1+e^{\tilde{x}})^2}\exp\left[-\int_{\tilde{x}}^x \Gamma_{n\to p}\frac{y}{\mathcal{H}(Q)}\left(1+e^{-y}\right)dy\right] \\ &= X_n^{\rm eq} + \int^x d\tilde{x}\frac{e^{\tilde{x}}}{(1+e^{\tilde{x}})^2}\exp\left[-\frac{255}{\mathcal{H}(Q)\,\tau_n}\int_{\tilde{x}}^x y^{-4}\left(y^2+16y+12\right)\left(1+e^{-y}\right)dy\right], \end{aligned} \tag{9.61}$$

and thus in the absence of neutron decay X_n would freeze out to the concentration $X_n(x\to\infty)$

$$X_n^f = \int_0^\infty d\tilde{x}\frac{e^{\tilde{x}}}{(1+e^{\tilde{x}})^2}\exp\left[-\frac{255}{\mathcal{H}(Q)\,\tau_n}\frac{\tilde{x}^2+3\tilde{x}+4+e^{-\tilde{x}}(\tilde{x}+4)}{\tilde{x}^3}\right] = 0.1480\,. \tag{9.62}$$

Nucleosynthesis begins at $T \simeq 0.079$ MeV, which corresponds to $t_{\rm BBN} = 210.6045$ [s]. Hence, the neutron concentration at BBN is

$$X_n^{\rm BBN} = X_n^f\,\exp\left(\frac{t_{\rm BBN}-t_n^f}{\tau_n}\right) = 0.1167\,. \tag{9.63}$$

and the primordial helium abundance is

$$Y_p \simeq 2X_n^{\rm BBN} = 0.2334. \tag{9.64}$$

These numerical results are also collected in Tables 9.1 and 9.2 in the bottom row.

Big Bang nucleosynthesis could not progress further in producing heavier elements with mass number $A > 7$ due to the Coulomb barrier and the lack of stable $A = 8$ nuclei. In the semianalytical approach, our discussion will end with the primordial helium synthesis. The title of this paper emphasizes "Big Bang nucleosynthesis" rather than the narrower "primordial helium synthesis", because we will proceed to investigate the synthesis of {D, ^{4}He, ^{7}Li} from the empirical approach.

9.8 Empirical constraints from D and ^{4}He abundances

So far we have calculated the primordial nucleosynthesis in $\mathscr{L} = \varepsilon^{2-2\beta}R^\beta + 16\pi m_{\rm Pl}^{-2}\mathscr{L}_m$ gravity and GR from the semianalytical approach. We have seen that primordial synthesis and abundances of the lightest elements (D, ^{4}He, and also ^{3}H, ^{3}He, ^{7}Li) rely on the baryon-to-photon ratio $\eta_{10} = 10^{10} \times n_b/n_\gamma$ and the expansion rate H of the Universe. In addition to the semianalytical approach, the abundances can be also be estimated in an empirical way at high accuracy [27, 28]. For modified gravity with a nonstandard Hubble expansion H, introduce the nonstandard-expansion parameter S as the ratio of H to the standard expansion $\mathcal{H} = 1/(2t)$ in GR, and this ratio varies among different gravity theories. In $\mathscr{L} = \varepsilon^{2-2\beta}R^\beta + 16\pi m_{\rm Pl}^{-2}\mathscr{L}_m$ gravity under discussion, one has

$$S \coloneqq \frac{H}{\mathcal{H}} \quad \Rightarrow \quad S = \beta\,, \tag{9.65}$$

and S takes such a concise form thanks to the exact solution $a \propto t^{\beta/2}$ and $H = \beta/(2t)$ for the radiation-dominated FRW Universe. It has been found that, for the priors $4 \lesssim \eta_{10} \lesssim 8$ and $0.85 \lesssim S \lesssim 1.15$, the primordial deuterium and ^{4}He abundances satisfy the best-fit formulae [27, 28]

$$y_{\rm D} \coloneqq 10^5 \times \frac{\rm D}{^1{\rm H}} = 46.5 \times (1 \pm 0.03) \times \left[\eta_{10} - 6(S-1)\right]^{-1.6} \tag{9.66}$$

and

$$Y_p = (0.2386 \pm 0.0006) + 2 \times 10^{-4} \times (\tau_n - 885.7) + \frac{\eta_{10}}{625} + \frac{S-1}{6.25}\,, \tag{9.67}$$

the reverse of which respectively yield

$$S = \frac{\eta_{10}}{6} - \frac{1}{6}\left[\frac{46.5 \times (1 \pm 0.03)}{y_{\rm D}}\right]^{1/1.6} + 1 \tag{9.68}$$

and

$$S = 6.25 \times \left[Y_p - (0.2386 \pm 0.0006) + 2 \times 10^{-4} \times (885.7 - \tau_n)\right] - \frac{\eta_{10}}{100} + 1\,. \tag{9.69}$$

Recall that we have the baryon-to-photon ratio $\eta_{10} = 6.0352 \pm 0.0739$ for $\Omega_b h^2 = 0.02207 \pm 0.00027$ as in Eq.(9.44), the neutron half life $\tau_n = 880.0 \pm 0.9$ [s], and the recommended values of the D and ^{4}He abundances from the Particle Data Group [23],

$$y_{\rm D} = 2.53 \pm 0.04 \quad , \quad Y_p = 0.2465 \pm 0.0097\,. \tag{9.70}$$

Thus, Eqs.(9.68) and (9.69) lead to

$$S = 0.9777 \pm 0.0708 \quad \text{or} \quad 0.9069 \leq S = \beta \leq 1.0485 \quad ({\rm D})\,, \tag{9.71}$$

$$S = 0.9961 \pm 0.1035 \quad \text{or} \qquad 0.8926 \le S = \beta \le 1.0997 \quad ({}^4\text{He})\,. \tag{9.72}$$

Here for the errors of mutually independent quantities in $\{x_i \pm \Delta x_i, x_j \pm \Delta x_j\} \mapsto y + \Delta y$, we have applied the propagation rules that $\Delta y = \sqrt{(\Delta x_i)^2 + \left(\Delta x_j\right)^2}$ for $y = x_i \pm x_j$, and $\frac{\Delta y}{y} = \sqrt{\left(\frac{\Delta x_i}{x_i}\right)^2 + \left(\frac{\Delta x_j}{x_j}\right)^2}$ for $y = x_i x_j$ or $y = x_i/x_j (i \neq j)$.

Combining Eq.(9.71) with Eq.(9.72), we find $0.8926 \le S = \beta \le 1.0485$, which satisfies the prior $0.85 \lesssim S \lesssim 1.15$; taking into account the positive energy density/positive temperature condition $1 < \beta < (4 + \sqrt{6})/5$ in Eq.(9.10), we further obtain $1 < S = \beta \le 1.0485$. Since S is related to the extra number of effective neutrino species by

$$S = \left(1 + \frac{7}{43}\Delta N_\nu\right)^{1/2} \quad \Rightarrow \quad \Delta N_\nu = \frac{43}{7}(\beta^2 - 1)\,, \tag{9.73}$$

thus for $1 < S = \beta \le 1.0485$, $\Delta N_\nu^{\text{eff}} := N_\nu^{\text{eff}} - 3$ is constrained by

$$0 < \Delta N_\nu^{\text{eff}} \le 0.6107\,. \tag{9.74}$$

Note that the theoretically predicted primordial abundance for ^{7}Li is found to respect the best-fit formula

$$y_{\text{Li}} := 10^{10} \times \frac{\text{Li}}{{}^1\text{H}} = \frac{(1 \pm 0.1)}{8.5} \times \left[\eta_{10} - 3(S - 1)\right]^2, \tag{9.75}$$

which, for the domain $1 < S = \beta \le 1.0485$, gives rise to

$$y_{\text{Li}} = 4.0892 \pm 0.0012\ (\beta = 1.0485) \quad \text{to} \quad 4.3022 \pm 0.0012\ (\beta = 1)\,. \tag{9.76}$$

Hence,

$$4.0880 \le y_{\text{Li}} < 4.3034\,, \tag{9.77}$$

which is much greater than the observed abundance $y_{\text{Li}} = 1.6 \pm 0.3$ [23]. This indicates that the lithium problem remains unsolved in $\mathscr{L} = \varepsilon^{2-2\beta} R^\beta + 16\pi m_{\text{Pl}}^{-2} \mathscr{L}_m$ gravity.

9.9 Consistency with gravitational baryogenesis

We just investigated the primordial nucleosynthesis in $\mathscr{L} = \varepsilon^{2-2\beta} R^\beta + 16\pi m_P^{-2} \mathscr{L}_m$ gravity from the semianalytical and the empirical approaches. The nucleons building the lightest nuclei come from the net baryons left after baryogenesis, and in this section we will quickly check the consistency of $\mathscr{L} = \varepsilon^{2-2\beta} R^\beta + 16\pi m_P^{-2} \mathscr{L}_m$ gravity with the baryon-antibaryon asymmetry using the framework of gravitational baryogenesis [30], which, compared with traditional Sakharov-type mechanisms, dynamically produces the required baryon asymmetry for an expanding Universe by violating the combined symmetry of charge conjugation, parity transformation and time reversal (CPT) while being in thermal equilibrium. In this mechanism, the dominance of baryons over antibaryons attribute to the coupling between the gradient of the Ricci curvature scalar R and some current J_B^μ leading to net baryon-lepton charges:

$$\int d^4x \sqrt{-g}\, \frac{\left(\partial_\mu R\right) J_B^\mu}{M_*^2} = \int d^4x \sqrt{-g}\, \frac{\dot{R}\,(n_B - n_{\bar{B}})}{M_*^2}\,, \tag{9.78}$$

where M_* refers to the cutoff scale of the effective theory, and is estimated to take the value of the reduced Plank mass $M_* \simeq m_P/\sqrt{8\pi}$.

