MEAN-FIELD DYNAMICS IN A CLASS OF OPEN QUANTUM SYSTEMS

by

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Abstract

We consider a system of N identical quantum particles coupled to an environment. The coupling is scaled in a mean-field way, and particles interact indirectly through the environment. There is no direct interaction between particles. The time evolution of the mean-field-scaled particles is called the mean-field dynamics and the limit of the evolution as $N \to \infty$ is called the mean-field limit. The study of mean-field limits is an active topic of research in many-body quantum theory. Previously, almost all research in this area has been carried out for directly interacting particles without interaction with an environment. In this thesis, we prove that under a suitable condition on the initial system states the mean-field limit in the above indirectly interacting particle system does exist. The condition is satisfied in particular for spin $\frac{1}{2}$ (qubit) systems. Assuming this condition, we show that the system dynamics is the free dynamics in the mean-field limit $N \to \infty$, and we find the first and second correction terms. We show that the particles have a collective effect on the dynamics of the environment (reservoir) which we derive analytically. We give examples to illustrate our results.

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Chapter 1

Introduction

Systems of interest in physics, chemistry, biology and applied sciences can be described by models with a large number of components. The microscopic behavior of such systems is driven by fundamental equations, such as the Schrödinger equation. However, because of the large number of degrees of freedom, working with evolution equations of such systems is not practical. Even for a few particles, the Schrödinger equation, for example, is prohibitively difficult to solve. One often tries to approximate the equations in different ways. One such approximation is the one approximating the solutions of linear N-particle Schrödinger equations in $3N$ variables by products of N single-particle functions in 3 variables. This approximation, which is called the **mean-field or self-consistent approximation**, results in a *non-linear* single-particle equation in 3 variables. It is especially effective when the number of particles is sufficiently large.

1.1 Mean-field regime

Consider a system of N identical quantum particles which can be described by a wave function $\psi_N \in L^2(\mathbb{R}^{3N}) \simeq L^2(\mathbb{R}^3) \otimes \cdots \otimes L^2(\mathbb{R}^3)$. We assume that the particles are Bosons, which means that the system can be described on the subspace $L^2_s(\mathbb{R}^{3N})$ of $L^2(\mathbb{R}^{3N})$ of all wave functions ψ_N symmetric with respect to arbitrary permutations of the N particles, i.e.

$$\psi_N(x_{\pi(1)}, \cdots, x_{\pi(N)}) = \psi_N(x_1, \cdots, x_N),$$

for all permutations $\pi \in S_N$.

The dynamics of the N-particle system, or in other words the dynamics of the wave

function ψ_N, is governed by the Schrödinger equation

$$i\partial_t \psi_{N,t} = H_N \psi_{N,t}, \tag{1.1}$$

with the initial condition $\psi_{N,0} = \psi_N$ where H_N is a self-adjoint operator on $L^2_s(\mathbb{R}^{3N})$, called the Hamiltonian of the system, given by

$$H_N = \sum_{j=1}^{N} -\Delta_j + \lambda \sum_{1 \le j < l \le N} V_{jl}. \tag{1.2}$$

Here, $\Delta_j = \Delta_{x_j}$ is the Laplacian so that the first sum yields the kinetic part of the Hamiltonian, generating the evolution of free particles. The operator $V_{jl} = V(x_j - x_l)$ is the interaction potential, describing the (two-body) interaction among particles. The parameter $\lambda \in \mathbb{R}$ is a coupling constant.

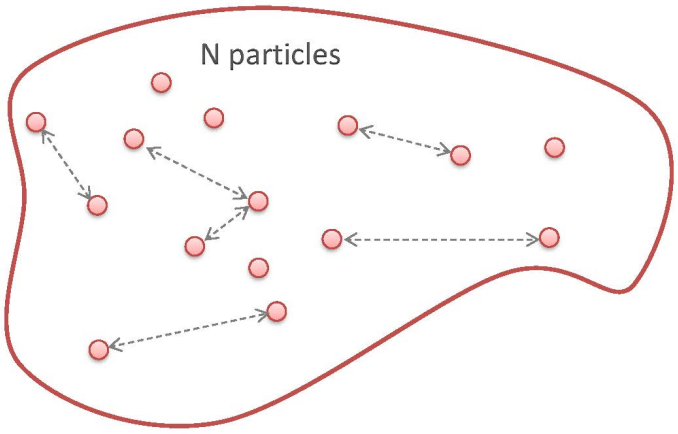

Figure 1: Direct interaction between particles

The N-particle Schrödinger equation has a unique solution

$$\psi_{N,t} = e^{-itH_N} \psi_N \tag{1.3}$$

obtained by the action of the one-parameter group of unitary transformations e^{-itH_N} on the initial wave function ψ_N. However, it is extremely difficult to solve it when N is large. Therefore, it is important to find effective equations which are (analytically or numerically) simple to solve and approximate the solution of the Schrödinger equation.

A simple but non-trivial regime that produces an effective equation for the dynamics of N-particle systems is the **mean-field regime** which is based on the assumption that the particles experience a large number of very weak collisions. It is realized by the

Hamiltonian of the form (1.2) when N is large and $|\lambda| \ll 1$ so that $N\lambda$ remains of order one, $N\lambda \approx 1$. This last condition assures that the total force acting on each particle, resulting from many weak collisions, is of order one and therefore (for large N) the potential and kinetic energy of the system are of the same order.

Thus, to study the mean-field regime, we consider the dynamics generated by the mean-field-scaled Hamiltonian

$$H_N^{mf} = \sum_{j=1}^{N} -\Delta_j + \frac{1}{N} \sum_{1 \le j < l \le N} V_{jl}, \tag{1.4}$$

in the limit $N \to \infty$. We consider an initial wave function $\psi_N \in L_s^2(\mathbb{R}^{3N})$ in factorized (or approximately factorized) form

$$\psi_N(x_1, x_2, \cdots, x_N) \approx \prod_{j=1}^{N} \phi(x_j), \tag{1.5}$$

for some $\phi \in L^2(\mathbb{R}^3)$. Because of interaction among particles, the factorization of wave function is not preserved under the time evolution. However, due to mean-field scaling $1/N$ in front of the interaction potential, one can expect that in the mean-field limit $N \to \infty$ the solution

$$\psi_{N,t} = e^{-itH_N^{mf}} \psi_N \tag{1.6}$$

of the Schrödinger equation to be still approximately factorized (in an appropriate sense):

$$\psi_{N,t}(x_1, x_2, \cdots, x_N) \approx \prod_{j=1}^{N} \phi_t(x_j). \tag{1.7}$$

It follows from (1.7) that the total potential experienced by a particle at site $x \in \mathbb{R}^3$ can be approximated by the convolution

$$V_{\phi_t}(x) := (V * |\phi_t|^2)(x) \tag{1.8}$$

and therefore the evolution of single-particle wave function ϕ_t is described by the non-linear Schrödinger equation

$$i\partial_t \phi_t = (-\Delta + V_{\phi_t})\phi_t, \tag{1.9}$$

of Hartree type, also called the **Hartree equation**. Thus, in the mean-field limit, the dynamics of the N-particle system reduces into the dynamics of a single-particle system.

Note that the approximation (1.7) is not true in the L^2-norm, i.e.

$$\left\| \psi_{N,t}(x_1, x_2, \cdots, x_N) - \prod_{j=1}^{N} \phi_t(x_j) \right\|_{L^2} \not\to 0 \quad \text{as} \quad N \to \infty. \tag{1.10}$$

In fact, a more useful and weaker indicator of convergence should depend only on a finite and fixed number n of particles. In order to obtain the precise mathematical statements about the relation between the many-body Schrödinger equation and the non-linear Hartree dynamics and also clarify in which sense the above factorization is approximately preserved in the mean-field limit, we need to introduce the notion of *reduced state* or *reduced density matrix*. Indeed, (1.7) should be thought of in terms of reduced density matrices in the trace norm topology.

For $n \in \{1, \cdots, N\}$, we define the n-particle reduced density matrix $\rho_{n,N}(t)$ associated with (1.6) by taking partial trace of $|\psi_{N,t}\rangle\langle\psi_{N,t}|$ over the last $N-n$ particle factors, where $|\psi_{N,t}\rangle\langle\psi_{N,t}|$ is the rank-one projection onto $\psi_{N,t}$. In other words,

$$\rho_{n,N}(t) = \mathrm{tr}_{[n+1,N]}(|\psi_{N,t}\rangle\langle\psi_{N,t}|). \tag{1.11}$$

Now, if the initial state of the system is the product state (1.5), then it follows that (1.7) can be precisely stated as

$$\lim_{N\to\infty} \rho_{n,N}(t) = |\phi_t\rangle\langle\phi_t|^{\otimes n} \tag{1.12}$$

in the trace norm for all $n \in \mathbb{N}$, where ϕ_t is the solution of the Hartree equation (1.9).

1.2 Other regimes

The Hartree equation is not the only non-linear equation that arises from mean-field limits. In (1.2), one can consider more general N-dependent interaction potentials

$$V_{\beta,N}(x) = N^{-1+3\beta} V(N^{\beta} x), \tag{1.13}$$

in the three dimensional case, where $\beta \in \mathbb{R}$ indicates the scaling behavior. The models with N-dependent potentials are used to describe systems of physical interest, such as a

Bose-Einstein condensate. Different regimes of β give different mean-field potentials and hence different non-linear equations. The case $\beta = 0$ yields the mean-field potential (1.8), which produces the non-linear Hartree equation (1.9). For $\beta = 1$, we obtain the mean-field potential

$$V_{\phi_t}(x) = \|V\|_{L^1}|\phi_t(x)|^2 \tag{1.14}$$

which produces the **Gross-Pitaevskii equation**. For $\beta < 1$, the many-body evolution can be approximated by a non-linear Schrödinger equation with a local cubic non-linearity. Results in this direction have been obtained in the case of one-dimensional N-dependent potentials in [1, 2, 3, 20], for the two-dimensional case in [44], and for the three dimensional case in [25]. One can also start with Hamiltonians with a three-body interaction potential and approximate the evolutions by a quintic non-linear Schrödinger equation, [18, 19]. We refer to [23, 26, 27, 28, 29] for details on the derivation of the Gross-Pitaevskii equation.

1.3 Mean-field approaches

We give a brief review of the literature on the different approaches to the mean-field (Hartree) dynamics in quantum systems. Mean-field theory has also been applied to classical systems. In this regards, we refer to [36] and the references therein.

Coherent state approach. The study of convergence in the mean-field limit and the first rigorous derivation of (1.7) was introduced by Hepp in [42], where he rigorously discussed the mean-field limit of quantum Bose gases for smooth and bounded interaction potentials. This approach is based on embedding the N-body Schrödinger system into the Fock-space representation and on the use of coherent states as initial states. The use of the Fock-space representation is especially dictated by the fact that coherent states do not have a fixed number of particles. The analysis of Hepp then was extended to the singular potentials by Ginbre and Velo in [34, 35]. In [42, 34, 35], the authors use the term 'semi-classical limit' which is mathematically equivalent to the mean-field limit described above.

This approach was further improved, in terms of the rate of convergence, by Rodnianski and Schlein in [59] where they considered Coulomb interaction potentials and derived a precise estimate for the rate of convergence in the mean-field limit, for both an initial coherent state as well as an initial factorized state. Further improvement on the rate of convergence was obtained by Chen, Lee, and Schlein in [17]. Higher order corrections to

Hartree dynamics have been considered in [37, 38], leading to a better approximation of the many-body evolution.

The coherent state method is particularly good for isolating the main (limit) part and studying the fluctuations around the limit. For details on the coherent state approach, we refer to [11] which is more recent.

The BBGKY approach. A set of recursive equations describing the dynamics of a system of $m+1$ interacting particles in terms of the dynamics of a system of m interacting particles is called a Bogoliubov-Born-Green-Kirkwood-Yvon or BBGKY hierarchy. Thus, a BBGKY hierarchy can describe the dynamics of a large number of interacting particles. The first rigorous proof of (1.7) based on a BBGKY hierarchy was obtained by Spohn in [62], generalizing the result of [42] for all bounded interaction potentials.

In this perturbative method, Spohn derives a BBGKY hierarchy for the time evolution of reduced density matrices, when the interaction potential is bounded. More precisely, he derives a (BBGKY) hierarchy of N equations

$$\begin{aligned} i\frac{d}{dt}\rho_{n,N}(t) &= \Big[\sum_{j=1}^{n} -\Delta_j + \frac{1}{N}\sum_{1\le j<l\le n} V_{jl},\ \rho_{n,N}(t)\Big] \\ &\quad + \frac{N-n}{N}\sum_{j=1}^{n} \mathrm{tr}_{n+1}\Big[V_{j(n+1)},\ \rho_{n+1,N}(t)\Big], \end{aligned} \tag{1.15}$$

describing the time evolution of the reduced density matrices, where $[.,.]$ is the commutator and $\rho_{n,N}(t)$ is given in (1.11). Based on the direct analysis of (1.15), Spohn proved that if the initial state of the system is a factorized state (1.5), then for all $t \in \mathbb{R}$ fixed,

$$\lim_{N\to\infty} \rho_{n,N}(t) = |\phi_t\rangle\langle\phi_t|^{\otimes n} \tag{1.16}$$

in the trace norm for all $n \in \mathbb{N}$, where ϕ_t is the solution of the Hartree equation (1.9).