The baryon asymmetry can be depicted by the dimensionless baryon-to-entropy ratio n_B/s of the radiation-dominated Universe, with

$$n_B \simeq \frac{1}{6} g_b \mu_B T^2 \quad \text{and} \quad s = \frac{2\pi^2}{45} g_{*s} T^3 \,, \tag{9.79}$$

where $g_b = 28 = 2\,(\text{photon}) + 2\times 8\,(\text{gluon}) + 3\times 3\,(W^\pm, Z^0) + 1\,(\text{Higgs})$ for $T > m(\text{top quark}) \simeq 1.733\times 10^5$ MeV, and $\mu_B := -\dot{R}/M_*^2$ acts as the effective chemical potential. Also, g_{*s} denotes the entropic effective number of degree of freedom, and is defined like g_* by

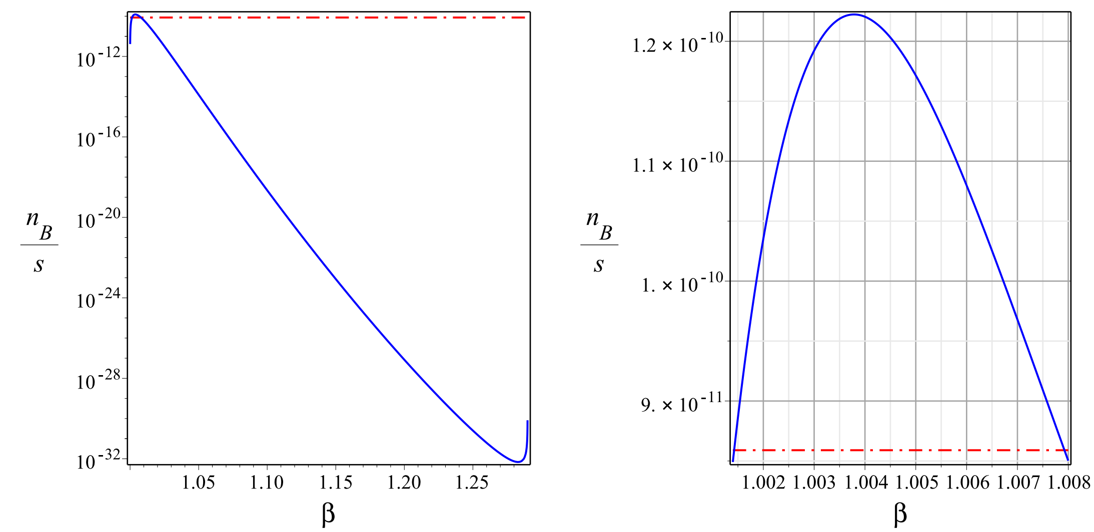
$$g_{*s} := \sum_{\text{boson}} g_i^{(b)} \left(\frac{T_i}{T}\right)^3 + \frac{7}{8} \sum_{\text{fermion}} g_j^{(f)} \left(\frac{T_j}{T}\right)^3 \,; \tag{9.80}$$

one has $g_{*s} = g_*$ at the baryogenesis era when all standard-model particles are relativistic and in equilibrium, $g_f = 2\times 3\,(\text{neutrino}) + 2\times 6\,(\text{charged lepton}) + 12\times 6\,(\text{quark}) = 90$, and $g_{*s} = g_* = g_b + \frac{7}{8} g_f = 106.75$ (Note that when calculating g_f, we use $N_\nu^{\text{eff}} = 3$ rather than $N_\nu^{\text{eff}} = 3.046$, because baryogenesis happens before primordial nucleosythesis and it's unnecessary to consider the "non-instantaneity" of neutrinos' decoupling.). In $\mathscr{L} = \varepsilon^{2-2\beta} R^\beta + 16\pi m_P^{-2} \mathscr{L}_m$ gravity for which $\partial_\mu R$ or $\dot{R}$ is nontrivial, Eqs.(9.14) and (9.79) lead to

$$\begin{aligned} \frac{n_B}{s} &= -\frac{15}{4\pi^2} \frac{g_b}{g_{*s}} \frac{\dot{R}}{M_*^2 T}\bigg|_{T_d} = \frac{45}{2\pi^2} \frac{g_b}{g_{*s}} \frac{\beta(\beta-1)}{t^3 M_*^2 T_d} \\ &= \frac{5\sqrt{3}}{2\pi^2} \frac{g_b}{g_{*s}} \frac{1}{\sqrt{\beta(\beta-1)}} \left(\sqrt{\frac{(\beta-1)\, g_*}{-5\beta^2 + 8\beta - 2}}\right)^{3/\beta} \left(\sqrt{\frac{32\pi^3}{30}} \frac{T_d^2}{\varepsilon m_P}\right)^{3/\beta} \frac{\varepsilon^3}{M_*^2 T_d} \,, \end{aligned} \tag{9.81}$$

where $T_d \simeq 3.3\times 10^{19}$ MeV is the upper bound on the tensor-mode fluctuations at the inflationary scale [31].

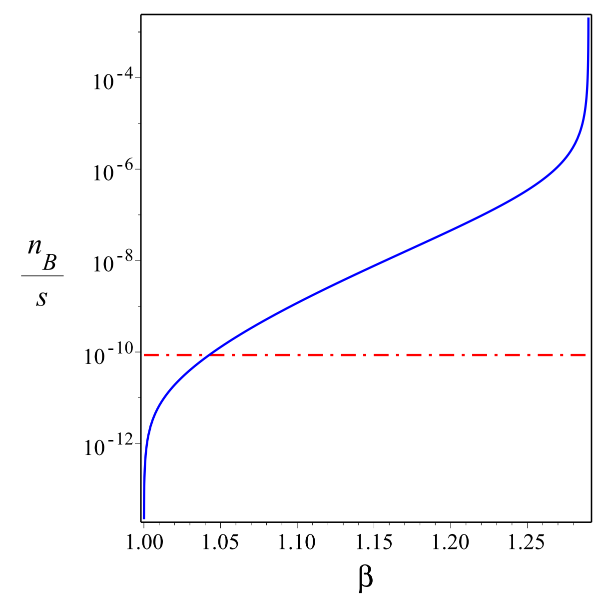
Following the observational value $\Omega_b h^2 = 0.02207 \pm 0.00027$ [24], we have the net-baryon-to-entropy ratio $n_b/s = \frac{n_b}{n_\gamma}/7.04 = 3.8920 \times 10^{-9} \Omega_b h^2 = (8.5897 \pm 0.1051) \times 10^{-11}$, which remains constant during the expansion of the early Universe and imposes a constraint to n_B/s. For $\varepsilon = \ [\text{s}^{-1}] = 6.58 \times 10^{-22}$ MeV, Eq.(9.81) respects this constraint for all $1 < \beta < (4 + \sqrt{6})/5$, as shown in Fig. 9.3a, with minor violation for $1.001426 < \beta < 1.007925$, as magnified in Fig. 9.3b; however, this minor violation can be easily removed by a fluctuation of M_* and T_d. For $\varepsilon = m_{\text{Pl}}$, this constraints is satisfied for $1 < \beta < 1.04255$, as shown in Fig. 9.4.



(a) **(b)**

Figure 9.3: n_B/s for $\varepsilon = 1\ [\mathrm{s}^{-1}] = 6.58 \times 10^{-22}$ MeV.

Figure 9.4: n_B/s for $\varepsilon = m_{\mathrm{Pl}}$



9.10 Conclusions

In this paper, we have reinvestigated the nonstandard BBN in $\mathscr{L} = \varepsilon^{2-2\beta}R^{\beta} + 16\pi m_{\text{Pl}}^{-2}\mathscr{L}_m$ gravity, which has overcome the inappropriateness in Refs.[8] and [9]. The main results, compared with the standard BBN or the GR limit in Sec. 9.7, manifest themselves as Eq.(9.13) for the nonstandard Hubble expansion, Eq.(9.14) for the generalized time-temperature correspondence, Eq.(9.21) for the neutrino decoupling temperature T_{ν}^{f}, Eq.(9.31) for the freeze-out temperature T_n^f of nucleons, Eq.(9.39) for the out-of-equilibrium concentration X_n, and Eq.(9.40) for the freeze-out concentration X_n^f. As reflected by the data points in Tables 9.1 and 9.2, we have shown that every step of BBN is considerably $\beta-$dependent when running over the entire domain $1 < \beta < (4 + \sqrt{6})/5$.

On the other hand, for the constants used in this paper, m_{Pl}, m_n, m_p, m_D, m_s, m_{μ}, m_{π^0}, m_c, m_{τ}, m_b, and G_F, their values are all taken from the latest recommended values from Particle Data Group [23]. In the semianalytical approach, β is constrained to $1 < \beta < 1.05$ for $\varepsilon = 1$ [s^{-1}] and $1 < \beta < 1.001$ for $\varepsilon = m_{\text{Pl}}$. In the empirical approach, we have found $1 < \beta \leq 1.0505$ which corresponds to an extra number of neutrino species by $0 < \Delta N_{\nu}^{\text{eff}} \leq 0.6365$. In theory, it might be possible for modified gravities to severely rescale the thermal history of the early Universe without changing the state of the current Universe. This requires a careful examination of the joint influences to BBN, cosmic radiation background and structure formation, and we will look into the possibility of such strongly modified gravities in our prospective studies.

Acknowledgement

This work was supported by NSERC grant 261429-2013.

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Chapter 10. Hot, warm and cold dark matter as thermal relics in power-law $f(R)$ gravity [arXiv:1512.09117]

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Abstract

We investigate the thermal relics as hot, warm and cold dark matter in $\mathscr{L} = \varepsilon^{2-2\beta}R^\beta + 16\pi m_{\text{Pl}}^{-2}\mathscr{L}_m$ gravity, where ε is a constant balancing the dimension of the field equation, and $1 < \beta < (4+\sqrt{6})/5$ for the positivity of energy density and temperature. If light neutrinos serve as hot/warm relics, the entropic number of statistical degrees of freedom g_{*s} at freeze-out and thus the predicted fractional energy density $\Omega_\psi h^2$ are β−dependent, which relaxes the standard mass bound Σm_ν. For cold relics, by exactly solve the simplified Boltzmann equation in both relativistic and nonrelativistic regimes, we show that the Lee-Weinberg bound for the mass of heavy neutrinos can be considerably relaxed, and the "WIMP miracle" for weakly interacting massive particles (WIMPs) gradually invalidates as β deviates from $\beta = 1^+$. The whole framework reduces to become that of GR in the limit $\beta \to 1^+$.

PACS numbers 26.35.+c, 95.35.+d, 04.50.Kd
Key words thermal relics, dark matter, $f(R)$ gravity

10.1 Introduction

With the development of observational astrophysics and cosmology, the investigations of galaxy rotation curves, gravitational lensing and large scale structures have provided strong evidences for the existence and importance of dark matter. The abundance of dark matter has been measured with increasingly high precision, such as $\Omega_{\text{dm}}h^2 = 0.1198 \pm 0.0026$ by the latest Planck data (Planck Collaboration, 2015); however, since our knowledge of dark matter exclusively comes from the gravitational effects, the physical nature of dark-matter particles remain mysterious.

Nowadays it becomes a common view that to account for the observed dark matter, one needs to go beyond the $\text{SU}(3)_c\times\text{SU}(2)_W\times\text{U}(1)_Y$ minimal standard model. There are mainly two leading classes of dark-matter candidates: axions that are non-thermally produced via quantum phase transitions in the early universe, and generic weakly interacting massive particles (WIMPs) (Lee & Weinberg, 1977) that freeze out of thermal equilibrium from the very early cosmic plasma and leave a relic density matching the present-day Universe. In this paper, we are interested in the latter class, i.e. dark matter created as thermal relics. We aim to correct and complete the pioneering investigations in Kang & Panotopoulos (2009) for cold relics in $\mathscr{L} = m_{\text{Pl}}^{2-2\beta}R^\beta + 16\pi m_{\text{Pl}}^{-2}\mathscr{L}_m$ gravity, and provide a comprehensive investigation of thermal relics as hot, warm and cold dark matter in $\mathscr{L} = \varepsilon^{2-2\beta}R^\beta + 16\pi m_{\text{Pl}}^{-2}\mathscr{L}_m$ gravity.

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This paper is organized as follows. Sec. 10.2 sets up the gravitational framework of $\mathscr{L} = \varepsilon^{2-2\beta}R^{\beta} + 16\pi m_{\rm Pl}^{-2}\mathscr{L}_m$ gravity, while Sec. 10.3 generalizes the time-temperature relation for cosmic expansion and derives the simplified Boltzmann equation. Sec. 10.4 studies hot/warm thermal relics, and shows the influences of β and ε to the bound of light neutrino mass. Sec. 10.5 investigates cold thermal relics by solving the simplified Boltzmann equation, while Sec. 10.6 rederives the Lee-Weinberg bound on fourth-generation massive neutrinos, and examines the departure from electroweak energy scale. Finally, the GR limit of the whole theory is studied in Sec. 7.

Throughout this paper, for the physical quantities involved in the calculations of thermal relics, we use the natural unit system of particle physics which sets $c = \hbar = k_B = 1$ and is related to le système international d'unités by 1 MeV $= 1.16\times10^{10}$ kelvin $= 1.78\times10^{-30}$ kg $= (1.97\times10^{-13}$ meters$)^{-1} = (6.58\times10^{-22}$ seconds$)^{-1}$. On the other hand, for the spacetime geometry, we adopt the conventions $\Gamma^{\alpha}_{\beta\gamma} = \Gamma^{\alpha}{}_{\beta\gamma}$, $R^{\alpha}{}_{\beta\gamma\delta} = \partial_\gamma\Gamma^{\alpha}_{\delta\beta}\cdots$ and $R_{\mu\nu} = R^{\alpha}{}_{\mu\alpha\nu}$ with the metric signature $(-,+++)$.

10.2 Gravitational framework of power-law $f(R)$ gravity

In this paper, DM thermal relics will be studied for the Universe governed by the power-law-type $f(R)$ gravity, which is given by the action

$$\mathcal{I} = \int d^4x\sqrt{-g}\left(\varepsilon^{2-2\beta}R^{\beta} + 16\pi m_{\rm Pl}^{-2}\mathscr{L}_m\right), \tag{10.1}$$

where β = constant > 0, R denotes the Ricci scalar of the spacetime, and ε is some constant balancing the dimensions of the field equation (see Sec.2 of Tian (2015) for a more detailed setup). Also, $m_{\rm Pl}$ refers to the Planck mass, which is related to Newton's constant G by $m_{\rm Pl} := 1/\sqrt{G}$ and takes the value $m_{\rm Pl} \simeq 1.2209\times10^{22}$ MeV. Variation of the action with respect to the inverse metric, i.e. $\delta\mathcal{I}/\delta g^{\mu\nu} = 0$ yields the field equation

$$\beta R^{\beta-1}R_{\mu\nu} - \frac{1}{2}R^{\beta}g_{\mu\nu} + \beta\left(g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu\right)R^{\beta-1} = 8\pi\varepsilon^{2\beta-2}m_{\rm Pl}^{-2}\mathcal{T}_{\mu\nu}, \tag{10.2}$$

where $\Box$ denotes the covariant d'Alembertian $\Box := g^{\alpha\beta}\nabla_\alpha\nabla_\beta$, and the stress-energy-momentum tensor $\mathcal{T}_{\mu\nu}$ is defined by the matter Lagrangian density $\mathscr{L}_m$ via $\mathcal{T}_{\mu\nu} := \frac{-2}{\sqrt{-g}}\frac{\delta\left(\sqrt{-g}\mathscr{L}_m\right)}{\delta g^{\mu\nu}}$. For the physical matter in the Universe, we will assume a perfect-fluid description $\mathcal{T}^{\mu}{}_{\nu} = \text{diag}[-\rho, P, P, P]$, where ρ and P are respectively the energy density and the pressure, and $\rho = 3P$ in the radiation dominated era for DM decoupling.

On the other hand, in the (t, r, θ, φ) comoving coordinates, the flat Friedmann-Robertson-Walker (FRW) metric for the spatially homogeneous and isotropic Universe reads

$$g_{\mu\nu}dx^{\mu}dx^{\nu} = ds^2 = -dt^2 + a(t)^2dr^2 + a(t)^2r^2\left(d\theta^2 + \sin^2\theta d\varphi^2\right), \tag{10.3}$$

where $a(t)$ denotes the cosmic scale factor. Under the flat FRW metric, the energy-momentum conservation equation $\nabla^{\mu}\mathcal{T}_{\mu\nu} = 0$ gives rise to the continuity equation

$$\dot{\rho} + 3\frac{\dot{a}}{a}(\rho + P) = 0, \tag{10.4}$$

which integrates to yields $\rho = \rho_0\left(\frac{a_0}{a}\right)^4 \propto a^{-4}$ with the constants $\{\rho_0, a_0\}$ being the present-day values of the radiation density and scale factor. Substituting $\rho = \rho_0 \left(\frac{a_0}{a}\right)^4$ and Eq.(10.3) into Eq.(10.2), one obtains the exact solution

$$a = a_0 t^{\beta/2} \propto t^{\beta/2}\,, \quad H := \frac{\dot{a}}{a} = \frac{\beta}{2t}\,, \tag{10.5}$$

along with the generalized Friedmann equation

$$\left[\frac{12(\beta-1)}{\beta}H^2\right]^{\beta} \frac{(-5\beta^2+8\beta-2)}{\beta-1} = 32\pi\varepsilon^{2\beta-2} m_{\rm Pl}^{-2}\rho\,, \tag{10.6}$$

where overdot denotes the temporal derivative and H refers to the cosmic Hubble parameter. Moreover, the weak, strong and dominant energy conditions for classical matter fields require the energy density ρ to be positive definite, and consequently, the positivity of the left hand side of Eq.(10.6) limits β to the domain

$$1 < \beta < \frac{4+\sqrt{6}}{5} \lesssim 1.2899\,; \tag{10.7}$$

note that the Ricci scalar for the flat FRW metric with $a = a_0 t^{\beta/2}$ reads

$$R = 6\left(\frac{\ddot{a}}{a} + \frac{\dot{a}^2}{a^2}\right) = \frac{3\beta(\beta-1)}{t^2}\,, \tag{10.8}$$

so $R > 0$ and R^β is always well defined in this domain.

10.3 Thermal relics

10.3.1 Time-temperature relation of cosmic expansion

For the very early Universe, the radiation energy density ρ attributes to all relativistic species, which are exponentially greater than those of the nonrelativistic particles, and therefore $\rho = \sum \rho_i(\text{boson}) + \frac{7}{8}\sum \rho_j(\text{fermion}) = \sum \frac{\pi^2}{30} g_i^{(b)} T_i^4(\text{boson}) + \frac{7}{8}\sum \frac{\pi^2}{30} g_j^{(f)} T_j^4(\text{fermion})$, where $\{g_i^{(b)}, g_j^{(f)}\}$ are the numbers of statistical degrees of freedom for relativistic bosons and fermions, respectively. More concisely, normalizing the temperatures of all relativistic species with respect to photons' temperature $T_\gamma \equiv T$, one has the generalized Stefan-Boltzmann law

$$\rho = \frac{\pi^2}{30} g_* T^4 \qquad \text{with} \qquad g_* := \sum_{\text{boson}} g_i^{(b)} \left(\frac{T_i}{T}\right)^4 + \frac{7}{8}\sum_{\text{fermion}} g_j^{(f)} \left(\frac{T_j}{T}\right)^4\,, \tag{10.9}$$

where, in thermodynamic equilibrium, T is the common temperature of all relativistic particles. To facilitate the discussion of thermal relics, introduce a dimensionless variable

$$x := \frac{m_\Psi}{T} \tag{10.10}$$

to relabel the time scale, where m_Ψ denotes the mass of dark-matter particles. x is a well defined variable since the temperature monotonically decreases after the Big Bang: Reheatings due to pair annihilations at $T \gtrsim 0.5486$ MeV $= m(e^\pm)$ only slow down the decrement of T rather than increase T (Scherrer & Turner, 1986).

Substitute Eq.(10.9) into Eq.(10.6), and it follows that the cosmic expansion rate is related to the radiation temperature by

$$
\begin{aligned}
H &= \sqrt{\frac{\beta}{12(\beta-1)}}\left(\sqrt{\frac{(\beta-1)\,g_*}{-5\beta^2+8\beta-2}}\right)^{1/\beta}\left(\sqrt{\frac{32\pi^3}{30}}\frac{T^2}{m_{\rm Pl}}\right)^{1/\beta}\varepsilon^{1-\frac{1}{\beta}} \\
&= \sqrt{\frac{\beta}{12(\beta-1)}}\left(\sqrt{\frac{(\beta-1)\,g_*}{-5\beta^2+8\beta-2}}\right)^{1/\beta}\left(\sqrt{\frac{32\pi^3}{30}}\frac{m^2}{m_{\rm Pl}}\right)^{1/\beta}\varepsilon^{1-\frac{1}{\beta}}x^{-2/\beta},
\end{aligned}
\tag{10.11}
$$

which can be compactified into

$$
H = H(m)x^{-2/\beta} \quad \text{with} \quad H(m) \coloneqq H(T=m_\psi)\,. \tag{10.12}
$$

As time elapses after the Big Bang, the space expands and the Universe cools. Eq.(10.11) along with $H = \beta/(2t)$ leads to $t = \frac{\beta}{2H} = \frac{\beta x^{2/\beta}}{2H(m)}$ and the time-temperature relation

$$
\begin{aligned}
t &= \sqrt{3\beta(\beta-1)}\left(\sqrt{\frac{-5\beta^2+8\beta-2}{(\beta-1)\,g_*}}\right)^{1/\beta}\left(\sqrt{\frac{30}{32\pi^3}}\frac{m_{\rm Pl}}{T^2}\right)^{1/\beta}\varepsilon^{1/\beta-1} \\
&= \sqrt{3\beta(\beta-1)}\left(\sqrt{\frac{-5\beta^2+8\beta-2}{(\beta-1)\,g_*}}\right)^{1/\beta}\left(\sqrt{\frac{30}{32\pi^3}}\frac{m_{\rm Pl}}{m_\psi^2}\right)^{1/\beta}\varepsilon^{1/\beta-1}x^{2/\beta}.
\end{aligned}
\tag{10.13}
$$

In the calculations below, we will utilize two choices of ε to balance the dimensions in $\mathscr{L} = \varepsilon^{2-2\beta}R^\beta + 16\pi m_{\rm Pl}^{-2}\mathscr{L}_m$ gravity:

(i) $\varepsilon = 1$ [sec^{-1}]. This choice can best respect and preserve existent investigations in mathematical relativity for the $f(R)$ class of modified gravity, which have been analyzed for $\widetilde{\mathscr{L}} = f(R) + 16\pi m_{\rm Pl}^{-2}\mathscr{L}_m$ without caring the physical dimensions.