As $N \to \infty$, the hierarchy (1.15) converges formally to the infinite hierarchy of equations

$$i\frac{d}{dt}\rho_{n,\infty}(t) = \Big[\sum_{j=1}^{n} -\Delta_j,\ \rho_{n,\infty}(t)\Big] + \sum_{j=1}^{n} \mathrm{tr}_{n+1}\Big[V_{j(n+1)},\ \rho_{n+1,\infty}(t)\Big] \tag{1.17}$$

for all $n \in \mathbb{N}$. Then, it follows that this infinite hierarchy of equations has a factorized

solution

$$\rho_{n,\infty}(t) = |\phi_t\rangle\langle\phi_t|^{\otimes n}, \tag{1.18}$$

given by products of solutions of the Hartree equation (1.9). Spohn's result is also valid for all one-particle density matrices (admitting mixed states).

In [30], Erdős and Yau extended Spohn's approach for a Coulomb interaction potential $V(x) = \text{const}/|x|$. Partial results for the Coulomb interaction were also obtained by Bardos, Golse, and Mauser in [9]. See also [24] for a derivation of the Hartree equation with Coulomb interaction for semi-relativistic Bosons. All the articles cited in the previous section are based mainly on the BBGKY approach.

Other approaches. Another different approach has been developed by Fröhlich et al. in [31, 32, 33], where the convergence of many-body evolution for a scalar bounded potential has been interpreted as an Egorov-type theorem, using dispersive estimates and counting of Feynman graphs.

Inspired by the Egorov-type approach, Ammari and Nier developed another method based on the construction of Wigner measures in the infinite-dimensional bosonic quantum field theory in [4], where Wigner measures were constructed and extended to the infinite-dimensional setting, as Borel probability measures under general assumptions. It was also explained how previous formulations of the mean-field limit are contained in the definition of these asymptotic Wigner measures, after a reformulation of the N-body problem as a semi-classical problem with the small parameter $\epsilon = 1/N \to 0$. The basic properties of these Wigner measures were considered and they were used to check that the mean-field dynamics for the coherent states and factorized states are essentially equivalent. The propagation of the Wigner measure for bosonic mean-field limit was studied in [6, 7]. Further progress in this direction are [5, 46].

And, there is a method introduced by Pickl in [55]. Pickl's approach involves a biased counting algorithm which counts the number of 'bad' particles of the evolved state $\psi_{N,t}$. The bad particles are the particles which become entangled and disrupt the product structure of the evolved state. In this method, Pickl introduces a counting measure $\alpha_N(t)$ such that for $t = 0$ most particles are good (initially almost factorized), $\alpha_N(0) \approx 0$. Then, it can be shown that $\alpha_N(0) \approx 0$ implies $\alpha_N(t) \approx 0$. The counting measure α also has the property that $\lim_{N\to\infty} \alpha_N(t) = 0$ implies the convergence of the one-particle reduced density matrices. Using the ideas of [55], further bounds on the rate of convergence towards the Hartree evolution have been obtained in [45, 56].

It should be finally mentioned that the mean-field convergence has also been studied for Fermionic systems, along with the study of Bosonic systems. In this regards, we only refer to [10] and the references therein. In contrast with the long list of articles concerning the mean-field dynamics of Bosons, much less is known about the mean-field limit of Fermionic systems.

1.4 Mean-field dynamics in open quantum systems

The convergence of the quantum dynamics has been studied on the aft-cited articles where most of the recent investigations rely mainly on the BBGKY hierarchy method with a focused interest on studying the singular interaction potentials and the rate of convergence, in the case of either a coherent state or a product (factorized) state as initial data. Even when such specific choices of initial data are avoided, the convergence for arbitrary states still has to be studied. Moreover, all research on the convergence of the mean-field quantum dynamics is concerned with closed quantum systems where there is no interaction with an 'environment' or 'reservoir'. The only known research on the convergence of mean-field dynamics in open quantum systems is the work of Berman and Merkli in [49] and the work of Mori in [52]. In [49], the authors consider an exactly solvable (energy-conserving) model of N identical quantum particles interacting indirectly via a common quantum heat bath (noise). More precisely, they consider the following situation. The Hilbert space of the system is

$$\mathcal{H}_N = \mathcal{H}^{\otimes N} \otimes \mathcal{F}_\beta, \tag{1.19}$$

where $\mathcal{H}$ is a finite-dimensional Hilbert space and $\mathcal{F}_\beta$ is the GNS Hilbert space of spatially infinitely extended KMS state of a free Bose field (heat bath) at temperature β. The dynamics is generated by the mean-field-scaled Hamiltonian

$$H_N = \sum_{j=1}^{N} A_j + K + \frac{\lambda}{\sqrt{N}} \sum_{j=1}^{N} W_j \otimes \varphi(f), \tag{1.20}$$

where A_j stands for the action of a fixed operator $A \in \mathcal{B}(\mathcal{H})$ on the j^{th} factor of $\mathcal{H}_N$, and $W_j \otimes \varphi(f) = W \otimes \varphi(f)$ acts on the j^{th} factor and the reservoir $\mathcal{F}_\beta$, with the evergy-conserving property $AW = WA$.

The Schrödinger dynamics of the reduced n-particle density matrix of the system is

given by

$$\rho_{n,N}(t) = \mathrm{tr}_{[n+1,N],R}\, e^{-itH_N}(\rho_0^{\otimes N} \otimes \rho_\beta)e^{itH_N}, \tag{1.21}$$

where ρ_0 is the single-particle initial state and ρ_β is the KMS state of the reservoir. Then, they prove that for fixed $t \in \mathbb{R}$ and $n \in \mathbb{N}$,

$$\lim_{N\to\infty} \rho_{n,N}(t) = \rho_1(t)^{\otimes n}, \tag{1.22}$$

in the trace norm. The single-particle density matrix $\rho_1(t)$ satisfies

$$i\frac{d}{dt}\rho_1(t) = [A, \rho_1(t)] + \lambda^2\, \mathrm{tr}_2[W_{\mathrm{eff}}(t), \rho_1(t) \otimes \rho_1(t)], \tag{1.23}$$

where $W_{\mathrm{eff}}(t) = 2\dfrac{d}{dt}S(t)(W \otimes W)$ is a time-dependent efficient two-body interaction with an explicit real-valued function S.

1.5 The structure of the thesis

This thesis has been an attempt to extend the result of [49] to a more general class of open quantum systems, relaxing the energy-conserving property of the above model.

A major challenge in the case of open systems is the proof of convergence of the mean-field dynamics. Even in the case of closed systems, one has to impose some conditions on the interaction potentials. By applying BBGKY approach or a direct analysis using Dyson expansion of the dynamics, we can show that relaxing the energy-conserving property in the above model, with the mean-field Hamiltonian (1.20), results in the divergence of the mean-field dynamics. The main source of divergence is the appearance of the (unbounded) bosonic quantum field operator $\varphi(f)$ in the interaction potential in (1.20). Thus, we have been guided to impose a certain physically sensible condition on initial system state, which is satisfied by a large class of physical systems, particularly in spin $\frac{1}{2}$ (qubit) systems, to prove the convergence of the mean-field dynamics. By imposing such a condition, the evolution of any sub-system observable becomes the free evolution as $N \to \infty$. However, it turns out that the system particles have a collective effect on the reservoir and the dynamics of the reservoir will not be free. In both cases of system and reservoir observables, we have obtained formulas for the rate of convergence in the first correction (error) terms which is of importance from computational point of view. The structure of the thesis is

as follows.

In chapter 2, we give a brief introduction to quantum mechanics that are relevant to this thesis. In chapter 3, we introduce the mathematical formalism of many-body quantum mechanics and the tools and terminology that we use in the thesis. The main results are presented in chapter 4, where we precisely state our problem and introduce a vanishing odd-moment condition on initial system states that enables us to prove the convergence of the mean-field quantum dynamics. The proof of our result about the evolution of system observables is given in the section 4.5 where we first prove the convergence of the dynamics based on a direct analysis of evolution operator and its Dyson expansion. Then, we extract the first and the second correction terms and the rate of convergence in each case. Here we consider a more general case where the interaction can be bounded or unbounded (Bosonic quantum field). In section 4.6, we prove the convergence of mean-field dynamics for the reservoir observables and derive the first correction term. We give examples, illustrating our results in concrete models. In particular, we consider a large number N of atoms interacting with the quantized electromagnetic field and apply one of our results to find the number of photons created by the process of emission of radiation induced by atom-field interaction. In chapter 5, we give an outline of future research. The results of current research is to be published in [51].

Chapter 2

Basics of Quantum Mechanics

We briefly present the essential concepts for the description of quantum mechanical systems which are relevant to this thesis. For more detailed description see for instance [13, 40, 41, 53, 60, 63] and also [14, 15, 16, 39, 64]. More details on the mathematical preliminaries can be found in [13, 40, 57, 58, 61, 65].

2.1 States and observables

Quantum mechanical systems are described by operators and vectors in a separable complex Hilbert space. Elementary version of the postulates of quantum theory are postulates P1-P5 below.

Let S be a quantum mechanical system (e.g. a free quantum particle). A complex Hilbert space $\mathcal{H}$ with the following additional specifications is assigned to S.

(P1) **Pure States.** They are unit vectors in $\mathcal{H}$. Two unit vectors ψ_1 and ψ_2 correspond to the same physical state if and only if $\psi_1 = c\psi_2$, where c is a complex number with $|c| = 1$. Such a c is often called a **phase**.

(P2) **Observables.** Corresponding to each physical quantity (observable) $\hat{A}$, there is a self-adjoint operator $A : \mathcal{H} \to \mathcal{H}$. (We usually drop the hat on A and refer to both an observable and its self-adjoint operator by the same letter A.)

Remark. (1) A finite-dimensional $\mathcal{H}$ is the n-dimensional complex Hilbert space $\mathbb{C}^n$. In particular, $\mathcal{H} = \mathbb{C}^2$ is used to describe a 2-level quantum system called spin $\frac{1}{2}$ or **qubit**. However, the finite-dimensional Hilbert space is considered only as a convenient

approximation for some quantum mechanical systems. If we want to investigate the fundamental properties of quantum systems, we have to work in an infinite-dimensional Hilbert space. The main infinite-dimensional $\mathcal{H}$ in quantum theory is the Lebesgue space $L^2(\mathbb{R}^3)$ of square-integrable complex-valued functions on $\mathbb{R}^3$. There is a simple correspondence between classical observables, real-valued functions on $\mathbb{R}^3$, and their quantum-mechanical counterparts, self-adjoint operators on $L^2(\mathbb{R}^3)$. The transition procedure from classical to quantum observables is called **quantization** procedure.

(2) Typical examples of observables in Schrödinger's theory (i.e. when $\mathcal{H} = L^2(\mathbb{R}^3)$) are the position and momentum operators, defined in Example A.2.2 of Appendix A.

(3) **Dirac bra-ket notation:** In quantum mechanics, the standard notation for a vector in a given Hilber space is $|\psi\rangle$. The entire object is usually called a **ket**. The only exception for this notation is the zero vector, because $|0\rangle$ is often used for a non-zero vector with a totally different meaning than the zero vector.

The **bra** notation $\langle\psi|$ is defined as the dual of the ket vector $|\psi\rangle$. Thus, it is a linear functional on the given Hilbert space. In the bra-ket notation, the inner product of two vectors $|\psi_1\rangle$ and $|\psi_2\rangle$ is denoted by $\langle\psi_1|\psi_2\rangle$, which implies the precise definition of a bra. That is, $\langle\psi|\big(|\phi\rangle\big) = \langle\psi|\phi\rangle$. Also, the notation $\langle\psi_1|A|\psi_2\rangle$ is used for the inner product of the vectors $|\psi_1\rangle$ and $A(|\psi_2\rangle)$. The notation for a tensor product is $|\psi_1\rangle \otimes |\psi_2\rangle$. Sometimes the abbreviated notation $|\psi_1\rangle|\psi_2\rangle$ or $|\psi_1, \psi_2\rangle$ is used for the tensor product of $|\psi_1\rangle$ and $|\psi_2\rangle$. Finally, there is a notion of outer product of vectors which is a linear transformation that uses the inner product.

If $|\psi\rangle$ is a vector in $\mathcal{H}$ and $|\phi\rangle$ is a vector in $\mathcal{K}$, then define $|\phi\rangle\langle\psi|$ as a linear transformation from $\mathcal{H}$ to $\mathcal{K}$ by

$$|\phi\rangle\langle\psi|\big(|\psi'\rangle\big) := |\phi\rangle\langle\psi|\psi'\rangle := \langle\psi|\psi'\rangle|\phi\rangle. \tag{2.1}$$

(P3) **Measurement.** If the system is in the state ψ and we measure the observable A, the outcome of the measurement is not deterministic. A measurement of A in the state ψ yields a result which is one of the eigenvalues $\lambda_1, \cdots, \lambda_d$ of A. The value λ_j is measured with a probability $p_j = \|P_j\psi\|^2 = \langle\psi, P_j\psi\rangle$, where P_j is the spectral projection of A associated to λ_j. Consequently, the statistical average of the measurement of A is

$$\sum_j \lambda_j p_j = \sum_j \lambda_j \langle\psi, P_j\psi\rangle = \Big\langle\psi, \Big(\sum_j \lambda_j P_j\Big)\psi\Big\rangle = \langle\psi, A\psi\rangle. \tag{2.2}$$

In the following, we use the notation $\langle A\rangle_\psi$ for $\langle \psi, A\psi\rangle$.

2.1.1 Quantum entanglement

For composite systems, we have the following postulate.

(P4) **Combined systems.** Let the Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ be assigned to two different systems S_1 and S_2, respectively. Then, the Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2$ is assigned to the combined (bipartite) system $S_1 + S_2$.