(ii) $\varepsilon = m_{\rm Pl} \simeq 0.1854\times 10^{44}$ [1/s], or $1/\ell_{\rm Pl}$ where $\ell_{\rm Pl} = \sqrt{G}$ refers to Planck length. The advantage of this choice is there is no need to employ extra parameters outside the mathematical expression $\widetilde{\mathscr{L}} = f(R) + 16\pi m_{\rm Pl}^{-2}\mathscr{L}_m$.

10.3.2 Boltzmann equation

For dark-matter particles ψ in the very early Universe (typically before the era of primordial nucleosynthesis), there are various types of interactions determining the ψ thermal relics, such as elastic scattering between ψ and standard-model particles, and self-annihilation $\psi+\psi \rightleftharpoons \psi+\psi+\cdots$. In this paper, we are interested in ψ initially in thermal equilibrium via the pair annihilation into (and creation from) standard-model particles $\ell = \gamma, e^\pm, \mu^\pm, \tau^\pm\cdots$,

$$
\psi + \bar{\psi} \rightleftharpoons \ell + \bar{\ell}\,. \tag{10.14}
$$

As the mean free path of ψ increases along the cosmic expansion, the interaction rate $\Gamma_{\psi\bar{\psi}}$ of Eq.(10.14) gradually falls below the Hubble expansion rate H, and the abundance of ψ freezes out. The number density of ψ satisfies the simplified Boltzmann equation

$$\dot{n}_\psi + 3Hn_\psi = -\langle\sigma v\rangle\left[n_\psi^2 - \left(n_\psi^{\rm eq}\right)^2\right], \tag{10.15}$$

where $\langle\sigma v\rangle$ is the thermally averaged cross-section. We employ the following quantity to describe the evolution of ψ at different temperature scales:

$$Y := \frac{n_\psi}{s} \propto \frac{n_\psi}{g_{*s}T^3}, \tag{10.16}$$

where s is the comoving entropy density $s := S/V$,

$$s = \sum_i \frac{\rho_i + P_i - \mu_i n_i}{T_i} \simeq \frac{2\pi^2}{45} g_{*s}T^3 \quad \text{with} \quad g_{*s} := \sum_{\text{boson}} g_i^{(b)}\left(\frac{T_i}{T}\right)^3 + \frac{7}{8}\sum_{\text{fermion}} g_j^{(f)}\left(\frac{T_j}{T}\right)^3. \tag{10.17}$$

Here we have applied $P_i = \rho_i/3$ and $\mu_i \ll T_i$ in s for relativistic matter, and g_{*s} denotes the entropic number of statistic degrees of freedom. According to the continuity equation Eq.(10.4) and the thermodynamic identities

$$\left.\frac{\partial P}{\partial T}\right|_\mu = s, \quad \left.\frac{\partial P}{\partial \mu}\right|_T = n, \tag{10.18}$$

one has

$$\frac{d(sa^3)}{dt} = -\frac{\mu}{T}\frac{d(na^3)}{dt}, \tag{10.19}$$

so the comoving entropy density sa^3 of a particle species is conserved when the comoving particle number density $n_\psi a^3$ is conserved or the chemical potential μ is far smaller than the temperature. Thus, $d(sa^3)/dt = 0 = a^3(\dot{s} + 3Hs)$, $\dot{s}/s = -3H$, and the time derivative of Y becomes

$$\frac{dY}{dt} = \frac{\dot{n}_\psi}{s} - \frac{\dot{s}}{s}Y = \frac{\dot{n}_\psi}{s} + 3HY = s^{-1}\left(\dot{n}_\psi + 3Hn_\psi\right). \tag{10.20}$$

Substitute the simplified Boltzmann equation (10.15) into Eq.(10.20), and one obtains

$$\frac{dY}{dt} = -s\langle\sigma v\rangle\left(Y^2 - Y_{\rm eq}^2\right). \tag{10.21}$$

Now rewrite dY/dt into dY/dx. Since

$$T = \left(\frac{30}{\pi^2 g_*}\rho\right)^{1/4} = \left\{\frac{30\varepsilon^{2-2\beta}m_{\rm Pl}^2(-5\beta^2 + 8\beta - 2)}{32\pi^3 g_*(\beta - 1)}\left[3\beta(\beta - 1)\right]^\beta\right\}^{1/4} t^{-\beta/2} \propto t^{-\beta/2}, \tag{10.22}$$

thus $\dot{T}/T = -\beta/(2t) = -H(t) = -H(x) = -H(m)x^{-2/\beta}$, and $\frac{dY}{dx}\frac{dx}{dT}\frac{dT}{dt} = \frac{dY}{dx}(-x)\frac{\dot{T}}{T} = \frac{dY}{dx}(-x)\left(-H(m)x^{-2/\beta}\right)$, which recast Eq.(10.21) into

$$\frac{dY}{dx} = -\frac{x^{\frac{2}{\beta}-1}}{H(m)}\langle\sigma v\rangle s\left(Y^2 - Y_{\rm eq}^2\right) = -\frac{\langle\sigma v\rangle s}{Hx}\left(Y^2 - Y_{\rm eq}^2\right). \tag{10.23}$$

Defining the annihilation rate of ψ as $\Gamma_\psi \coloneqq n_{\rm eq} \langle \sigma v \rangle$, then Eq.(10.23) can be rewritten into the form

$$\frac{x}{Y_{\rm eq}} \frac{dY}{dx} = -\frac{n_{\rm eq}}{H} \langle \sigma v \rangle \left[\left(\frac{Y}{Y_{\rm eq}} \right)^2 - 1 \right] = -\frac{\Gamma_\psi}{H} \left[\left(\frac{Y}{Y_{\rm eq}} \right)^2 - 1 \right] , \tag{10.24}$$

which will be very useful in calculating the freeze-out temperature of cold relics in Sec. 10.5.

10.4 Hot/warm relic dark matter and light neutrinos

10.4.1 Generic bounds on ψ mass

Having set up the modified cosmological dynamics and Boltzmann equations in $\mathscr{L} = \varepsilon^{2-2\beta} R^\beta + 16\pi m_{\rm Pl}^{-2} \mathscr{L}_m$ gravity, we will continue to investigate hot dark matter which is relativistic for the entire history of the Universe until now, and warm dark matter which is relativistic at the time of decoupling but become nonrelativistic nowadays.

In the relativistic regime $T \gg 3m_\psi$ or equivalently $0 < x \ll 3$, the abundance of m_ψ is given by

$$Y_{\rm eq} = Y_{\rm eq}^{\rm (R)} = \frac{45\zeta(3)}{2\pi^4} \frac{b_\psi g_\psi}{g_{*s}} \simeq 0.2777 \frac{b_\psi g_\psi}{g_{*s}} , \tag{10.25}$$

where $\zeta(3) = 1.20206$, $b_\psi = 1$ for bosons and $b_\psi = 3/4$ for fermions. $Y_{\rm eq}$ only implicitly depends on x through the evolution of g_{*s} along the temperature scale. Then, the relic abundance is still given by $Y_{\rm eq}$ at the time of freeze-out x_f:

$$Y_\infty \coloneqq Y(x \to \infty) = Y_{\rm eq}^{\rm (R)}(x_f) = 0.2777 \times \frac{b_\psi g_\psi}{g_{*s}(x_f)} . \tag{10.26}$$

At the present time with $T_{\rm cmb} = 2.7255\, K$ (Particle Data Group, 2015), the entropy density is

$$s_0 = \frac{2\pi^2}{45} g_{*s0} T_{\rm cmb}^3 = 2891.2 \text{ cm}^{-3} , \tag{10.27}$$

where in the minimal standard model with three generations of light neutrinos ($N_\nu = 3$),

$$g_{*s0} = 2 + \frac{7}{8} \times 2 \times N_\nu \times \left(\frac{T_{\nu 0}}{T_{\rm cmb}} \right)^3 \simeq 3.9091 . \tag{10.28}$$

Thus, the present-day number density and energy density of hot/warm relic ψ can be found by

$$n_{\psi 0} = s_0 Y_\infty = 802.8862 \times \frac{b_\psi g_\psi}{g_{*s}(x_f)} \text{ cm}^{-3} , \tag{10.29}$$

$$\rho_{\psi 0} = m_\psi n_{\psi 0} = 802.8862 \times \frac{b_\psi g_\psi}{g_{*s}(x_f)} \left(\frac{m_\psi}{\rm eV} \right) \frac{\rm eV}{\rm cm^3} , \tag{10.30}$$

which, for $\rho_{\rm crit} = 1.05375 \times 10^4\, h^2 \text{ eV/cm}^3$, correspond to the fractional energy density

$$\Omega_\psi h^2 = \frac{\rho_{\psi 0}}{\rho_{\rm crit}} h^2 \times \frac{b_\psi g_\psi}{g_{*s}(x_f)} \left(\frac{m_\psi}{\rm eV} \right) = 0.0762 \times \frac{b_\psi g_\psi}{g_{*s}(x_f)} \left(\frac{m_\psi}{\rm eV} \right) . \tag{10.31}$$

This actually stands for an attractive feature of the paradigm of thermal relics: the current abundance $\Omega_\psi h^2$ of relic dark matter (hot, warm, or cold) can be predicted by ψ's microscopic properties like mass, annihilation cross-section, and statistical degrees of freedom.

Since hot/warm relics can at most reach the total dark matter density $\Omega_\psi h^2 = 0.1198 \pm 0.0026$ (Particle Data Group, 2015), $\Omega_\psi h^2$ has to satisfy $\Omega_\psi h^2 \lesssim 0.1198$, and it follows from Eq.(10.31) that m_ψ is limited by the upper bound

$$m_\psi \lesssim 1.5723 \times \frac{g_{*s}(x_f)}{b_\psi g_\psi}\ \mathrm{eV}\,. \tag{10.32}$$

Moreover, particles of warm dark matter become nonrelativistic at present time, which imposes a lower bound to m_ψ,

$$m_\psi \gtrsim T_{\psi 0} = T_{\psi f}\frac{a_f}{a_0} = \left(\frac{g_{*s0}}{g_{*s}(x_f)}\right)^{1/3} T_{\mathrm{cmb}} = 2.3496 \times 10^{-4} \times \left(\frac{3.9091}{g_{*s}(x_f)}\right)^{1/3}\ \mathrm{eV}\,, \tag{10.33}$$

where we have applied $g_{*s}^{1/3} aT = \text{constant}$ due to $sa^3 = \text{constant}$. Eqs.(10.32) and (10.33) lead to the mass bound for warm relics that

$$2.3496 \times 10^{-4} \times \left(\frac{3.9091}{g_{*s}(x_f)}\right)^{1/3} \lesssim \frac{m_\psi}{\mathrm{eV}} \lesssim 1.5723 \times \frac{g_{*s}(x_f)}{b_\psi g_\psi}\,. \tag{10.34}$$

10.4.2 Example: light neutrinos as hot relics

Light neutrinos are the most popular example of hot/warm dark matter (Lesgourgues & Pastor, 2006). One needs to figure out the temperature T_f^ν and thus $g_{*s}(T = T_f^\nu)$ when neutrinos freeze out from the cosmic plasma. The decoupling occurs when the Hubble expansion rate H balances neutrinos' interaction rate Γ_ν. For the cosmic expansion, it is convenient to write Eq.(10.11) into

$$H = 0.2887 \times \sqrt{\frac{\beta}{\beta-1}} \times \left(\sqrt{\frac{(\beta-1)\,g_*}{-5\beta^2+8\beta-2}}\right)^{1/\beta} \left(0.7164 \cdot T_{\mathrm{MeV}}^2\right)^{1/\beta} \varepsilon_s^{\,1-\frac{1}{\beta}}\ [1/\mathrm{s}]\,, \tag{10.35}$$

where T_{MeV} refers to the value of temperature in the unit of MeV, $T = T_{\mathrm{MeV}} \times\ [1\,\mathrm{MeV}]$, ε_s is the value of ε in the unit of [1/s], and numerically $T^2/m_{\mathrm{Pl}} = T_{\mathrm{MeV}}^2/8.0276$ [1/s].

On the other hand, the event of neutrino decoupling actually indicates the beginning of primordial nucleosynthesis, when neutrinos are in chemical and kinetic equilibrium with photons, nucleons and electrons via weak interactions and elastic scattering. The interaction rate Γ_ν is (Kolb & Turner, 1990)

$$\Gamma_\nu \simeq 1.3 G_F^2 T^5 \simeq 0.2688\, T_{\mathrm{MeV}}^5\ [1/\mathrm{s}]\,, \tag{10.36}$$

where G_F is Fermi's constant in beta decay and generic weak interactions, and $G_F = 1.1664 \times 10^{-11}\mathrm{MeV}^{-2}$. Neutrinos decouple when $\Gamma_\nu = H$, and according to Eqs.(10.35) and (10.36), the weak freeze-out temperature T_ν^f is the solution to

$$T_{\mathrm{MeV}}^{5-2/\beta} = 1.0741 \times \sqrt{\frac{\beta}{\beta-1}} \times \left(0.7164 \cdot \sqrt{\frac{(\beta-1)\,g_*}{-5\beta^2+8\beta-2}}\right)^{1/\beta} \varepsilon_s^{1-1/\beta}\,. \tag{10.37}$$

Figs. 10.1 and 10.2 have shown the dependence of T_ν^f on β for $\varepsilon = 1\ \mathrm{sec}^{-1} = 6.58 \times 10^{-22}$ MeV and $\varepsilon = m_{\rm Pl} = 1.2209 \times 10^{-22}$ MeV, respectively. Fig. 10.2 clearly illustrates that T_ν^f spreads from 1.3030 MeV to over 1000 MeV, which goes far beyond the scope of $1 \sim 10$ MeV; thus, as shown in Table 10.1, g_{*s} varies and the mass bound Σm_ν in light of Eq.(10.34) is both $\beta-$dependent and $\varepsilon-$dependent.

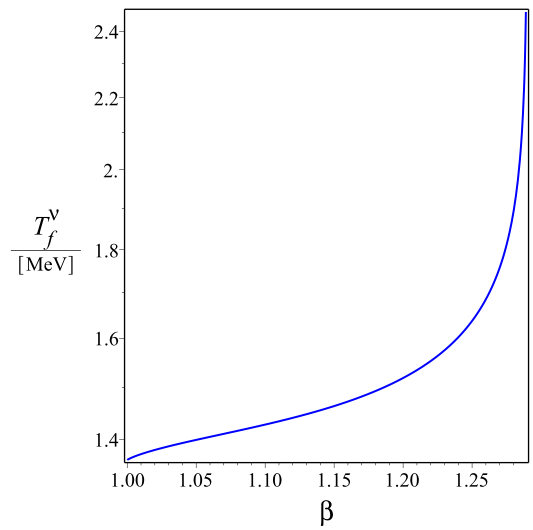

Figure 10.1: T_ν^f (in MeV) for $\varepsilon = 1\ \mathrm{sec}^{-1} = 6.58 \times 10^{-22}$ MeV

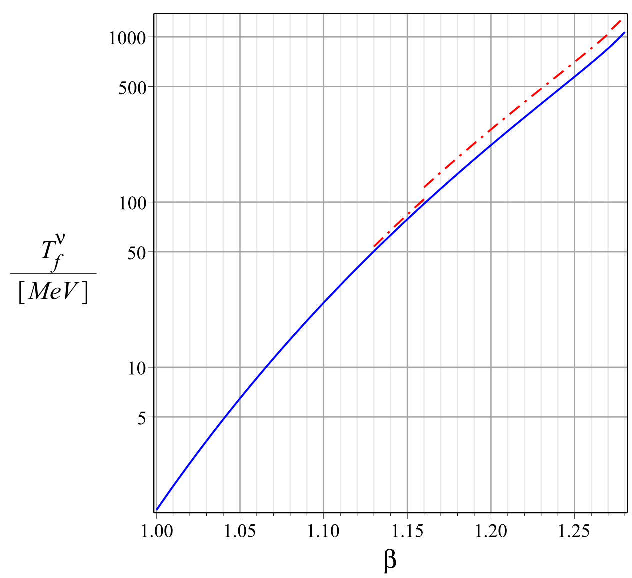

Figure 10.2: T_ν^f (in MeV) for $\varepsilon = m_{\rm Pl} = 1.2209 \times 10^{-22}$ MeV

10.5 Cold relic dark matter

Now let's consider cold dark matter which is already nonrelativistic at the time of decoupling. In the nonrelativistic regime $T \ll 3m_\psi$ or equivalently $x \gg 3$, the number density and entropy density are given by

Table 10.1: g_{*s} for the T_f^γ in Fig. 10.2, based on the data of Particle Data Group. Note that between 100~200 MeV, g_{*s} is also subject to the phase transition of quantum chromodynamics for strange quarks.

Temperature	Temperature (in MeV)	g_{*s}
$m_e < T < m_s$ (strange)	$0.5110 < T < 95$	43/4
$m_s < T < m_\mu$	$95 < T < 105.6584$	57/4
$m_\mu < T < m_\pi$	$105.6584 < T < 134.9766$	69/4
$m_\pi < T < T_c$	$134.9766 < T < T_c$	205/4
$T_c < T < m_c$ (charm)	$T_c < T < 1275$	247/4
$m_c < T < m_\tau$	$1275 < T < 1776.82$	289/4
$m_\tau < T < m_b$ (bottom)	$1776.82 < T < 4180$	303/4

$$n_\psi = g_\psi \left(\frac{m_\psi^2}{2\pi}\right)^{3/2} x^{-3/2} e^{-x}\,, \qquad s = \frac{2\pi^2}{45} g_{*s} m_\psi^3 x^{-3} = s(m)\, x^{-3}\,, \tag{10.38}$$

so one obtains the equilibrium abundance of nonrelativistic ψ particles

$$Y_{\rm eq} = Y_{\rm eq}^{\rm (NR)} = \frac{45}{4\pi^4}\left(\frac{\pi}{2}\right)^{1/2} \frac{g_\psi}{g_{*s}} x^{3/2} e^{-x} \simeq 0.1447 \times \frac{g_\psi}{g_{*s}} x^{3/2} e^{-x}\,. \tag{10.39}$$

Thus, n_ψ and $Y_{\rm eq} = Y_{\rm eq}^{\rm (NR)}$ are exponentially suppressed when the temperature drops below m_ψ. Moreover, since cold relics are nonrelativistic when freezing out, one can expand the thermally averaged cross-section by $\langle\sigma v\rangle = c_0 + c_1 v^2 + c_2 v^4 + \cdots + c_q v^{2q} + \cdots$, where c_0 corresponds to the decay channel of $s-$wave, c_1 to $p-$wave, c_2 to $d-$wave, and so forth; recalling that $\langle\sigma v\rangle \sim \sqrt{T}$ in light of the Boltzmann velocity distribution, thus the annihilation cross-section can be expanded by the variable x into

$$\langle\sigma v\rangle = \langle\sigma v\rangle_0\, x^{-n} \quad \text{with} \quad n = q/2\,. \tag{10.40}$$

Then the Boltzmann equation (10.23) becomes

$$\frac{dY}{dx} = -\frac{s(m)\,\langle\sigma v\rangle_0}{H(m)} x^{\frac{2}{\beta}-4-n}\left(Y^2 - Y_{\rm eq}^2\right) = -\frac{s(m)\,\langle\sigma v\rangle_0}{H(m)} x^{\frac{2}{\beta}-4-n}\left[Y^2 - 0.0209\left(\frac{g_\psi}{g_{*s}}\right)^2 x^3 e^{-2x}\right], \tag{10.41}$$

where

$$\frac{s(m)\,\langle\sigma v\rangle_0}{H(m)} = \frac{1.519525}{(5.750944)^{1/\beta}} \sqrt{\frac{\beta-1}{\beta}} \left(\sqrt{\frac{-5\beta^2+8\beta-2}{\beta-1}}\right)^{1/\beta} \frac{g_{*s}}{(\sqrt{g_*})^{1/\beta}}\, \varepsilon^{\frac{1}{\beta}-1}\, m^{3-\frac{2}{\beta}}\, m_{\rm Pl}^{1/\beta} \,\langle\sigma v\rangle_0\,. \tag{10.42}$$