Remark. If the systems are indistinguishable, then we need to modify the tensor product space to a symmetrized or anti-symmetrized space, as we shall discuss in the next chapter.

In general, a state $\psi \in \mathcal{H}_1 \otimes \mathcal{H}_2$ is expressed as a linear combination of elements $\psi_j^{(1)} \otimes \psi_k^{(2)} \in \mathcal{H}_1 \otimes \mathcal{H}_2$.

Definition 2.1.1. If a state $\psi \in \mathcal{H}_1 \otimes \mathcal{H}_2$ can be written as $\psi = \psi_1 \otimes \psi_2$ with $\psi_j \in \mathcal{H}_j$, then it is called a (tensor) **product state** or a **separable state**, or a **disentangled state**. A non-separable state, on the other hand, is called an **entangled state**.

Example 2.1.2. Using the Dirac notation, the state $\psi \in \mathbb{C}^2 \otimes \mathbb{C}^2$ given by

$$\psi = \frac{|00\rangle + |11\rangle}{\sqrt{2}} := \frac{1}{\sqrt{2}}\left[\begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix} + \begin{pmatrix}0\\1\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix}\right] \tag{2.3}$$

which is a state of two spins, is an entangle state. Indeed, any decomposition

$$\begin{aligned} \psi &= \psi_1 \otimes \psi_2 \\ &= [\lambda_1|0\rangle + \mu_1|1\rangle] \otimes [\lambda_2|0\rangle + \mu_2|1\rangle] \\ &= \lambda_1\lambda_2|00\rangle + \lambda_1\mu_2|01\rangle + \lambda_2\mu_1|10\rangle + \mu_1\mu_2|11\rangle. \end{aligned}$$

leads to the inconsistent relations

$$\lambda_1\lambda_2 = \mu_1\mu_2 = \frac{1}{\sqrt{2}}, \quad \lambda_1\mu_2 = \lambda_2\mu_1 = 0. \tag{2.4}$$

2.2 Statistical mechanical states

"In practice, physics is often concerned with large assemblies of particles of which we have only a very imperfect knowledge. We can scarcely hope to determine the state of all

molecules in a liter of gas. In classical mechanics, such systems are handled by means of statistical averages and we should like to do the same in quantum theory." [41]

We remember that all vectors (states) that are complex multiples of each other correspond to the same physical state and it is really the one-dimensional subspace spanned by unit vector $\psi \in \mathcal{H}$ which is physically significant and not ψ itself. This subspace is determined by the rank-one orthogonal projection P_ψ onto $\mathbb{C}\psi$ given by

$$P_\psi(\chi) := \langle \psi, \chi \rangle \psi. \tag{2.5}$$

Let $\{\psi_j\}$ be an orthonormal basis in $\mathcal{H}$. If A is an observable, then

$$\langle \psi_j, P_\psi A \psi_j \rangle = \langle \psi_j, \langle \psi, A\psi_j \rangle \psi \rangle = \langle \psi_j, \psi \rangle \langle \psi, A\psi_j \rangle. \tag{2.6}$$

Summing over all vectors ψ_j, we obtain

$$\operatorname{tr}(P_\psi A) = \langle \psi, A\psi \rangle \tag{2.7}$$

which shows explicitly how to recover the expectation of A from the projection. Suppose now that $\{\psi_j\}$ is an orthonormal basis and the probability that we find the system in the state ψ_j be p_j. The expected value of any observable A should be given by the weighted average

$$\sum_j p_j \langle A \rangle_{\psi_j} = \sum_j p_j \operatorname{tr}(P_{\psi_j} A) = \operatorname{tr}\Big(\sum_j p_j P_{\psi_j} A \Big). \tag{2.8}$$

The relations (2.7) and (2.8) suggest that such a statistical system is best described by the operator

$$\rho := \sum_j p_j P_{\psi_j}. \tag{2.9}$$

The operator ρ is a non-negative, and hence self-adjoint, operator because the projections are self-adjoint and all probabilities are non-negative real numbers. Moreover,

$$\operatorname{tr}(\rho) = \sum_j p_j \operatorname{tr}(P_{\psi_j}) = \sum_j p_j = 1. \tag{2.10}$$

The above discussion motivates the following definition.

Definition 2.2.1. A non-negative trace-class operator $\rho : \mathcal{H} \to \mathcal{H}$ with $\mathrm{tr}(\rho) = 1$ is called a **density operator**. The set of all density operators on $\mathcal{H}$ is usually denoted by $\mathcal{S}(\mathcal{H})$. In a quantum statistical system whose state is described by a mixture of states or a density operator ρ, the expectation of the observable A is given by the **Born-von Neumann** formula

$$\langle A \rangle_\rho = \mathrm{tr}(\rho A). \tag{2.11}$$

If we know that the state of the system is precisely ψ, then $\rho = P_\psi$ and one applies the 'pure' quantum theory.

Definition 2.2.2. States described by the rank-one projections $\rho = P_\psi$ are called **pure states**. The states which are not pure are called **mixed states**.

There is an easy way to recognize the density operators and determine which of them describe pure states. The proof of the following proposition is straightforward.

Proposition 2.2.3. *The set $\mathcal{S}(\mathcal{H})$ of all density operators is a convex set in the set $\mathcal{L}(\mathcal{H})$ of linear operators on $\mathcal{H}$. Any density operator ρ satisfies*

$$0 \leq \rho^2 \leq \rho \leq 1, \tag{2.12}$$

hence $\mathrm{tr}(\rho^2) \leq 1$. Moreover, ρ is pure if and only if $\rho^2 = \rho$ if and only if $\mathrm{tr}(\rho^2) = 1$.

2.2.1 Entanglement entropy

The notions of product and entangled states which were defined for pure states can be extended to density operators. Entangled pure states arise when we consider linear combinations of (tensor) product pure states that cannot be written as a (tensor) product state, such as the state (2.3) that we considered in the previous section.

Definition 2.2.4. A bipartite mixed state or density matrix ρ is called **entangled (mixed) state** if it cannot be written as a convex combination of pure product states. That is, it cannot be written as

$$\rho = \sum_j p_j P_{\psi_j} \otimes P_{\chi_j}, \tag{2.13}$$

where p_j's are probabilities. A bipartite mixed state that can be expressed as a convex combination of pure states is called a **product (separable) state**.

We can quantify the entanglement of a state by finding its von Neumann entropy. The von Neumann entropy is an important tool in quantum statistical mechanics and thermodynamics. It is the quantum analog of the classical **Shannon information entropy**

$$H(X) = -\sum_x p(x) \log p(x), \tag{2.14}$$

where $p(x) := p(X = x)$ is the probability distribution of a random variable X, and log is taken to be in base 2 since we are transmitting messages with binary bits. We set $0 \log 0 := \lim_{s \to 0^+} s \log s = 0$.

Definition 2.2.5. The **von Neumann entropy** of the density operator $\rho \in \mathcal{S}(\mathcal{H})$ is defined by $S(\rho) := -\operatorname{tr}(\rho \log(\rho))$. If the trace is not finite, we set $S(\rho) = +\infty$.

If we use the spectral decomposition $\rho = \sum_j p_j P_{\psi_j}$, we find the representation

$$S(\rho) = -\sum_j p_j \log(p_j), \tag{2.15}$$

which shows that the von Neumann entropy is equal to Shannon entropy $H(\{p_j\})$ of the random variable J with the distribution $p_j := \mu(J = j)$, given by the spectral decomposition of the density operator ρ.

We use the notion of a **partial trace**, defined in Definition A.2.14 of Appendix A, to define the reduced density operators and their entanglement entropies.

Definition 2.2.6. Let $\mathcal{H} := \mathcal{H}_A \otimes \mathcal{H}_B$ be the Hilbert space of a bipartite system made up of two systems A and B, and $\rho := \rho_{AB}$ be a combined density operator of the systems, defined on $\mathcal{H}$.

(1) The **reduced density operator** ρ_A is defined by

$$\rho_A := \operatorname{tr}_B(\rho). \tag{2.16}$$

Similarly, we define $\rho_B := \operatorname{tr}_A(\rho)$.

(2) The **entanglement entropy** of ρ_{AB} with respect to the system A is defined as $S(\rho_A)$, the von Neumann entropy of the reduced state ρ_A.

The notion of a reduced density operator (taking partial trace) is the quantum version of creating a classical marginal probability distribution $p(x) = \sum_y p(x, y)$ from a classical joint probability distribution $p(x, y)$ over two variables.

The entropy of entanglement is one of the many entanglement measures, although for bipartite pure states it is the unique measure of entanglement in the sense that it is the only function that satisfies certain properties required of an entanglement measure. For a comprehensive review of entanglement measures see [43].

We conclude this section by some of the basic properties of entropy. For more details we refer to [53].

Proposition 2.2.7. *The entropy $S(\rho)$ is a non-negative function. Moreover,*

(1) The state ρ is pure if and only if $S(\rho) = 0$.

(2) In a d-dimensional Hilbert space, the entropy is at most $\log d$. The maximum entropy is taken by a completely mixed state. More precisely, $S(\rho) = \log d$ if and only if the system is in the completely mixed state $\rho = \mathbb{1}/d$, where $\mathbb{1}$ is the identity operator.

(3) For a bipartite pure state $\rho \in \mathcal{H}_A \otimes \mathcal{H}_B$, $S(\rho_A) = S(\rho_B)$.

(4) The entropy $S(\rho)$ is additive for independent subsystems:

$$S(\rho_A \otimes \rho_B) = S(\rho_A) + S(\rho_B), \tag{2.17}$$

while it is sub-additive in general:

$$|S(\rho_A) - S(\rho_B)| \leq S(\rho) \leq S(\rho_A) + S(\rho_B). \tag{2.18}$$

*This triangle inequality is called the **Araki-Lieb inequality**.*

(5) In the case of three subsystems, the entropy is strongly sub-additive:

$$S(\rho_{ABC}) + S(\rho_B) \leq S(\rho_{AB}) + S(\rho_{BC}). \tag{2.19}$$

*This inequality is called the **Lieb-Ruskai inequality**.*

2.3 Quantum dynamics

The following postulate describes the evolution of the states of a closed system in time. We denote by $\psi(t)$ the state $\psi \in \mathcal{H}$ at time t.

(P5) **Dynamics.** The time evolution of the pure state ψ of the system S is given by the **Schrödinger equation**

$$i\hbar \frac{d}{dt}\psi(t) = H\psi(t), \tag{2.20}$$

where H is a self-adjoint operator corresponding to the energy of the system and is called the **Hamiltonian**. The constant $\hbar$ is the Planck constant, which as is customary in mathematical literature, we take it to be 1, by a change of units.

The time evolution of a mixed state is given by the Liouville-von Neumann equation.

Proposition 2.3.1. *The time evolution of a density operator ρ is given by the* ***Liouville-von Neumann equation***

$$i\frac{d}{dt}\rho(t) = [H, \rho(t)]. \tag{2.21}$$

Proof. The proof is easy. It follows by writing the spectral decomposition of $\rho(t)$ and using the Schrödinger equation and its adjoint. ■

If for simplicity we assume that the Hamiltonian H is time-independent, then the Schrödinger equation (2.20) has the formal solution

$$\psi(t) = e^{-itH}\psi(0), \tag{2.22}$$

given the initial state $\psi(0)$. Using this solution in the spectral decomposition

$$\rho(t) = \sum_j p_j P_{\psi_j(t)} \tag{2.23}$$

we find the time evolution

$$\rho(t) = e^{-itH}\rho(0)e^{itH} \tag{2.24}$$

of the mixed states, which gives the solution of the Liouville-von Neumann equation. Note also that the operator $U(t)$ given by

$$U(t) := e^{-itH} \tag{2.25}$$

defines a strongly continuous one-parameter unitary group. Indeed, since H is a self-adjoint operator, we have $U(t)^* = U(-t)$ and thus

$$U(t)^* U(t) = U(0) = \mathbb{1} = U(t)U(t)^* \tag{2.26}$$

which shows that $U(t)$ is unitary. The unitarity of $U(t)$ gives

$$\|\psi(t)\|^2 = \|U(t)\psi(0)\|^2 = \|\psi(0)\|^2 \tag{2.27}$$

which confirms that the time evolution does not change the normalization of ψ. The unitary operator $U(t)$ is called the **time-evolution operator**.

2.3.1 Time evolution of open systems

An **open quantum system** S is a quantum system interacting with another (very large) quantum system E, called an environment. The combined system $S + E$ is assumed to be closed, hence its dynamics is governed by a unitary evolution operator. Using the notion of partial trace, we can derive the dynamics of an open quantum system S, considered as a sub-system of $S + E$.

Let the Hilbert space $\mathcal{H}_{SE} := \mathcal{H}_S \otimes \mathcal{H}_E$ be assigned to the combined system $S + E$, and H_{SE} be the Hamiltonian of the combined system. Such a Hamiltonian can always be decomposed into a sum of three terms as

$$H_{SE} = H_S \otimes \mathbb{1}_E + \mathbb{1}_S \otimes H_E + H_I, \tag{2.28}$$

where H_S, H_E and H_I are the Hamiltonians of the system, environment, and system-environment interaction, respectively. The interaction Hamiltonian may be written as

$$H_I = \sum_j G_j \otimes B_j, \tag{2.29}$$

where G_j and B_j are system and environment operators, respectively.