Though initially in equilibrium $Y \approx Y_{\rm eq} = Y_{\rm eq}^{\rm (NR)}$, the actual abundance Y gradually departures from the equilibrium value $Y_{\rm eq}^{\rm (NR)}$ as the temperature decreases; Y freezes out and escapes the exponential Boltzmann suppression when the interaction rate Γ_ψ equates the cosmic expansion rate H. Transforming Eq.(10.41) into the form

$$\frac{x}{Y_{\rm eq}}\frac{dY}{dx} = -\frac{s(m)\,\langle\sigma v\rangle_0}{H(m)}Y_{\rm eq}\left[\left(\frac{Y}{Y_{\rm eq}}\right)^2 - 1\right]x^{\frac{2}{\beta}-3-n} = -\frac{\Gamma_\psi}{H}\left[\left(\frac{Y}{Y_{\rm eq}}\right)^2 - 1\right], \tag{10.43}$$

and the coupling condition $\Gamma_\psi(x_f) = H(x_f)$ at the freeze-out temperature $T_f^\psi = m_\psi/x_f$ yields

$$\frac{\Gamma_\psi}{H}(x_f) = 1 = \frac{s(m)\,\langle\sigma v\rangle_0}{H(m)}Y_{\rm eq}x^{\frac{2}{\beta}-3-n} \simeq 0.1447\frac{s(m)\,\langle\sigma v\rangle_0}{H(m)}\frac{g_\psi}{g_{*s}}x^{\frac{2}{\beta}-3/2-n}e^{-x}\,. \tag{10.44}$$

Thus, it follows that

$$\begin{aligned} e^{x_f} &= 0.1447\frac{s(m)\,\langle\sigma v\rangle_0}{H(m)}\frac{g_\psi}{g_{*s}}x^{\frac{2}{\beta}-3/2-n} \\ &= \frac{0.2199}{(5.7509)^{1/\beta}}\sqrt{\frac{\beta-1}{\beta}}\left(\sqrt{\frac{-5\beta^2+8\beta-2}{\beta-1}}\right)^{1/\beta}\frac{g_\psi}{(\sqrt{g_*})^{1/\beta}}\,\varepsilon^{\frac{1}{\beta}-1}\,m^{3-\frac{2}{\beta}}\,m_{\rm Pl}^{1/\beta}\,\langle\sigma v\rangle_0\,x_f^{\frac{2}{\beta}-3/2-n}\,. \end{aligned} \tag{10.45}$$

After taking the logarithm of both side, Eq.(10.45) can be iteratively solved to obtain

$$\begin{aligned} x_f =& \ln\left[\frac{0.2199}{(5.7509)^{1/\beta}}\sqrt{\frac{\beta-1}{\beta}}\left(\sqrt{\frac{-5\beta^2+8\beta-2}{\beta-1}}\right)^{1/\beta}\frac{g_\psi}{(\sqrt{g_*})^{1/\beta}}\,\varepsilon^{\frac{1}{\beta}-1}\,m^{3-\frac{2}{\beta}}\,m_{\rm Pl}^{1/\beta}\,\langle\sigma v\rangle_0\right] \\ &+\left(\frac{2}{\beta}-\frac{3}{2}-n\right)\ln\left[\ln\left(\frac{0.2199}{(5.7509)^{1/\beta}}\sqrt{\frac{\beta-1}{\beta}}\left(\sqrt{\frac{-5\beta^2+8\beta-2}{\beta-1}}\right)^{1/\beta}\frac{g_\psi}{(\sqrt{g_*})^{1/\beta}}\,\varepsilon^{\frac{1}{\beta}-1}\,m^{3-\frac{2}{\beta}}\,m_{\rm Pl}^{1/\beta}\,\langle\sigma v\rangle_0\right)\right] \\ &+\left(\frac{2}{\beta}-\frac{3}{2}-n\right)\ln\Big[\cdots\cdots\Big], \end{aligned} \tag{10.46}$$

where g_* has been treated as a constant, as the time scale over which g_* evolves is much greater than the time interval near x_f.

10.5.1 Abundance Y before freeze-out

To work out the actual abundance Y before the decoupling of ψ, employ a new quantity $\Delta := Y - Y_{\rm eq}$, and then Eq.(10.41) can be recast into

$$\frac{d\Delta}{dx} = -\frac{s(m)\,\langle\sigma v\rangle_0}{H(m)}x^{\frac{2}{\beta}-4-n}\Delta\left(\Delta + 2Y_{\rm eq}\right) - \frac{dY_{\rm eq}}{dx}\,. \tag{10.47}$$

In the high-temperature regime $x \ll x_f$ before ψ freezes out, Y is very close to $Y_{\rm eq}$, so that $\Delta \ll Y_{\rm eq}$ and $d\Delta/dx \ll -dY_{\rm eq}/dx$. With $Y_{\rm eq} = Y_{\rm eq}^{\rm (NR)}$ in Eq.(10.39), Eq.(10.47) can be algebraically solved to obtain

$$\Delta = -\frac{dY_{\rm eq}}{dx}\frac{H(m)}{s(m)\,\langle\sigma v\rangle_0}\frac{x^{n+4-\frac{2}{\beta}}}{2Y_{\rm eq}+\Delta} = \left(1-\frac{3}{2x}\right)\frac{H(m)}{s(m)\,\langle\sigma v\rangle_0}\frac{x^{n+4-\frac{2}{\beta}}}{2+Y_{\rm eq}/\Delta} \simeq \left(1-\frac{3}{2x}\right)\frac{H(m)}{2s(m)\,\langle\sigma v\rangle_0}x^{n+4-\frac{2}{\beta}}, \tag{10.48}$$

and consequently

$$
\begin{aligned}
Y = \Delta + Y_{\rm eq} &= \left(1 - \frac{3}{2x}\right) \frac{H(m)}{s(m)\,\langle\sigma v\rangle_0} \frac{x^{n+4-\frac{2}{\beta}}}{2 + Y_{\rm eq}/\Delta} + \frac{45}{4\pi^4}\left(\frac{\pi}{2}\right)^{1/2} \frac{g_\Psi}{g_{*s}} x^{3/2} e^{-x} \\
&\simeq \left(1 - \frac{3}{2x}\right) \frac{H(m)}{2s(m)\,\langle\sigma v\rangle_0} x^{n+4-\frac{2}{\beta}} + 0.1447 \times \frac{g_\Psi}{g_{*s}} x^{3/2} e^{-x}\,.
\end{aligned}
\tag{10.49}
$$

10.5.2 Freeze-out abundance Y_∞

After the decoupling of ψ particles, the actual number density n_Ψ becomes much bigger than the ideal e-quilibrium value $n_\Psi^{\rm eq}$. One has $Y \gg Y_{\rm eq}$, $Y \approx \Delta$, and the differential equations (10.41) or (10.47) leads to

$$
\frac{dY}{dx} = -\frac{s(m)\,\langle\sigma v\rangle_0}{H(m)} x^{\frac{2}{\beta}-4-n}\, Y^2 \quad \text{or} \quad \frac{dY}{dx} = -\frac{s(m)\,\langle\sigma v\rangle_0}{H(m)} x^{\frac{2}{\beta}-4-n}\, Y^2\,,
\tag{10.50}
$$

which integrates to yield the freeze-out abundance $Y_\infty := Y(x = x_f) \approx Y(x \to \infty)$ that

$$
\begin{aligned}
Y_\infty &= \left(3 + n - \frac{2}{\beta}\right) \frac{H(m)}{s(m)\,\langle\sigma v\rangle_0} x_f^{3+n-\frac{2}{\beta}} \\
&= \frac{\left(3 + n - \frac{2}{\beta}\right) x_f^{3+n-\frac{2}{\beta}}}{\frac{1.5195}{(5.7509)^{1/\beta}} \sqrt{\frac{\beta-1}{\beta}} \left(\sqrt{\frac{-5\beta^2+8\beta-2}{\beta-1}}\right)^{1/\beta} \frac{g_{*s}}{(\sqrt{g_*})^{1/\beta}}\, \varepsilon^{\frac{1}{\beta}-1}\, m^{3-\frac{2}{\beta}}\, m_{\rm Pl}^{1/\beta} \,\langle\sigma v\rangle_0}\,.
\end{aligned}
\tag{10.51}
$$

Following Y_∞, the number density and energy density of ψ are directly are directly found to be

$$
n_{\Psi 0} = s_0 Y_\infty = \frac{2891.2 \left(3 + n - \frac{2}{\beta}\right) x_f^{3+n-\frac{2}{\beta}}}{\frac{1.5195}{(5.7509)^{1/\beta}} \sqrt{\frac{\beta-1}{\beta}} \left(\sqrt{\frac{-5\beta^2+8\beta-2}{\beta-1}}\right)^{1/\beta} \frac{g_{*s}}{(\sqrt{g_*})^{1/\beta}}\, \varepsilon^{\frac{1}{\beta}-1}\, m^{3-\frac{2}{\beta}}\, m_{\rm Pl}^{1/\beta} \,\langle\sigma v\rangle_0}\ {\rm cm}^{-3}\,,
\tag{10.52}
$$

$$
\rho_{\Psi 0} = m_\Psi n_{\Psi 0} = \frac{2891.2 \left(3 + n - \frac{2}{\beta}\right) x_f^{3+n-\frac{2}{\beta}}}{\frac{1.5195}{(5.7509)^{1/\beta}} \sqrt{\frac{\beta-1}{\beta}} \left(\sqrt{\frac{-5\beta^2+8\beta-2}{\beta-1}}\right)^{1/\beta} \frac{g_{*s}}{(\sqrt{g_*})^{1/\beta}}\, \varepsilon^{\frac{1}{\beta}-1}\, m^{2-\frac{2}{\beta}}\, m_{\rm Pl}^{1/\beta} \,\langle\sigma v\rangle_0}\ \frac{\rm eV}{{\rm cm}^3}\,,
\tag{10.53}
$$

which gives rise to the fractional energy density

$$
\Omega_\psi h^2 = \frac{\rho_{\Psi 0}}{\rho_{\rm crit}} h^2 = \frac{2743.7248 \left(3 + n - \frac{2}{\beta}\right) x_f^{3+n-\frac{2}{\beta}}}{\frac{1.5195}{(5.7509)^{1/\beta}} \sqrt{\frac{\beta-1}{\beta}} \left(\sqrt{\frac{-5\beta^2+8\beta-2}{\beta-1}}\right)^{1/\beta} \frac{g_{*s}}{(\sqrt{g_*})^{1/\beta}}\, \varepsilon^{\frac{1}{\beta}-1}\, m^{2-\frac{2}{\beta}}\, m_{\rm Pl}^{1/\beta} \,\langle\sigma v\rangle_0}\,.
\tag{10.54}
$$

Unlike Eq.(10.31) for hot/warm relics, the relic density $\Omega_\psi h^2$ for cold dark matter is not only much more sensitive to the temperature of cosmic plasma, but also relies on the annihilation cross-section.