Definition 2.3.2. Let $U(t) = e^{-itH_{SE}}$ be the unitary time-evolution operator of the combined system $S + E$, and

$$\rho_{SE}(t) = U(t)\rho(0)U(t)^* \tag{2.30}$$

be the time evolution of the combined system, where $\rho(0) = \rho_{SE}(0) = \rho_S(0) \otimes \rho_E(0)$ is the initial state of the combined system which is assumed to be initially disentangled. Then, the time evolution of the open system S is the map $\rho_S(0) \to \rho_S(t)$ given by the **reduced density operator**

$$\rho_S(t) := \mathrm{tr}_E \left(U(t)\rho(0)U(t)^* \right). \tag{2.31}$$

In section 3.3, we give some more details about the mathematical structure of the environment E when we consider the interacting particle-field systems.

2.3.2 Pictures of quantum mechanics

There are three mathematical formulations of quantum dynamics, known as pictures of quantum mechanics. These are Schrödinger picture, Heisenberg picture, and Dirac or interaction picture.

In the Schrödinger picture, states evolve in time but observables are stationary. In the Heisenberg picture, it is the other way round: states are stationary but observables evolve in time. The interaction picture encompasses both pictures: both states and observables evolve in time. Relevant equations of motion are as follows.

Let $U(t) := e^{-itH}$ and $\psi(t)$ be a state in the Schrödinger picture, i.e. $\psi(t) = U(t)\psi(0)$ is the solution of the Schrödinger equation and let A be an observable. Denote by $\psi_H(t)$ a state and by $A_H(t)$ an observable in the Heisenberg picture.

Definition 2.3.3. In the **Heisenberg picture** of quantum mechanics, the states and observables evolve according to the equations

$$\begin{aligned} \psi_H(t) &:= U(t)^*\psi(t) \\ A_H(t) &:= U(t)^*AU(t). \end{aligned}$$

Thus, in this picture states are stationary and observables evolve in time. We set $\psi_H(0) =$

$\psi(0)$.

It is easy to see that the time evolution of observables in Heisenberg picture is given by the differential equation

$$i\frac{d}{dt}A_H(t) = [A_H(t), H]. \tag{2.32}$$

Both Schrödinger and Heisenberg pictures give the same time evolution for expected values and, for this reason, they are considered equivalent.

Proposition 2.3.4. *The Schrödinger and Heisenberg picture give the same expected values.*

Proof. One can write

$$\begin{aligned}
\left\langle A_H(t)\right\rangle_{\psi_H(0)} &= \left\langle \psi_H(0), A_H(t)\psi_H(0)\right\rangle \\
&= \left\langle \psi_H(0), U(t)^* A U(t)\psi_H(0)\right\rangle \\
&= \left\langle U(t)\psi_H(0), A U(t)\psi_H(0)\right\rangle \\
&= \left\langle U(t)\psi(0), A U(t)\psi(0)\right\rangle \\
&= \left\langle \psi(t), A\psi(t)\right\rangle \\
&= \langle A\rangle_{\psi(t)},
\end{aligned}$$

which clearly shows that the expected value of an observable, in an initial state $\psi_H(0)$, in the Heisenberg picture is the same as the expected value of the observable, in the time-evolved state $\psi(t)$, in the Schrödinger picture. ■

In the language of density operators, we may use the cyclicity of trace to write

$$\begin{aligned}
\left\langle A_H(t)\right\rangle_{\rho(0)} &= \mathrm{tr}(\rho(0)A_H(t)) \\
&= \mathrm{tr}(\rho(0)U(t)^* A U(t)) \\
&= \mathrm{tr}(U(t)\rho(0)U(t)^* A) \\
&= \mathrm{tr}(\rho(t)A) \\
&= \langle A\rangle_{\rho(t)}.
\end{aligned}$$

In fact, both Schrödinger and Heisenberg pictures of quantum mechanics are special cases of the interaction picture, which compares the actual evolution with another evolution chosen to serve as a reference.

Definition 2.3.5. Let $V(t) = e^{-itH_0}$ be the reference evolution operator. In the **interaction or Dirac picture**, the states and observables evolve according to the equations

$$\begin{aligned} \psi_I(t) &:= V(t)^* U(t)\psi(0); \\ A_I(t) &:= V(t)^* A V(t). \end{aligned}$$

Note that when $V(t) = \mathbb{1}$, we obtain the Schrödinger picture, and when $V(t) = U(t)$ we obtain the Heisenberg picture. The choice of $V(t)$ should not affect the quantities of physical interest.

Proposition 2.3.6. *In the interaction picture, the expected value of an observable $A_I(t)$ in the state $\psi_I(t)$ is independent of the choice of the reference $V(t)$.*

Proof. Since $V(t)$ is unitary and its inverse is $V(t)^*$,

$$\begin{aligned} \big\langle A_I(t) \big\rangle_{\psi_I(t)} &= \big\langle \psi_I(t), A_I(t)\psi_I(t) \big\rangle \\ &= \big\langle V(t)^* U(t)\psi(0), V(t)^* A V(t) V(t)^* U(t)\psi(0) \big\rangle \\ &= \big\langle U(t)\psi(0), A U(t)\psi(0) \big\rangle \end{aligned}$$

is independent of $V(t)$. ■

Thus, by the last two propositions, the Heisenberg, Schrödinger, and interaction pictures all give the same expected values.

Finally, it is easy to see that the time evolution of states and observables in the interaction picture satisfy the differential equations

$$\begin{aligned} i\frac{d}{dt}\psi_I(t) &= \Big(V(t)^*(H - H_0)V(t)\Big)\psi_I(t); \\ i\frac{d}{dt}A_I(t) &= [A_I(t), H_0]. \end{aligned}$$

We will have a closer look at the interaction picture in the next section.

2.3.3 Time-dependent perturbation theory

The interaction picture is very useful for the systems with complicated Hamiltonians so that one can compare the Hamiltonian of the system with a simpler Hamiltonian of a

reference system, which is supposed to be understood. In such cases, the complicated Hamiltonian H can be written as $H = H_0 + H_I$, where H_0 is the simpler (unperturbed) Hamiltonian while $H_I = H - H_0$ is some perturbation of the system.

As before, let $V(t) = e^{-itH_0}$ be the reference evolution operator and let $U(t) = e^{-itH}$. For any given observable A, define

$$\tau^t(A) := U(t)^* A U(t). \tag{2.33}$$

$$\tau_0^t(A) := V(t)^* A V(t). \tag{2.34}$$

Note that $\tau_0^t(A)$ is the observable $A_I(t)$ in the interaction picture and $\tau^t(A)$ is the observable in the Heisenberg picture. We are interested in a representation of τ^t in terms of τ_0^t and the time-dependent perturbation

$$H_I(t) := V(t)^* H_I V(t), \tag{2.35}$$

also called the time-dependent interaction Hamiltonian.

Proposition 2.3.7 (**Dyson series**). *Let $H_I(t)$ be a bounded operator in some time interval J. Then, for any observable A, the time evolution operator τ^t has the Dyson series expansion*

$$\tau^t(A) = \tau_0^t(A) + \sum_{k=1}^{\infty} i^k \int_0^t dt_1 \int_0^{t_2} \cdots \int_0^{t_{k-1}} dt_k [H_I(t_k), [\cdots, [H_I(t_1), \tau_0^t(A)] \cdots]]. \tag{2.36}$$

Proof. For any observable Y,

$$\frac{d}{dt}(\tau^t \circ \tau_0^{-t}(Y)) = \frac{d}{dt}(e^{itH} e^{-itH_0} Y e^{itH_0} e^{-itH}) = i\tau^t([H_I, \tau_0^{-t}(Y)]), \tag{2.37}$$

and hence

$$(\tau^t \circ \tau_0^{-t})(Y) = Y + i \int_0^t dt_1 \; \tau^{t_1}([H_I, \tau_0^{-t_1}(Y)]). \tag{2.38}$$

Set $Y = \tau_0^t(A)$. Then,

$$\begin{aligned} \tau^t(A) &= \tau_0^t(A) + i \int_0^t dt_1 \; \tau^{t_1}([H_I, \tau_0^{t-t_1}(A)]) \\ &= \tau_0^t(A) + i \int_0^t dt_1 \; \tau^{t_1} \circ \tau_0^{-t_1}([H_I(t_1), \tau_0^t(A)]). \end{aligned} \tag{2.39}$$

The result follows if we iterate the last equation, using (2.38). The series is norm-convergent by the Weierstrass M-test, as it is bounded by

$$\|A\| \sum_{k=0}^{\infty} \frac{(2tM_t)^k}{k!} = \|A\| e^{2tM_t}, \tag{2.40}$$

where $M_t = \sup_{0 \le s \le t} \|H_I(s)\|$. ■

In chapter 4, we will discuss the convergence of the Dyson series when the interaction Hamiltonian is unbounded. In fact, this is the main issue we are dealing with: the interaction depends on an unbounded parameter (N) and we need to control the series and its convergence uniformly in this parameter!

2.4 Algebraic quantum theory

The algebraic formulation of quantum mechanics is a more abstract version of Heisenberg's approach. In the algebraic theory, one uses only the algebraic properties of observables without insisting that they should be linear operators, and replaces states by the expected values. The need for extension beyond Hilbert space initially arose in quantum statistical mechanics in attempts at a mathematically rigorous theory of systems with an infinite number of degrees of freedom, see [14, 15].

The algebraic formulation of quantum theory assumes that the observables of a quantum system are described by the self-adjoint elements of a non-abelian C^*-algebra.

A **C^*-algebra** is a complex algebra $\mathcal{A}$ that is complete in a norm $\|.\|$ satisfying $\|ab\| \le \|a\|\|b\|$ for all $a, b \in \mathcal{A}$, and has an involution $a \mapsto a^*$ such that $\|a^*a\| = \|a\|^2$. The self-adjoint elements are the elements a with $a^* = a$. A basic example of a C^*-algebra is the algebra $M_n(\mathbb{C})$ of all complex $n \times n$ matrices, which describes an n-level system. Another example is the algebra $\mathcal{B}(\mathcal{H})$ of all bounded operators on a Hilbert space $\mathcal{H}$. This is indeed a generalization of the former example.

Further structure than the C^*-algebraic one is needed to describe the system completely, for example to describe the time evolution of the system.

2.4.1 States, representations, and GNS construction

In the algebraic quantum theory, states of a quantum system are non-negative linear functionals $\omega : \mathcal{A} \to \mathbb{C}$ with $\omega(\mathbb{1}) = 1$. This postulate is based on the properties of the

expected values of observables: the expected values of observables are real and non-negative, and the expected value of a linear combination of observables is the linear combination of the expected values of the observables. Note that in (unital) C^*-algebras, the positivity condition $\omega(A^*A) \geq 0$, for all $A \in \mathcal{A}$, is equivalent to assuming that ω is bounded and $\|\omega\| = \omega(\mathbb{1})$.

We now face the question of how the abstract algebraic structure can be used for concrete physical problems, calculations and predictions. In the abelian case, which provides the algebraic theory of classical mechanics, the Gelfand-Naimark theory implies that abelian C^*-algebras are represented by algebras of continuous functions on a compact space. By the **Gelfand-Naimark Theorem**, any C^*-algebra is isomorphic to an algebra of bounded operators on a Hilbert space. Thus, observables again correspond to Hilbert space operators. Also, in the non-abelian case, the following **Gelfand-Naimark-Segal (GNS) construction**, defines a concrete realization of a C^*-algebra as operators on a Hilbert space and relates states of the algebraic theory with vector states in the Hilbert space.

Theorem 2.4.1 (GNS, [14]). *Given a C^*-algebra $\mathcal{A}$ (with identity) and a state $\omega : \mathcal{A} \to \mathbb{C}$, there is a Hilbert space $\mathcal{H}_\omega$ and a representation $\pi_\omega : \mathcal{A} \to \mathcal{B}(\mathcal{H}_\omega)$, such that*

1. *$\mathcal{H}_\omega$ contains a cyclic vector Ψ_ω;*
2. *$\omega(A) = \langle \Psi_\omega, \pi_\omega(A)\Psi_\omega \rangle$, for all $A \in \mathcal{A}$, hence $\|\Psi_\omega\| = 1$;*
3. *every other representation π in a Hilbert space $\mathcal{H}_\pi$ with a cyclic vector Ψ such that $\omega(A) = \langle \Psi, \pi(A)\Psi \rangle$ is unitarily equivalent to π_ω, i.e. there exists an isometry $U : \mathcal{H}_\pi \to \mathcal{H}_\omega$ such that*

$$U\Psi = \Psi_\omega, \quad U\pi(A)U^{-1} = \pi_\omega(A). \tag{2.41}$$

We recall that, given a representation π in a Hilbert space $\mathcal{H}$, a vector $\Psi \in \mathcal{H}$ is **cyclic** if $\pi(\mathcal{A})\Psi$ is dense in $\mathcal{H}$. The triple $(\mathcal{H}_\omega, \pi_\omega, \Psi_\omega)$ is called the **GNS representation** of $(\mathcal{A}, \omega)$ defined by the state ω.

Finally, let us define the mixed states in the algebraic quantum theory.

Definition 2.4.2. A state ω in the C^*-algebra $\mathcal{A}$ is called a **mixed state** if it can be written as a convex combination

$$\omega = \lambda\omega_1 + (1-\lambda)\omega_2, \quad (0 < \lambda < 1) \tag{2.42}$$

of states ω_1 and ω_2. A state is called a **pure state** if it cannot be written as a convex combination of other states; equivalently, if the only non-negative linear functionals 'majorized' by ω are of the form $\lambda\omega, 0 < \lambda < 1$.

A representation $\pi : \mathcal{A} \to \mathcal{B}(\mathcal{H})$ is **irreducible** if $\{0\}$ and $\mathcal{H}$ are the only closed subspaces invariant under $\pi(\mathcal{A})$. One can prove that the GNS representation defined by a state ω is irreducible if and only if ω is pure. Therefore, a mixed state ω cannot be represented by a state vector of an irreducible representation. A mixed state is rather represented by a density operator in an irreducible representation.

Proposition 2.4.3. *Let ω be a mixed state in a C^*-algebra $\mathcal{A}$, and $\pi : \mathcal{A} \to \mathcal{B}(\mathcal{H})$ be an irreducible representation in $\mathcal{H}$. Then, there is a non-negative trace-class operator $\rho : \mathcal{H} \to \mathcal{H}$ with $\mathrm{tr}(\rho) = 1$ such that*

$$\omega(A) = \mathrm{tr}(\rho\ \pi(A)), \quad (A \in \mathcal{A}). \tag{2.43}$$

Given a representation π, the set of all states of the form (2.43) is called the **folium of the representation** π. This set includes, as a special case, the state vectors when ρ is a rank-one projection.

For more details on the (more general) algebraic formulation of quantum mechanics and physical motivations, see [14, 15, 39, 63, 64].

Chapter 3

Many-body Quantum Mechanics

In this chapter, we describe some basic tools of many-particle quantum systems, relevant to this thesis. More details can be found in [15, 12, 22, 47, 60].

3.1 Fock space

In N-body quantum theory, the Hilbert space of a system of N identical particles is the N-fold tensor product of the single-particle Hilbert space. Yet, as is fundamental in describing many-particle systems, a more general Hilbert space, called **Fock space**, is constructed and assigned to a system with an arbitrary (non-fixed) number of identical particles. Even when one deals with a system of fixed number N of particles, using this general Hilbert space gives some technical flexibilities.

Definition 3.1.1. Let $\mathcal{H}$ be a Hilbert space and $\mathcal{H}^n$ be the n-fold product $\mathcal{H} \otimes \cdots \otimes \mathcal{H}$.

(1) The **total Fock space** over $\mathcal{H}$ is denoted by $\mathcal{F}(\mathcal{H})$ and defined as

$$\mathcal{F}(\mathcal{H}) := \bigoplus_{n \geq 0} \mathcal{H}^n, \tag{3.1}$$

where we set $\mathcal{H}^0 = \mathbb{C}$. Any element ψ in $\mathcal{F}(\mathcal{H})$ is a sequence $\psi = \{\psi_n\}_{n \geq 0}$ with $\psi_n \in \mathcal{H}^n$.

(2) The Hilbert space $\mathcal{H}^n$, identified as a sub-space of $\mathcal{F}(\mathcal{H})$, is called the **n-sector**. In particular, the zero-sector $\mathbb{C}$ is called the **vacuum sector**. We also use the notation $[\psi]_n$ for the n-component ψ_n.

(3) The inner product of $\psi = \{\psi_n\}_{n\geq 0}$ and $\chi = \{\chi_n\}_{n\geq 0}$ in $\mathcal{F}(\mathcal{H})$ is defined by

$$\langle \psi, \chi \rangle := \sum_{n\geq 0} \langle \psi_n, \chi_n \rangle_{\mathcal{H}^n}, \tag{3.2}$$

where $\langle \psi_n, \chi_n \rangle_{\mathcal{H}^n}$ is the inner product in the n-sector $\mathcal{H}^n$:

$$\langle f_1^{(n)} \otimes \cdots \otimes f_n^{(n)}, g_1^{(n)} \otimes \cdots \otimes g_n^{(n)} \rangle_{\mathcal{H}^n} = \prod_{j=1}^{n} \langle f_j^{(n)}, g_j^{(n)} \rangle_{\mathcal{H}}. \tag{3.3}$$

(4) The element $\Omega \in \mathcal{F}(\mathcal{H})$ given by

$$[\Omega]_0 = 1 \in \mathbb{C}, \qquad [\Omega]_n = 0 \in \mathcal{H}^n, \quad (\text{for all } \ n \in \mathbb{N}). \tag{3.4}$$

is called the **vacuum vector** or just **the vacuum**. In other words, $\Omega = \{1, 0, 0, \cdots\}$.

Remark. If $\mathcal{H}$ is separable, so is $\mathcal{F}(\mathcal{H})$.

3.1.1 The particle number operator

One of the important operators defined on a Fock space is the number operator.

Definition 3.1.2. The self-adjoint operator $\mathcal{N} : \mathcal{F}(\mathcal{H}) \to \mathcal{F}(\mathcal{H})$ defined by

$$\mathcal{N}\{\psi_n\}_{n\geq 0} := \{n\psi_n\}_{n\geq 0}, \tag{3.5}$$

for all $\{\psi_n\}_{n\geq 0}$ in a dense domain $D(\mathcal{N}) \subset \mathcal{F}(\mathcal{H})$ is called the **number operator**.

Remark. (1) One can easily calculate $D(\mathcal{N})$. Indeed,

$$\begin{aligned} D(\mathcal{N}) &= \Big\{ \psi \in \mathcal{F}(\mathcal{H}) \;\Big|\; \|\mathcal{N}\psi\| < \infty \Big\} \\ &= \left\{ \psi \in \mathcal{F}(\mathcal{H}) \;\middle|\; \Big(\sum_{n\geq 0} \|n\psi_n\|^2 \Big)^{\frac{1}{2}} < \infty \right\} \\ &= \left\{ \psi \in \mathcal{F}(\mathcal{H}) \;\middle|\; \sum_{n\geq 0} n^2 \|\psi_n\|^2 < \infty \right\}. \end{aligned} \tag{3.6}$$

(2) The spectrum of $\mathcal{N}$ is the discrete set $\mathbb{N} \bigcup \{0\}$.

(3) By the definition of $\mathcal{N}$, the eigenspace of n is $\mathcal{H}^n$. Thus, the direct sum (3.1) is indeed the decomposition of the Fock space into the spectral eigenspaces of the number operator.

(4) The one-dimensional kernel of $\mathcal{N}$ is spanned by the vacuum vector Ω.

3.1.2 Creation and annihilation operators

Definition 3.1.3. Let $f \in \mathcal{H}$. The **annihilation operator** $a(f) : \mathcal{F}(\mathcal{H}) \to \mathcal{F}(\mathcal{H})$ is defined sector-wise as follows: for $n \geq 1$ it maps $\mathcal{H}^n$ into $\mathcal{H}^{n-1}$ by

$$f_1 \otimes \cdots \otimes f_n \mapsto \sqrt{n}\langle f, f_1\rangle_{\mathcal{H}}\ f_2 \otimes \cdots \otimes f_n. \tag{3.7}$$

For $n = 0$, we set $\mathcal{H}^{n-1} = \{0\} \subset \mathcal{F}(\mathcal{H})$. Thus, $a(f)$ maps the vacuum sector $\mathcal{H}^0 = \mathbb{C}$ into $\{0\} \subset \mathcal{F}(\mathcal{H})$. The **creation operator** $a^*(f) : \mathcal{F}(\mathcal{H}) \to \mathcal{F}(\mathcal{H})$ is defined sector-wise, mapping $\mathcal{H}^n$ into $\mathcal{H}^{n+1}$ with

$$f_1 \otimes \cdots \otimes f_n \mapsto \sqrt{n+1}\ f \otimes f_1 \otimes \cdots \otimes f_n, \quad (n \geq 1). \tag{3.8}$$

In other words, if $\psi = \{\psi_n\}_{n\geq 0}$ and $\psi_n = f_1^{(n)} \otimes f_2^{(n)} \otimes \cdots \otimes f_n^{(n)}$, then $[a^*(f)\psi]_0 = 0$, $[a^*(f)\psi]_1 = f$, and

$$[a^*(f)\psi]_{n+1} = \sqrt{n+1}\ f \otimes f_1^{(n)} \otimes \cdots \otimes f_n^{(n)} \quad n \geq 1. \tag{3.9}$$

Note that the map $f \mapsto a(f)$ is anti-linear, while $f \mapsto a^*(f)$ is linear. Also, note that the domains of the definitions of $a(f)$ and $a^*(f)$ are extended to $\mathcal{H}^n$ by linearity. The proof of the following relations is straightforward, [15, 47].

Proposition 3.1.4. *Let $f \in \mathcal{H}$ and $\psi_n \in \mathcal{H}^n$. Then,*

$$\|a(f)\psi_n\| \leq \sqrt{n}\ \|f\|\|\psi_n\|, \tag{3.10}$$

$$\|a^*(f)\psi_n\| = \sqrt{n+1}\ \|f\|\|\psi_n\|. \tag{3.11}$$

It follows from the above (continuity) relations that the domains of $a(f)$ and $a^*(f)$ can be extended to the domain $D(\mathcal{N}^{1/2}) \subset \mathcal{F}(\mathcal{H})$, and for all $\psi \in D(\mathcal{N}^{1/2})$,

$$\|a^{\#}(f)\psi\| \leq \|f\|\ \|(\mathcal{N}+1)^{1/2}\psi\|, \tag{3.12}$$

where $a^{\#}(f)$ denotes either $a(f)$ or $a^*(f)$.

Finally, we can show that $a(f)^* = a^*(f)$. That is, the adjoint of $a(f)$ is indeed $a^*(f)$, and appearance of star in $a^*(f)$ is not arbitrary.

3.2 Bosons and Fermions

Assume that S is a system of indistinguishable particles. The indistinguishability is reflected in the symmetry of the state vector (wave function) under the exchange of particle labels. In such cases, the particles are called **Bosons**. If the state vectors are anti-symmetric under permutation of indices, then the particles are called **Fermions**.

If $f_1, \cdots, f_n \in \mathcal{H}$ are n state vectors of a single particle, the vector $f_1 \otimes \cdots \otimes f_n \in \mathcal{H}^n$ is the state of an n-particle system, where the particle labeled by k is in the state f_k. Now, the state describing n Bosons, one of which (we cannot say which one because the particles are indistinguishable) is in the state f_1, one of which is in the state f_2, and so on, is given by the symmetric state vector

$$P_+^{(n)}(f_1 \otimes \cdots \otimes f_n) \in \mathcal{H}^n \tag{3.13}$$

where $P_+^{(n)}$ is the **symmetrization operator**. On the other hand, the state vector of n Fermions is given by

$$P_-^{(n)}(f_1 \otimes \cdots \otimes f_n) \in \mathcal{H}^n \tag{3.14}$$

where $P_-^{(n)}$ is the **anti-symmetrization operator**.

Definition 3.2.1. (1) The **symmetrization** (P_+) and the **anti-symmetrization** (P_-) **operators** are the operators $P_\pm := \bigoplus_{n\geq 0} P_\pm^{(n)}$ defined on $\mathcal{F}(\mathcal{H})$ section-wise as

$$P_+^{(n)}(f_1 \otimes \cdots \otimes f_n) := \frac{1}{n!}\sum_{\pi\in S_n} f_{\pi(1)} \otimes \cdots \otimes f_{\pi(n)}, \tag{3.15}$$

$$P_-^{(n)}(f_1 \otimes \cdots \otimes f_n) := \frac{1}{n!}\sum_{\pi\in S_n} \sigma(\pi) f_{\pi(1)} \otimes \cdots \otimes f_{\pi(n)}, \tag{3.16}$$

where $\sigma(\pi)$ is the signature of the permutation π. We set $P_\pm\Omega = \Omega$.

(2) The **Bosonic Fock space** $\mathcal{F}_+(\mathcal{H})$ and the **Fermionic Fock space** $\mathcal{F}_-(\mathcal{H})$ are

defined as the symmetric and anti-symmetric part of $\mathcal{F}(\mathcal{H})$:

$$\mathcal{F}_{\pm}(\mathcal{H}) := P_{\pm}\mathcal{F}(\mathcal{H}) = \bigoplus_{n\geq 0} P_{\pm}^{(n)}\mathcal{H}^n. \tag{3.17}$$

(3) The **Bososnic** (+) and **Fermionic** (-) **creation and annihilation operators** are defined on $\mathcal{F}_{\pm}(\mathcal{H})$ by

$$a_{\pm}^*(f) = P_{\pm}a^*(f)P_{\pm} \quad \text{and} \quad a_{\pm}(f) = P_{\pm}a(f)P_{\pm}. \tag{3.18}$$

Remark. The operators $P_{\pm}$ are orthogonal projections. That is, $P_{\pm}^2 = P_{\pm} = P_{\pm}^*$. Thus, $\|P_{\pm}\| = 1$. It follows from the definitions that $a_{\pm}(f) = a(f)P_{\pm}$ and $a_{\pm}^*(f) = P_{\pm}a^*(f)$.

3.2.1 Canonical (anti-)commutation relations

Bososnic creation and annihilation operators satisfy the **canonical commutation relations (CCR)**

$$[a_+(f), a_+^*(g)] = \langle f, g\rangle \, \mathbb{1}_{\mathcal{F}_+(\mathcal{H})}, \tag{3.19}$$

$$[a_+(f), a_+(g)] = [a_+^*(f), a_+^*(g)] = 0, \tag{3.20}$$

for any $f, g \in \mathcal{H}$, where $[x, y] = xy - yx$ is the commutator. Fermionic creation and annihilation operators satisfy the **canonical anti-commutation relations (CAR)**

$$\{a_-(f), a_-^*(g)\} = \langle f, g\rangle \, \mathbb{1}_{\mathcal{F}_-(\mathcal{H})}, \tag{3.21}$$

$$\{a_-(f), a_-(g)\} = \{a_-^*(f), a_-^*(g)\} = 0, \tag{3.22}$$

for any $f, g \in \mathcal{H}$, where $\{x, y\} = xy + yx$ is the anti-commutator.