10.6 Example: Fourth generation massive neutrinos and Lee-Weinberg bound

An example of cold relics can be the hypothetical fourth generation massive neutrinos (Lee & Weinberg, 1977, Kolb & Olive, 1986, Lesgourgues & Pastor, 2006). For the Dirac-type neutrinos whose annihilations are dominated by $s-$wave ($n = 0$), the interaction cross-section reads

$$\langle \sigma v \rangle_0 \simeq G_F^2 m^2 = 1.3604 \times 10^{-10} \left(\frac{m_\Psi}{\text{GeV}} \right)^2 \ \text{GeV}^{-2} \tag{10.55}$$

where G_F is Fermi's constant in beta decay and generic weak interactions, and $G_F = 1.16637 \times 10^{-5}\text{GeV}^{-2}$. Then with $g_\Psi = 2$ and $g_* \sim 60$, the neutrinos decouple at

$$\begin{aligned} \tilde{x}_f = & \ln \left[\frac{0.5983 \times 10^{-10}}{(44.5463)^{1/\beta}} \sqrt{\frac{\beta - 1}{\beta}} \left(\sqrt{\frac{-5\beta^2 + 8\beta - 2}{\beta - 1}} \right)^{1/\beta} \varepsilon^{\frac{1}{\beta}-1} m^{5-\frac{2}{\beta}} m_{\text{Pl}}^{1/\beta} \right] \\ & + \left(\frac{2}{\beta} - \frac{3}{2} - n \right) \ln \left[\ln \left(\frac{0.5983 \times 10^{-10}}{(44.5463)^{1/\beta}} \sqrt{\frac{\beta - 1}{\beta}} \left(\sqrt{\frac{-5\beta^2 + 8\beta - 2}{\beta - 1}} \right)^{1/\beta} \varepsilon^{\frac{1}{\beta}-1} m^{5-\frac{2}{\beta}} m_{\text{Pl}}^{1/\beta} \right) \right] \\ & + \left(\frac{2}{\beta} - \frac{3}{2} - n \right) \ln \left[\cdots\cdots \right], \end{aligned} \tag{10.56}$$

which, through Eq.(10.57), gives rise to the fractional energy density

$$\Omega_\psi h^2 = \frac{\rho_{\Psi 0}}{\rho_{\text{crit}}} h^2 = \frac{2743.7248 \times 10^{10} \times \left(3 + n - \frac{2}{\beta}\right) \tilde{x}_f^{3+n-\frac{2}{\beta}}}{\frac{0.5983}{(44.5463)^{1/\beta}} \sqrt{\frac{\beta-1}{\beta}} \left(\sqrt{\frac{-5\beta^2+8\beta-2}{\beta-1}} \right)^{1/\beta} \varepsilon^{\frac{1}{\beta}-1} m^{5-\frac{2}{\beta}} m_{\text{Pl}}^{1/\beta}} . \tag{10.57}$$

With the same amount of anti-particles, we finally have $\Omega_{\Psi\bar{\Psi}0} h^2 = 2\Omega_\psi h^2 \lesssim 0.1198$. Thus the Lee-Weinberg bound (Lee & Weinberg, 1977, Kolb & Olive, 1986) for massive neutrinos are relaxed in $\mathscr{L} = \varepsilon^{2-2\beta} R^\beta + 16\pi m_{\text{Pl}}^{-2} \mathscr{L}_m$ gravity.

10.7 Conclusions

In this paper, we have comprehensively investigated the thermal relics as hot, warm and cold dark matter in $\mathscr{L} = \varepsilon^{2-2\beta} R^\beta + 16\pi m_{\text{Pl}}^{-2} \mathscr{L}_m$ gravity. When light neutrinos act as hot and warm neutrinos, the upper limit of neutrino mass Σm_ν relies on the value of β and the choice of ε. For cold relics, we have derived the freeze-out temperature $T_f = m/x_f$ in Eq.(10.46), Y before the freeze-out in Eq.(10.49), the freeze-out value Y_∞ in Eq.(10.51), and the dark-matter fractional density $\Omega_\psi h^2$ in Eq.(10.57). Note that we focused on power-law $f(R)$ gravity because unlike the approximated power-law ansatz $a = a_0 t^\alpha$ ($\alpha =$ constant > 0) for generic $f(R)$ gravity, $a = a_0 t^{\beta/2}$ is an exact solution to $\mathscr{L} = \varepsilon^{2-2\beta} R^\beta + 16\pi m_{\text{Pl}}^{-2} \mathscr{L}_m$ gravity for the radiation-dominated Universe; for GR with $\beta \to 1^+$, Eq.(10.5) reduces to recover the behavior $a \propto t^{1/2}$ which respects $3\dot{a}^2/a^2 = -8\pi m_{\text{Pl}}^{-2} \rho_0 a^{-4}$.

When light neutrinos serve as hot/warm relics, the entropic number of statistical degrees of freedom g_{*s} at freeze-out and thus the predicted fractional energy density $\Omega_\Psi h^2$ are $\beta-$dependent, which relaxes the standard mass bound Σm_ν. For cold relics, by exactly solve the simplified Boltzmann equation in both relativistic and nonrelativistic regimes, we show that the Lee-Weinberg bound for the mass of heavy neutrinos can be considerably relaxed, and the "WIMP miracle" for weakly interacting massive particles (WIMPs) gradually becomes invalid when β departs $\beta = 1^+$. The whole framweork reduces to become that of GR in the limit

$\beta \to 1^+$.

Acknowledgement

This work was supported by NSERC grant 261429-2013.

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Chapter 11

Summary and prospective research

Based on the concordant observations from high-redshift type-Ia supernovae, galaxy clusters, and cosmic microwave anisotropy, an amazing fact has been established that the Universe is undergoing accelerated expansion. Within general relativity and in light of the second Friedmann equation $\frac{\ddot{a}}{a} = -\frac{4\pi G}{3}(\rho + 3P)$, the Universe must be dominated by some exotic dark energy with large negative pressure that violate the standard energy conditions. Quite a few models of dark energy have been developed, such as the cosmological constant Λ with the equation of state parameter $w = -1$, extra scalar fields (quintessence $-1 < w < -1/3$, phantom $w < -1$, quintom), generalized Chaplygin gas, and phenomenological modifications of Friedmann equations. However, to date our knowledge of dark energy solely comes from the gravitational consequences at large cosmic scales, and its nature in particle physics is totally mysterious.

Alternatively, instead of considering dark energy, one can go beyond the gravitational framework of general relativity, explaining the cosmic acceleration and reconstructing the entire expansion history in modified theories of relativistic gravity. Such modified gravities actually encode the possible ways to go beyond Lovelock's theorem and its necessary conditions, which limit the second-order field equation in four dimensions to $R_{\mu\nu} - Rg_{\mu\nu}/2 + \Lambda g_{\mu\nu} = 8\pi G T^{(\mathrm{m})}_{\mu\nu}$, i.e. Einstein's equation supplemented by the cosmological constant. These directions can allow for, for example, fourth and even higher order gravitational field equations like $f(R)$ gravity, more than four spacetime dimensions like Gauss-Bonnet and Lovelock gravities, extensions of pure pseudo-Riemannian geometry and metric gravity like Einstein-Cartan and teleparallel gravities, extra physical degrees of freedom like Brans-Dicke and Chern-Simmons gravities, and nonminimal curvature-matter couplings like $f(R, \mathscr{L}_m)$ gravity.

This thesis studied the theories and phenomenology of modified gravity, along with the applications in cosmology, astrophysics, and effective dark energy. To begin with, Chapter 1 has reviewed the fundamentals of general relativity, dark energy, modified gravity, the standard ΛCDM model, and observational cosmology. These are the preparations for the discussion in Chapters 3~10.

Chapter 3 has proposed the $\mathscr{L} = f(R, R_c^2, R_m^2, \mathscr{L}_m)$ class of modified gravity that allows for nonminimal matter-curvature couplings ($R_c^2 := R_{\mu\nu}R^{\mu\nu}$, $R_m^2 := R_{\mu\alpha\nu\beta}R^{\mu\alpha\nu\beta}$). This framework unifies most of existing fourth-order gravities. When the "coherence condition" $f_{R^2} = f_{R_m^2} = -f_{R_c^2}/4$ is satisfied for explicit R^2−dependence, it has a smooth limit to the $f(R, \mathcal{G}, \mathscr{L}_m)$ generalized Gauss-Bonnet gravity. Furthermore, it is promoted to the $f(R, \mathcal{R}_1, \ldots, \mathcal{R}_n, \mathscr{L}_m)$ theory to investigate the stress-energy-momentum conservation, and conjectured that $f_{\mathscr{L}_m}\nabla^\mu T^{(m)}_{\mu\nu} = (\mathscr{L}_m g_{\mu\nu} - T^{(m)}_{\mu\nu})\nabla^\mu f_{\mathscr{L}_m}$. Also, the equations of nongeodesic motions, the generalized energy conditions and their consequences on black holes, the conditions to maintain traversable wormholes by nonminimal couplings, the $\mathscr{L} = f(R, R_c^2, R_m^2, T^{(m)})$ gravity which contains $f(R, \mathcal{G}, T^{(m)})$, are all discussed.

Chapter 4 has developed a unified formulation to derive the Friedmann equations from (non)equilibrium thermodynamics for modified gravities $R_{\mu\nu} - Rg_{\mu\nu}/2 = 8\pi G_{\text{eff}} T^{(\text{eff})}_{\mu\nu}$, and applied this formulation to the Friedman-Robertson-Walker Universe governed by $f(R)$, generalized Brans-Dicke, scalar-tensor-chameleon, quadratic, $f(R,\mathcal{G})$ generalized Gauss-Bonnet and dynamical Chern-Simons gravities. Ref.[3] extended Hayward's unified first law from equilibrium to nonequilibrium thermodynamics, found out the evolution of the effective gravitational coupling strength $\dot{G}_{\text{eff}}$ as the only source of irreversible energy dissipation and entropy production, and generalized the Hawking and the Misner-Sharp masses. Moreover, a self-inconsistency of $f(R,\mathcal{G})$ gravity due to the non-uniqueness of G_{eff} is discovered.