The CCR and CAR relations are understood in the strong sense on $D(\mathcal{N})$, on which the products of two creation and annihilation operators are defined. We say that the operator identity $A = B$ holds in the strong sense on a domain D if $Ax = Bx$ for all $x \in D$. This is important if A and B are unbounded operators.

It turns out that Fermionic creation and annihilation operators extend to bounded operators. Indeed, it follows from CAR relations that

$$\|a_-^{\#}(f)\| = \|f\|. \tag{3.23}$$

However, the Bosonic creation and annihilation operators are unbounded operators. The unboundedness stems from the fact that there is no bound on the number of particles that can have the same one-particle state. This is not true for Fermions, as it is impossible to have more than one particle being in the same one-particle state. This is called the **Pauli principle**, expressed mathematically as

$$a_-^*(f)a_-^*(f) = 0, \tag{3.24}$$

for all $f \in \mathcal{H}$ which follows from (3.22).

The set of all Fermionic creation and annihilation operators generates a unital C^*-algebra of operators on $\mathcal{F}_-(\mathcal{H})$. Since the Bosonic creation and annihilation operators are unbounded, the set of Bosonic creation and annihilation operators are replaced by a set of bounded operators that in some sense are equivalent to the set of Bosonic creation and annihilation operators. These bounded operators are Weyl operators, defined in (3.29), in the following section. The set of all Weyl operators generates a unital C^*-algebra of operators on $\mathcal{F}_+(\mathcal{H})$, defined more precisely in the Definition 3.2.3.

3.2.2 Bosonic quantum fields

Since we are going to deal only with the Bosonic operators, we drop the index $+$ of the associated operators in the following. In this section, $\mathcal{H} = L^2(\mathbb{R}^3)$, the Lebesgue space of square-integrable functions on $\mathbb{R}^3$ with respect to the Lebesgue measure on $\mathbb{R}^3$.

Definition 3.2.2. A **Bosonic quantum field** (or reservoir) is a family of operators on $D(\mathcal{N}^{1/2}) \subset \mathcal{F}_+(\mathcal{H})$ defined by

$$\varphi(f) := \frac{a_+(f) + a_+^*(f)}{\sqrt{2}}, \tag{3.25}$$

where $f \in \mathcal{H}$.

Fermionic quantum fields are defined in a similar way, using the Fermionic creation and annihilation operators. It can be shown, [15, 47, 58], that $\varphi(f)$ is essentially self-adjoint on the finite-particle subspace

$$\mathcal{F}_+^0(\mathcal{H}) := \Big\{ \{\psi_n\}_{n\geq 0} \;\Big|\; \psi_n = 0, \text{ except for finitely many } n \Big\} \subset \mathcal{F}_+(\mathcal{H}). \tag{3.26}$$

Note that $\mathcal{F}_+^0(\mathcal{H}) \subset D(\mathcal{N}^\nu)$, for any $\nu > 0$. We denote by the same notation the

self-adjoint closure of $\varphi(f)$. The mapping $\mathcal{H} \to \mathcal{F}_+(\mathcal{H})$ given by

$$f \mapsto \varphi(f) \tag{3.27}$$

is called the **Segal quantization** over $\mathcal{H}$. Note that the Segal quantization is a real linear (and not a complex linear) operator since $f \mapsto a(f)$ is anti-linear and $f \mapsto a^*(f)$ is linear.

For the Bosonic field operators, we have the CCR

$$[\varphi(f), \varphi(g)] = i \ \mathrm{Im}\langle f, g\rangle, \tag{3.28}$$

understood in the strong sense on $D(\mathcal{N})$.

Finally, using $\varphi(f)$, we define the **Weyl operator** $W(f) : \mathcal{F}_+(\mathcal{H}) \to \mathcal{F}_+(\mathcal{H})$, for $f \in \mathcal{H}$, by

$$W(f) := e^{i\varphi(f)}. \tag{3.29}$$

As stated before, the Weyl operators generate a unital C^*-algebra of operators. More precisely,

Definition 3.2.3. Let $\mathfrak{D} \subset \mathcal{H}$ be the **test function space** which is the set of all compactly supported functions in $C^\infty(\mathbb{R}^3)$. Then, the unital C^*-algebra generated by all Weyl operators $W(f)$, $f \in \mathfrak{D}$, satisfying the relations

$$W(-f) = W(f)^*, \quad W(f)W(g) = e^{-\frac{i}{2}\mathrm{Im}\langle f,g\rangle} W(f+g), \tag{3.30}$$

is called the **Weyl algebra** or **CCR algebra** over $\mathcal{F}_+(\mathfrak{D})$, which is denoted by $\mathrm{CCR}(\mathfrak{D})$. Note that $W(0) = \mathbb{1}$.

The relations (3.30) are obtained from (3.28) and (3.29). In particular, one has the Baker-Campell-Hausdorff formula

$$W(f)W(g) = e^{-\frac{i}{2}\mathrm{Im}\langle f,g\rangle} W(f+g) = e^{-i\mathrm{Im}\langle f,g\rangle} W(g)W(f), \tag{3.31}$$

also called the **Weyl form of CCR**.

3.2.3 Quasi-free states and Wick's Theorem

Let R be a reservoir, represented by a Bosonic quantum field. The evaluation of a reservoir state on the products of Bosonic field operators appears in many calculations related to Bosonic systems. The following result, known as **Wick's Theorem**, shows that the value of a **quasi-free** state on any polynomial of Bosonic field operators is completely determined by evaluating the state on products of pairs of field operators, or the so-called **two-point functions** of the given state.

Definition 3.2.4. Let ω be a state on the Weyl algebra $\mathrm{CCR}(\mathfrak{D})$, defined in the Definition 3.2.3. Then, $\omega(\varphi(f)\varphi(g))$, viewed as a function on $\mathfrak{D}\times\mathfrak{D}$ is called the **two-point function** of the state ω. More precisely, the two-point function of ω is the function $\mathfrak{D}\times\mathfrak{D}\to\mathbb{C}$ given by

$$(f,g)\mapsto\omega(\varphi(f)\varphi(g)).$$

Any state which is determined uniquely by its one- and two-point functions is called a **quasi-free** state.

Note that although ω is defined on Weyl operators, yet we can evaluate it on field operators. In particular,

$$\omega(\varphi(f)\varphi(g))=-\partial_{t_1}\partial_{t_2}|_{t_1=t_2=0}\,\omega\big(W(t_1f)W(t_2g)\big),$$

where ∂_t stands for the partial derivative with respect to t.

The **Fock state** ω_F defined by $\omega_F(W(f)):=\langle\Omega,W(f)\Omega\rangle$ is a basic example of a quasi-free state, where Ω is the vacuum, defined in the Definition 3.1.1. An easy calculation yields $\omega_F(W(f))=e^{-\frac{1}{4}\|f\|^2}$.

Theorem 3.2.5 (Wick)**.** *Let ω be a quasi-free state on the Weyl algebra $\mathrm{CCR}(\mathfrak{D})$, and $f_1,\cdots,f_n\in\mathfrak{D}$. Then,*

$$\omega(\varphi(f_1)\cdots\varphi(f_n))=0 \tag{3.32}$$

if n is odd. For $n=2k,k\in\mathbb{N}$, we have

$$\omega(\varphi(f_1)\cdots\varphi(f_n))=\sum_{\Lambda_k}\prod_{m=1}^{k}\omega(\varphi(f_{\alpha_m})\varphi(f_{\beta_m})), \tag{3.33}$$

where the summation is over the set Λ_k *of all partitions* $\Big\{\{\alpha_1,\beta_1\},\cdots,\{\alpha_k,\beta_k\}\Big\}$ *of* $\{1,\cdots,2k\}$ *into pairs* $\{\alpha_j,\beta_j\}$ *with* $\alpha_j<\beta_j, j=1,\cdots,k$. *Note that* $|\Lambda_k|=\frac{(2k)!}{k!2^k}$.

For a proof, see [54].

3.3 Interacting particle-field systems

Assume that S is a system of quantum particles. As mentioned before, S is an open quantum system if it interacts with another system, generally called environment. A **reservoir** R refers to an environment with an infinite number of degrees of freedom, usually a Bosonic quantum field. The term **bath or heat bath** refers to a reservoir which is in a thermal equilibrium state.

The combined system $S+R$ is described on the Hilbert space $\mathcal{H}_S\otimes\mathcal{H}_R$ where $\mathcal{H}_S$ is the state space of the open system S, and $\mathcal{H}_R$ is the reservoir state space. The Hamiltonian of the composite system is given as

$$H_{total}=H_{free}+H_{interaction}=H_S\otimes\mathbb{1}_R+\mathbb{1}_S\otimes H_R+\lambda H_I, \tag{3.34}$$

where H_S (H_R) is called the **free Hamiltonian** of the system S (the reservoir R), and H_I, called the **interaction Hamiltonian**, describes the interaction of the particles and the Bosonic field. Here, $\lambda\in\mathbb{R}$ is a coupling constant. Usually, the symbol $\otimes$ is assumed to be implicit and we simply write

$$H_{SR}=H_S+H_R+\lambda H_I, \tag{3.35}$$

so that H_S+H_R is the free Hamiltonian of the combined system $S+R$.

The structure of the open system $\{\mathcal{H}_S,H_S\}$ is simple. Assuming S is a system of N identical (but distinguishable) particles, the Hilbert space $\mathcal{H}_S$ of the system is given by

$$\mathcal{H}_S=\mathcal{H}\otimes\cdots\otimes\mathcal{H}\qquad(N\ \text{ times}), \tag{3.36}$$

where $\mathcal{H}$ is a finite-dimensional Hilbert space. The free Hamiltonian H_S is a bounded self-adjoint element of the C^*-algebra of bounded operators on $\mathcal{H}_S$.

The reservoir $\{\mathcal{H}_R,H_R\}$ is defined precisely as follows. The state space $\mathcal{H}_R$ of the

reservoir is the Bosonic Fock space

$$\mathcal{H}_R = \mathcal{F}(L^2(\mathbb{R}^3, d^3k)), \tag{3.37}$$

and the free Hamiltonian H_R of the reservoir is the second quantization of the multiplication by the dispersion relation w, a real-valued function that for us (when the particles are photons) is defined by $w(k) = |k|$.

We recall that the **second quantization** of a self-adjoint operator A, acting on a Hilbert space $\mathcal{H}$, is defined on the n-sector $L^2(\mathbb{R}^3, d^3k) \otimes_s \cdots \otimes_s L^2(\mathbb{R}^3, d^3k)$ of $\mathcal{H}_R$ by

$$A \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1} + \mathbb{1} \otimes A \otimes \cdots \otimes \mathbb{1} + \cdots + \mathbb{1} \otimes \mathbb{1} \otimes \cdots \otimes A, \tag{3.38}$$

and extends to the whole $\mathcal{H}_R$ by linearity. Here, the notation $\otimes_s$ refers to the symmetric tensors. The second quantization of A is denoted by $d\Gamma(A)$. With this notation,

$$H_R = d\Gamma(|k|).$$

We observe that $d\Gamma(\mathbb{1}) = \mathcal{N}$, the number operator.

Finally, the interaction Hamiltonian H_I is defined on $\mathcal{H}_S \otimes \mathcal{H}_R$ by

$$G \otimes \varphi(f), \tag{3.39}$$

where G, a bounded self-adjoint operator acting on $\mathcal{H}_S$, is the interaction Hamiltonian of the open system and, for a given $f \in L^2(\mathbb{R}^3)$, the Bosonic field operator $\varphi(f)$, defined in (3.25), is the interaction Hamiltonian of the reservoir.

Then, the full dynamics of the interacting particle-field system is given by

$$\tau_t(A) = e^{itH_{SR}} A e^{-itH_{SR}}, \tag{3.40}$$

for all observables A acting on $\mathcal{H}_S \otimes \mathcal{H}_R$, where H_{SR} is the total Hamiltonian in (3.35).

Chapter 4

Main Results: Mean-field Dynamics in Open Systems

4.1 Statement of the problem

Consider a system of N identical quantum particles interacting indirectly through a reservoir R. We would like to consider a fixed n-particle sub-system of the large N-particle system and study its evolution.

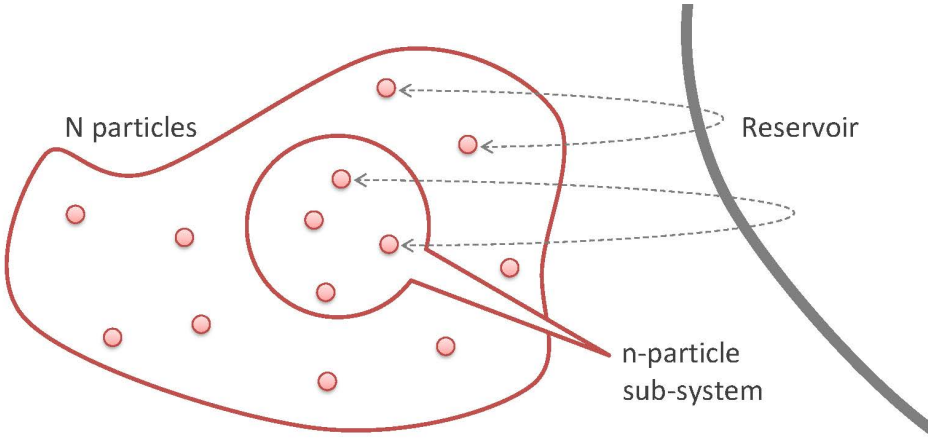

Figure 2: Indirect interaction through a reservoir

The Hilbert space of the system-reservoir is given by $\mathcal{H}_{N,R} := \mathcal{H} \otimes \cdots \otimes \mathcal{H} \otimes \mathcal{H}_R$, where tensor product $\mathcal{H} \otimes \cdots \otimes \mathcal{H}$ is an N-fold product of a single-particle finite-dimensional Hilbert space $\mathcal{H}$, and $\mathcal{H}_R$ is the Hilbert space assigned to the reservoir.