Chapter 5 has systematically restudied the thermodynamics of the Universe in ΛCDM and modified gravities by requiring its compatibility with the holographic-style gravitational equations. Possible solutions to the long-standing confusions regarding the temperature of the cosmological apparent horizon and the failure of the second law of thermodynamics in cosmology are proposed. We concluded that the Cai-Kim temperature is more suitable than Hayward-Kodama, and both temperatures are independent of the inner or outer trappedness. Moreover, the Cai-Kim-Clausius equation $T_{\text{A}} dS_{\text{A}} = -A_{\text{A}} \boldsymbol{\psi}_t$ encodes the *positive heat out* sign convention, which adjusts the traditional positive-heat-in Gibbs equation of laboratory thermodynamics into $dE_m = -T_m dS_m - P_m dV$. This way, it is also shown that the Bekenstein-Hawking and Wald entropies only apply to the apparent horizon, the phantom dark energy is less favored than the cosmological constant and the quintessence from a thermodynamic perspective, the artificial "local equilibrium assumption" can be abandoned, the apparent horizon is a natural infrared cutoff for holographic dark energy for the late-time Universe, and an existing model of QCD ghost dark energy fails to carry positive energy density.

Chapter 6, inspired by Lovelock's theorem, has proposed the Lovelock-Brans-Dicke theory of alternative gravity with $\mathscr{L}_{\text{LBD}} = \frac{1}{16\pi}\left[\phi\left(R + \frac{a}{\sqrt{-g}}{}^*RR + b\mathcal{G}\right) - \frac{\omega_{\text{L}}}{\phi}\nabla_\alpha\phi\nabla^\alpha\phi\right]$, where ${}^*RR$ and $\mathcal{G}$ respectively denote the topological Chern-Pontryagin and Gauss-Bonnet invariants. This theory reduces to general relativity in the limit $\omega_{\text{L}} \to \infty$ unless the "topological balance condition" holds, it can be conformally transformed into dynamical Chern-Simons gravity and Gauss-Bonnet dark energy, and allows for the late-time cosmic acceleration without dark energy. Furthermore, LBD gravity is generalized into the Lovelock-scalar-tensor gravity, and its equivalence to fourth-order modified gravities is established. As a quick application of Chapter 6, Chapter 7 has looked into traversable wormholes and energy conditions in Lovelock-Brans-Dicke gravity, along with an extensive comparison to wormholes in Brans-Dicke gravity.

Chapter 8, for a large class of scalar-tensor-like gravity $\mathcal{S} = \int d^4x\sqrt{-g}\left(\mathscr{L}_{\text{HE}} + \mathscr{L}_{\text{G}} + \mathscr{L}_{\text{NC}} + \mathscr{L}_\phi\right) + \mathcal{S}_m$ whose action contains nonminimal couplings between a scalar field $\phi(x^\alpha)$ and generic curvature invariants $\{\mathcal{R}\}$ beyond the Ricci scalar, has proved the local energy-momentum conservation and introduced the "Weyl/-conformal dark energy".

Chapter 9 has investigated the primordial nucleosynthesis in $\mathscr{L} = \varepsilon^{2-2\beta}R^\beta + 16\pi m_{Pl}^{-2}\mathscr{L}_m$ gravity. From the semianalytical approach, the influences of β to the decoupling of neutrinos, the freeze-out temperature and concentration of nucleons, the opening of deuterium bottleneck, and the ^{4}He abundance are all extensively analyzed; then β is constrained to $1 < \beta < 1.05$ for $\varepsilon = 1$ [1/s] and $1 < \beta < 1.001$ for $\varepsilon = m_{Pl}$ (Planck mass), which correspond to the extra number of neutrino species $0 < \Delta N_\nu^{\text{eff}} \leq 0.6296$ and $0 < \Delta N_\nu^{\text{eff}} \leq 0.0123$, respectively. Supplementarily, abundances of the lightest elements (D, ^{4}He, ^{7}Li) are computed by the model-independent best-fit empirical formulae for nonstandard primordial nucleosynthesis, and we find the constraint $1 < \beta \leq 1.0505$ and equivalently $0 < \Delta N_\nu^{\text{eff}} \leq 0.6365$; also, the ^{7}Li abundance problem cannot be solved by $\mathscr{L} = \varepsilon^{2-2\beta}R^\beta + 16\pi m_{Pl}^{-2}\mathscr{L}_m$ gravity for this domain of β. Finally, consistency with the mechanism of gravitational baryogenesis is estimated.

Still in $\mathscr{L} = \varepsilon^{2-2\beta} R^\beta + 16\pi m_{\rm Pl}^{-2} \mathscr{L}_m$ gravity, Chapter 10 has studied thermal relics as hot, warm, and cold dark matter. If light neutrinos serve as hot/warm relics, the predicted fractional energy density $\Omega_\psi h^2$ and the mass bound Σm_ν are $\beta-$ and $\varepsilon-$dependent. For cold relics, by exactly solving the simplified Boltzmann equation in both relativistic and nonrelativistic regimes, we show that the Lee-Weinberg bound for the mass of heavy neutrinos can be considerably relaxed, and the "WIMP miracle" for weakly interacting massive particles gradually invalidates as β deviates from $\beta = 1^+$.

We believe that theoretical physicists should keep close eyes on the progress of experiments and observations. In prospective research, we will continue applying relativistic gravities to physical problems in astrophysics and precision cosmology. Here are some of our projects in progress or under preparation.

(1) Test and constrain dark energy and modified gravity by the expansion history and structure growth of the Universe, using the observations of type-Ia supernovae (Union 2.1 compilation), anisotropy of cosmic microwave background (WMAP, Planck), baryon acoustic oscillation (SDSS, BOSS), direct Hubble rate $H(z)$ (differential age, clustering of galaxies/quasars), and so forth.

(2) In minimally coupled modified gravities and with respective to the $\mathrm{SU}(3)_c \times \mathrm{SU}(2)_W \times \mathrm{U}(1)_Y$ minimal standard model, study the gravitationally induced baryogenesis by nonstandard cosmic expansion; investigate hot, warm and cold dark matter as thermal relics of the very early Universe; calculate the primordial helium synthesis from the semi-analytical approach, and nucleosynthesis of deuterium and lithium from the empirical approach; and look into hydrogen recombination and cosmic microwave background.

(3) The very early Universe in $f(R, T^{(m)}) = R + 2\lambda R T^{(m)}$ gravity: Impacts of nonminimal curvature-matter coupling to gravitational baryogenesis, thermal-relic dark matter, and primordial nucleosynthesis.

One typical curvature-matter coupling is the $\mathscr{L} = f(R, T^{(m)}) + 16\pi m_{\rm Pl}^{-2} \mathscr{L}_m$ model [57], where the Ricci scalar R is nonminimally coupled to the trace of the stress-energy-momentum tensor $T^{(m)} = g^{\mu\nu} T^{(m)}_{\mu\nu}$. The field equation is

$$-\frac{1}{2} f\, g_{\mu\nu} + f_R \cdot R_{\mu\nu} + \left(g_{\mu\nu}\Box - \nabla_\mu \nabla_\nu\right) f_R = -f_{T^{(m)}} \cdot (T^{(m)}_{\mu\nu} + \Theta_{\mu\nu}) + 8\pi m_{\rm Pl}^{-2} T^{(m)}_{\mu\nu} \,,$$

where $-f_{T^{(m)}}\,(T^{(m)}_{\mu\nu} + \Theta^{(m)}_{\mu\nu})$ comes from the $T^{(m)}$-dependence in $f(R, T^{(m)})$, and

$$\Theta^{(m)}_{\mu\nu} := \frac{g^{\alpha\beta}\,\delta T^{(m)}_{\alpha\beta}}{\delta g^{\mu\nu}} = -2T^{(m)}_{\mu\nu} + g_{\mu\nu}\mathscr{L}_m - 2g^{\alpha\beta}\,\frac{\partial^2 \mathscr{L}_m}{\partial g^{\mu\nu}\partial g^{\alpha\beta}} \,.$$

For $\mathscr{L} = R + 8\lambda\pi m_{\rm Pl}^{-2} T^{(m)} + 16\pi m_{\rm Pl}^{-2}\mathscr{L}_m$, where λ is a constant and $\Theta^{(m)}_{\mu\nu} = -2T^{(m)} + P_m g_{\mu\nu}$, we have the modified Friedmann equations $3H^2 = 8\pi m_{\rm Pl}^{-2}(1 + \frac{4}{3}\lambda)\rho_m$ and $3\dot{H} = -16\pi m_{\rm Pl}^{-2}(1 + \lambda)\rho_m$ for the radiation-dominated era. Thus $\dot{H} + \dfrac{2(1+\lambda)}{1+\frac{4}{3}\lambda} H^2 = 0$, which integrates to yield the exact solutions

$$H = \frac{1 + \frac{4}{3}\lambda}{2(1+\lambda)} t^{-1} \quad \text{and} \quad a(t) = a_0 t^{\frac{1+\frac{4}{3}\lambda}{2(1+\lambda)}} \,.$$

With H and a obtained, it becomes possible to calculate gravitational baryogenesis, relic dark matter and primordial nucleosynthesis in $f(R, T^{(m)}) = R + 2\lambda R T^{(m)}$ gravity, and thus construct the thermal history of the early Universe, which is expected to constrain the possible domain of λ. Also, one should keep in mind the "matter creation effect" due to the nontrivial conservation $\nabla^\mu T^{(m)}_{\mu\nu} \neq 0$ under $R - T^{(m)}$ coupling. (In fact, it is difficult to solve the Friedmann equations in modified gravity, so every exact solution of $a(t)$ is valuable!)

(4) Following particle physics, it is natural to assume the interactions of dark energy with dark matter and even the cosmic neutrino background. We will look into the consequences of such interactions: (i) curvature oscillation $\Box R$ in a local region (galaxies, clusters, etc.) with dense ($\rho \gg \rho_{\text{cr0}}$) and evolving($\rho = \rho(t)$) matter fields, along with the occurrence and removal of curvature singularities; (ii) enhancement of the matter power spectra by massive neutrinos, and constraints on the summed neutrino mass.

(5) Neutron stars can form in iron core-collapse or electron capture supernovae – in the latter case [71], a $8 - 10 M_\odot$ massive star with a degenerate ONeMg core collapses as the capture of electrons destroys the internal equilibrium by a sudden loss of hydrostatic pressure. This mechanism is far from being fully understood, and we will study the conditions for electron capture along with their influences to the neutron star's characteristic parameters, propagation of the neon burning front towards the stellar center, and impact to the population of binary and isolated neutron stars in globular clusters.

The projects I will be working on will be subject to the accumulations of my physics knowledge, the progress of my skills on numerical calculations, and my inspirations from the arXiv daily updates. Physics is the most attractive career to me, and I will try to advance my professional attainment with heart and soul.

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