Let $\mathfrak{M}$ be the algebra of observables on the Hilbert space $\mathcal{H}_{N,R}$, and $\mathfrak{M}_R$ be the algebra

of observables acting only on the reservoir factor $\mathcal{H}_R$ of $\mathcal{H}_{N,R}$. Also, assume that $\mathfrak{M}_{\leq k}$ is the algebra of observables acting on the first k system factors, i.e.

$$\mathfrak{M}_{\leq k} := \mathfrak{M}_1 \otimes \cdots \otimes \mathfrak{M}_k, \tag{4.1}$$

where $\mathfrak{M}_j$ is the algebra of observables on $\mathcal{H}$, acting on the j^{th} factor of $\mathcal{H}^{\otimes N}$. In other words, the elements of $\mathfrak{M}_j$ are the elements of the form

$$\mathbb{1} \otimes \cdots \otimes \mathbb{1} \otimes Y_j \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1}, \quad (Y_j \text{ is in the } j^{th} \text{ factor}), \tag{4.2}$$

and the elements of $\mathfrak{M}_{\leq k}$ are sums of elements of the form

$$Y_1 \otimes Y_2 \otimes \cdots \otimes Y_k \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1}, \quad (N-k+1 \text{ times } \mathbb{1}). \tag{4.3}$$

Similarly, the elements of $\mathfrak{M}_R$ are of the form

$$\mathbb{1} \otimes \cdots \otimes \mathbb{1} \otimes Z, \quad (N \text{ times } \mathbb{1}). \tag{4.4}$$

As is usual, we assume that the symbol $\otimes$ is implicit and denote (4.2)-(4.4) simply by Y_j, $Y_1 \otimes Y_2 \otimes \cdots \otimes Y_k$, and Z, respectively.

The total Hamiltonian H_N, as a self-adjoint operator on $\mathcal{H}_{N,R}$, is given in the mean-field way by

$$H_N = \sum_{j=1}^{N} A_j + H_R + \frac{\lambda}{\sqrt{N}} \sum_{j=1}^{N} G_j \otimes B, \tag{4.5}$$

in which particle interactions are scaled by an N-dependent coupling factor, called **mean-field scaling**. Here, $A_j, G_j \in \mathfrak{M}_j$, H_R and B are self-adjoint operators acting on $\mathcal{H}_R$, and $\lambda \in \mathbb{R}$ is a coupling constant. Since the particles are identical, for all j, we write

$$A_j = \mathbb{1} \otimes \cdots \otimes \mathbb{1} \otimes A \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1}, \tag{4.6}$$

$$G_j = \mathbb{1} \otimes \cdots \otimes \mathbb{1} \otimes G \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1}, \tag{4.7}$$

for some one-particle Hamiltonians A and G.

We denote by $\omega : \mathfrak{M} \to \mathbb{C}$ the initial state of the system+reservoir, and by

$$\tau^t_{\lambda,N}(Y) := e^{itH_N} Y e^{-itH_N}, \tag{4.8}$$

the Heisenberg evolution of the n-particle observable $Y \in \mathfrak{M}_{\leq n}$. Then, our problem precisely is the study of

$$\omega(\tau^t_{\lambda,N}(Y)) \tag{4.9}$$

for large N and a suitable choice of the initial state ω.

4.2 States with vanishing odd-moment condition

In this section, we introduce a condition on initial system states which is satisfied by a large class of systems. It will enable us to prove the existence of mean-field limit in a class of open quantum systems.

Definition 4.2.1 (**Vanishing Odd-moment Condition**)**.** For all $1 \leq j \leq N$, let $G_j(t) := e^{itA_j} G_j e^{-itA_j}$ and let $\mathcal{G}_j^{p_j} \in \mathfrak{M}_j$ be a p_j-fold product of G_j's at different times:

$$\mathcal{G}_j^{p_j} = \begin{cases} \prod_{k=1}^{p_j} G_j(t_{j_k}), & p_j \geq 1 \\ \mathbb{1}, & p_j = 0. \end{cases} \tag{4.10}$$

Fix $n \geq 1$. We say that the initial N-particle system state ω_S satisfies **the vanishing odd-moment condition** for n, if for all $\mathcal{O}_n \in \mathfrak{M}_{\leq n}$ and all N

$$\omega_S\big(\mathcal{O}_n \otimes \mathcal{G}_{n+1}^{p_{n+1}} \otimes \cdots \otimes \mathcal{G}_N^{p_N}\big) = 0, \quad \text{if any } p_j \text{ is odd.} \tag{4.11}$$

The initial state ω satisfies **the vanishing odd-moment condition** for $n = 0$ if for all N,

$$\omega_S\big(\mathcal{G}_1^{p_1} \otimes \cdots \otimes \mathcal{G}_N^{p_N}\big) = 0, \quad \text{if any } p_j \text{ is odd.} \tag{4.12}$$

Note that this condition depends on the value of n. The case $n = 0$ can be viewed an n-independent version of this condition.

A collection of examples satisfying (4.11) and (4.12) may be constructed in the class of spin $\frac{1}{2}$ (qubit) systems. Denote by ω_n the initial n-particle system state. For any $Y \in \mathfrak{M}_{\leq n}$, this means $\omega_n(Y) := \omega_S(Y \otimes \mathbb{1}_{N-n})$, where $\mathbb{1}_{N-n}$ is the identity operator on the factors $n+1, \cdots, N$ of $\mathcal{H}^{\otimes N}$.

Example 4.2.2 (Qubits)**.** Let $\mathcal{H} = \mathbb{C}^2$ and $\mathfrak{M}_1 = \mathcal{B}(\mathbb{C}^2)$. Take

$$A = \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \text{ and } G = \sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

Then, for any n-particle system state ω_n, the N-particle system state

$$\omega_S := \omega_n \otimes \omega_1 \otimes \cdots \otimes \omega_1, \quad (N - n \text{ times } \omega_1) \tag{4.13}$$

satisfies the vanishing odd-moment condition (4.11) if the single-particle system state $\omega_1 : \mathfrak{M}_1 \to \mathbb{C}$ is defined by

$$\omega_1(.) = \mathrm{tr}(\rho\, .),$$

where

$$\rho = \begin{bmatrix} p & 0 \\ 0 & 1-p \end{bmatrix}, \quad p \in [0,1].$$

Indeed, we calculate

$$e^{itA} = \begin{bmatrix} e^{it} & 0 \\ 0 & e^{-it} \end{bmatrix}, \; G(t) := e^{itA}\, G\, e^{-itA} = \begin{bmatrix} 0 & e^{2it} \\ e^{-2it} & 0 \end{bmatrix}, \tag{4.14}$$

and for all $k \in \mathbb{N}$, we observe that

$$\omega_1(G(t_1)\cdots G(t_{2k-1})) \;=\; \omega_1\left(\begin{bmatrix} 0 & e^{2it'_{2k-1}} \\ e^{-2it'_{2k-1}} & 0 \end{bmatrix}\right) = 0,$$

and

$$\omega_1(G(t_1)\cdots G(t_{2k})) \;=\; \omega_1\left(\begin{bmatrix} e^{-2it'_{2k}} & 0 \\ 0 & e^{2it'_{2k}} \end{bmatrix}\right) \neq 0,$$

where $t'_J = \sum_{r=1}^{J} (-1)^{r+1} t_r$.

It is evident that if, in (4.13), we replace ω_n by the n-fold tensor product $\omega_1 \otimes \cdots \otimes \omega_1$, then the resulting N-particle state satisfies the vanishing odd-moment condition (4.12).

Therefore, referring to ρ above, we see that the vanishing odd-moment condition is satisfied e.g. for the (pure) **spin up/down states** as well as for the (mixed) **thermal equilibrium state**. The thermal equilibrium state of a spin at the inverse temperature β, which is a simple and physically important example for ω_1, is given by the density matrix

$\propto e^{-\beta\sigma_z}$.

4.3 Main results

In the following, we consider the initial system states that satisfy the vanishing odd-moment condition, defined in the previous section. This enables us to find the mean-field limit of (4.9). It turns out that by imposing such a condition the evolution of any sub-system observable becomes the free evolution in the limit $N \to \infty$, however the system particles have a collective effect on the reservoir and the dynamics of the reservoir will not be free. The free dynamics of the system is given by

$$\tau^t_{0,N}(Y) := e^{itH_{0,N}} Y e^{-itH_{0,N}}, \quad (Y \in \mathfrak{M}_{\leq n}) \tag{4.15}$$

where $H_{0,N} := \sum_{j=1}^{N} A_j + H_R$ is the free Hamiltonian of the system+reservoir. For n-particle sub-system, we set $H^S_{0,n} := \sum_{j=1}^{n} A_j$ and

$$\tau^t_{0,n}(Y) := e^{itH^S_{0,n}} Y e^{-itH^S_{0,n}}, \quad (Y \in \mathfrak{M}_{\leq n}). \tag{4.16}$$

Note that $\tau^t_{0,N}(Y) = \tau^t_{0,n}(Y)$.

Here is the first result.

Theorem 4.3.1. *Let $n \in \mathbb{N}$ be fixed and $\omega = \omega_S \otimes \omega_R$ be the initial system-reservoir state where*

$$\omega_S = \omega_n \otimes \omega_1 \otimes \cdots \otimes \omega_1, \quad (N - n \text{ times } \omega_1). \tag{4.17}$$

If the initial system state ω_1 satisfies the vanishing odd-moment condition (4.11), then $\exists t_0 > 0$ such that $\forall t \in [0, t_0)$ and for all observables $Y \in \mathfrak{M}_{\leq n}$,

$$\omega(\tau^t_{\lambda,N}(Y)) \;\; = \;\; \omega_n(\tau^t_{0,n}(Y)) + \frac{\lambda}{\sqrt{N}}\omega^{(1)}_{n,t}(Y) + O(\frac{\lambda^2}{N}), \tag{4.18}$$

where the first correction term $\omega^{(1)}_{n,t}(Y)$ is given in the Lemma 4.5.6 below. Moreover, $t_0 = \infty$ when B is a bounded operator. If $B = \varphi(f)$, the Bosonic field operator, and ω_R is

the vacuum state, then

$$t_0 = \left(2|\lambda|\|G\|\|f\|\sqrt{2(n^2+1)}\ \right)^{-1}. \tag{4.19}$$

As can be seen from the proof of the Theorem, for the existence of the limit, as $N \to \infty$, the product structure of ω_S is not required. However, to obtain the first correction term, the initial state ω_S must be a product state.

A similar scenario is not valid for reservoir observables. That is, the dynamics of the reservoir observables, when the initial state of the system satisfies the vanishing odd-moment condition, is not free, as stated in the following theorem.

Theorem 4.3.2. *Let $Z \in \mathfrak{M}_R$, and $Z(t) = e^{itH_R} Z e^{-itH_R}$. If $\omega = \omega_S \otimes \omega_R$ is the initial system-reservoir state where $\omega_S = \omega_1 \otimes \cdots \otimes \omega_1$, N times ω_1, and the initial system state ω_S satisfies the vanishing odd-moment condition (4.12), then $\exists s_0 > 0$ such that $\forall t \in [0, s_0)$ and all observables $Z \in \mathfrak{M}_R$, we have*

$$\omega(\tau^t_{\lambda,N}(Z)) \quad = \quad K_\lambda(Z(t)) + O(\frac{\lambda^2}{N}), \tag{4.20}$$

where $K_\lambda(Z(t))$, defined in (4.88) and (4.87), is an N-independent function of λ which is analytic at $\lambda = 0$. Furthermore, if B is a bounded operator, then $s_0 = \infty$. When B is the Bosonic field operator $\varphi(f)$ and ω_R is the vacuum state, then $s_0 = (2\sqrt{2}|\lambda|\|f\|\|G\|)^{-1}$.

Before we apply Theorem 4.3.2 to a concrete model, we calculate the first truncation $K^{(j)}_\lambda(Z(t))$ of $K_\lambda(Z(t))$, which gives the lowest order term in λ, up to order $2j$.

Example 4.3.3. By the j^{th} truncation $K^{(j)}_\lambda(Z(t))$ of $K_\lambda(Z(t))$, we mean equation (4.88) in which the series has been replaced by the sum $\sum_{k=0}^{j}$, i.e.,

$$\begin{aligned} K^{(j)}_\lambda(Z(t)) \quad := \quad & \sum_{k=0}^{j} (\lambda i)^{2k} \int_0^t dt_1 \cdots \int_0^{t_{2k-1}} dt_{2k} \sum_{\Lambda_k} \sum^{2^{2k}} \prod_{m=1}^{k} \\ & \omega_1(G(t_{\alpha'_m}) G(t_{\beta'_m}))\ \omega_R(\mathcal{B}^{2k}(Z(t))). \end{aligned} \tag{4.21}$$

We extract and simplify $K^{(1)}_\lambda(Z(t))$ as follows. (The reader may want to refer to (4.84) for seeing how the terms in the sums arise.) Thus, by referring to (4.84) and (4.83), we see that

$$K^{(0)}_\lambda(Z(t)) = \omega_R(Z(t)) \tag{4.22}$$

and

$$K^{(1)}_{\lambda,N}(Z(t)) = \omega_R(Z(t)) + (\frac{\lambda i}{\sqrt{N}})^2 \int_0^t dt_1 \int_0^{t_1} dt_2 \sum_{\Lambda_1}^{*} \omega([G_{j_2}(t_2) \otimes B(t_2), [G_{j_1}(t_1) \otimes B(t_1), Z(t)]]), \quad (4.23)$$

where the star sum is the sum over the only pairing $j_1 = j_2$ of indices, i.e.,

$$\sum_{\Lambda_1}^{*} = \sum_{j_1=j_2=1}^{N} .$$

The expansion of the multi-commutator in (4.23) yields a sum of four terms:

$$G_{j_2}(t_2)G_{j_1}(t_1)B(t_2)B(t_1)Z(t) - G_{j_2}(t_2)G_{j_1}(t_1)B(t_2)Z(t)B(t_1)$$
$$-G_{j_1}(t_1)G_{j_2}(t_2)B(t_1)Z(t)B(t_2) + G_{j_1}(t_1)G_{j_2}(t_2)Z(t)B(t_1)B(t_2).$$

Thus,

$$\begin{aligned} K^{(1)}_{\lambda,N}(Z(t)) = \omega_R(Z(t)) + (\frac{\lambda i}{\sqrt{N}})^2 \int_0^t dt_1 \int_0^{t_1} dt_2 \sum_{j_1=j_2=1}^{N} \Big(\\ \omega_S(G_{j_2}(t_2)G_{j_1}(t_1))\ \omega_R(B(t_2)B(t_1)Z(t)) \\ -\omega_S(G_{j_2}(t_2)G_{j_1}(t_1))\ \omega_R(B(t_2)Z(t)B(t_1)) \\ -\omega_S(G_{j_1}(t_1)G_{j_2}(t_2))\ \omega(B(t_1)Z(t)B(t_2)) \\ +\omega_S(G_{j_1}(t_1)G_{j_2}(t_2))\ \omega_R(Z(t)B(t_1)B(t_2))\Big), \end{aligned}$$

so that, by reducing the sum, we obtain

$$\begin{aligned} K^{(1)}_{\lambda}(Z(t)) = \omega_R(Z(t)) + \lambda^2 \int_0^t dt_1 \int_0^{t_1} dt_2 \Big(\\ -\omega_1(G(t_2)G(t_1))\ \omega_R(B(t_2)B(t_1)Z(t)) \\ +\omega_1(G(t_2)G(t_1))\ \omega_R(B(t_2)Z(t)B(t_1)) \\ +\omega_1(G(t_1)G(t_2))\ \omega_R(B(t_1)Z(t)B(t_2)) \\ -\omega_1(G(t_1)G(t_2))\ \omega_R(Z(t)B(t_1)B(t_2))\Big). \end{aligned} \quad (4.24)$$

Now, we are ready to apply the above results to some concrete models.

4.4 Concrete examples

We consider a large number N of atoms interacting with the quantized electromagnetic field. Each atom is modeled simply by a two-level quantum system, having a ground and an excited state with energies $E_0 < E_1$, associated with an energy gap

$$\epsilon = E_1 - E_0. \tag{4.25}$$

At an initial time, all atoms are in their excited state and the field is in its vacuum state, showing no photons. The atom-field interaction induces the process of emission of radiation. Namely, atoms transition from their excited state to the ground state and emit a photon into the field, which carries an energy compensating the energy loss of the atom. Starting with all atoms excited and no photons, one thus expects a production of photons due to the atomic emission. We now apply Theorem 4.3.2 to this situation and calculate the number of photons created by this process, as a function of time.

Example 4.4.1 (Spins, and Bose field in the vacuum state)**.** In a system of N atoms interacting with the quantized electromagnetic field, the Hilbert space of each atom is $\mathcal{H} = \mathbb{C}^2$, and the algebra of system observables is the space $\mathcal{M}_2(\mathbb{C})$ of all complex 2×2 matrices. It is convenient to have a basis for the space of observables. One such basis is the set of the identity matrix and the three Pauli matrices:

$$\mathbb{1} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{4.26}$$

The Hilbert space of the quantum field is the Bosonic Fock space $\mathcal{H}_R = \mathcal{F}(\mathcal{K})$ over $\mathcal{K} = L^2(\mathbb{R}^3, d^3k)$. The algebra of field observables is the space $\mathfrak{M}_R$ of (bounded) operators on $\mathcal{H}_R$. The total Hamiltonian is given by (4.5) with the following specifications.

Regarding the system, we take

$$A = \frac{\epsilon}{2}\sigma_z = \frac{\epsilon}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad \text{and} \quad G = \sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \tag{4.27}$$

so that

$$e^{itA} = \begin{bmatrix} e^{\frac{i\epsilon t}{2}} & 0 \\ 0 & e^{\frac{-i\epsilon t}{2}} \end{bmatrix} \quad \text{and} \quad G(t) = e^{itA} G e^{-itA} = \begin{bmatrix} 0 & e^{i\epsilon t} \\ e^{-i\epsilon t} & 0 \end{bmatrix}. \tag{4.28}$$

Moreover,

$$G(t_1)G(t_2) = \begin{bmatrix} e^{i\epsilon(t_1-t_2)} & 0 \\ 0 & e^{-i\epsilon(t_1-t_2)} \end{bmatrix}. \tag{4.29}$$

The initial density matrix of the system is the spin-up state

$$\rho := |\uparrow\rangle\langle\uparrow| = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}. \tag{4.30}$$

Thus,

$$\begin{aligned} \omega_1(G(t_1)G(t_2)) &= \mathrm{tr}(\rho\, G(t_1)G(t_2)) \\ &= \mathrm{tr}\left(\begin{bmatrix} e^{i\epsilon(t_1-t_2)} & 0 \\ 0 & 0 \end{bmatrix}\right) \\ &= e^{i\epsilon(t_1-t_2)}. \end{aligned} \tag{4.31}$$

The quantum field is the Bosonic field operator $B = \varphi(f)$, for a form factor $f \in \mathcal{H} = L^2(\mathbb{R}^3)$. The operator H_R is the free Hamiltonian of the Bosonic reservoir R, defined in section 3.3, that is $H_R = d\Gamma(|k|)$. The relevant field observable is the number operator $Z = \mathcal{N}$ (see subsection 3.1.1). Note that $Z = \mathcal{N}$ is not a bounded operator (so it is not in $\mathfrak{M}_R$), but the derivation of the result still holds: the only thing that contains Z is the bound on β in (4.78), which we should get for $Z = \mathcal{N}$. (See (4.81) and (4.82) and note that $\|(\mathcal{N}+1)^{\frac{1}{2}}\varphi(f)^{k-1}\Omega\| \leq \sqrt{k}\|\varphi(f)^{k-1}\Omega\|$).

The initial state ω_R of the quantum field is the vacuum state

$$\omega_R(K) := \langle\Omega, K\Omega\rangle, \quad (\Omega \text{ is the vacuum vector}). \tag{4.32}$$

Thus, $\omega_R(\mathcal{N}) = 0$, and we have

$$\omega_R(B(t_2)B(t_1)\mathcal{N}(t)) = 0 = \omega_R(\mathcal{N}(t)B(t_1)B(t_2)). \tag{4.33}$$

We recall that $\mathcal{N}(t) := e^{itH_R}\mathcal{N}e^{-itH_R} = \mathcal{N}$ and $B(t) := e^{itH_R}\varphi(f)e^{-itH_R} = \varphi(f_t)$ with $f_t = e^{itw(k)}f$, where $w(k) = |k|$ is the dispersion relation. Since $B(t)\Omega$ is a one-particle

state, $\mathcal{N}B(t)\Omega = B(t)\Omega$. Thus, we have

$$\begin{aligned}\omega_R(B(t_1)\mathcal{N}(t)B(t_2)) &= \omega_R(B(t_1)B(t_2)) \\ &= \frac{1}{2}\langle e^{i|k|t_1}f, e^{i|k|t_2}f\rangle \\ &= \frac{1}{2}\langle e^{i|k|(t_1-t_2)}f, f\rangle \\ &= \frac{1}{2}\int_{\mathbb{R}^3}|f(k)|^2 e^{-i|k|(t_1-t_2)}d^3k. \end{aligned} \tag{4.34}$$

We apply Theorem 4.3.2 to this situation and calculate $\langle\mathcal{N}\rangle_t = \omega(\tau^t_{\lambda,N}(\mathcal{N}))$, to the lowest non-trivial order in λ, using (4.24). Using (4.31) and (4.34) in (4.24) and obtain

$$\begin{aligned}K^{(1)}_\lambda(\mathcal{N}(t)) &= \lambda^2\int_0^t dt_1\int_0^{t_1}dt_2\Big(\omega_1(G(t_2)G(t_1))\ \omega_R(B(t_2)\mathcal{N}(t)B(t_1)) \\ &\quad +\omega_1(G(t_1)G(t_2))\ \omega_R(B(t_1)\mathcal{N}(t)B(t_2))\Big) \\ &= \frac{\lambda^2}{2}\int_0^t dt_1\int_0^{t_1}dt_2\Big(e^{i\epsilon(t_2-t_1)}\int_{\mathbb{R}^3}|f(k)|^2e^{-i|k|(t_2-t_1)}d^3k \\ &\quad +e^{i\epsilon(t_1-t_2)}\int_{\mathbb{R}^3}|f(k)|^2e^{-i|k|(t_1-t_2)}d^3k\Big) \\ &= \frac{\lambda^2}{2}\int_0^t dt_1\int_0^{t_1}dt_2\int_{\mathbb{R}^3}|f(k)|^2d^3k\Big(e^{i(\epsilon-|k|)(t_1-t_2)}+e^{-i(\epsilon-|k|)(t_1-t_2)}\Big) \\ &= \lambda^2\int_{\mathbb{R}^3}|f(k)|^2d^3k\int_0^t dt_1\int_0^{t_1}dt_2\cos\Big((\epsilon-|k|)(t_1-t_2)\Big) \\ &= \lambda^2\int_{\mathbb{R}^3}\frac{1-\cos\Big((\epsilon-|k|)t\Big)}{(\epsilon-|k|)^2}|f(k)|^2d^3k. \end{aligned} \tag{4.35}$$

Thus, we find the following result:

$$\langle\mathcal{N}\rangle_t = (4.35) + O(\lambda^4). \tag{4.36}$$

As already mentioned, $K^{(1)}_\lambda(Z(t))$ yields, to the lowest order in λ, the number of photons emitted at time t by the sea ($N\to\infty$) of all two-level atoms, initially in their exited state. In particular, we see that for small t (4.35) is roughly proportional to $\lambda^2t^2\|f\|^2$ and the initial photon production behaves quadratically in time. In addition, the rate of photon emission for large t can be obtained as follows.

Using

$$\lim_{t\to\infty}\frac{1}{t}\int_0^\infty h(s)\frac{\sin^2(\frac{s}{2}t)}{s^2}ds=\frac{\pi}{4}h(0), \tag{4.37}$$

we calculate

$$\begin{aligned}(4.35) &= 2\lambda^2 t\int_{\mathbb{R}^3}\frac{\sin^2(\frac{\epsilon-|k|}{2}t)}{t(\epsilon-|k|)^2}|f(k)|^2d^3k\\ &= 2\lambda^2 t\int_0^\infty\rho^2\,\frac{\sin^2(\frac{\epsilon-\rho}{2}t)}{t(\epsilon-\rho)^2}\int_{S^2}|f(\rho,\Sigma)|^2d\Sigma\;d\rho\\ &\propto 2\lambda^2\frac{\pi}{4}t\epsilon^2\int_{S^2}|f(\epsilon,\Sigma)|^2d\Sigma\quad(\text{as } t\to\infty).\end{aligned} \tag{4.38}$$

So, the asymptotic (t large) rate of photon emission is

$$R=\frac{\pi\lambda^2}{2}\epsilon^2\int_{S^2}|f(\epsilon,\Sigma)|^2d\Sigma. \tag{4.39}$$

In the next example, we apply Theorem 4.3.1.

Example 4.4.2 (Spins, and Bose field in a coherent state)**.** We calculate $\omega_{n,t}^{(1)}(Y)$ in Theorem 4.3.1, given precisely in (4.63), to the lowest order in λ for spin systems, (4.27), when $n=1$ and the system state $\omega_n=\omega_1$ is the spin-up state, (4.30), and

$$Y=\begin{bmatrix}c & z\\ \bar{z} & d\end{bmatrix} \tag{4.40}$$

is a general system observable, where $c,d\in\mathbb{R}$ and $z\in\mathbb{C}$. As the reservoir, we take a single-mode Bose field, namely a single harmonic oscillator at frequency μ_R, with the interaction operator

$$B=a^*+a,\quad(a\text{ is the annihilation operator}). \tag{4.41}$$

Here, $H_R=\mu_R a^*a$. We take $\mu_R=1$. The initial state of the oscillator is a coherent state given by

$$\omega_R(a)=\alpha,\quad(\alpha\in\mathbb{C}). \tag{4.42}$$

We recall that the vector ψ is a coherent state if it is an eigenvector of the annihilation

operator, i.e. $a\psi = \alpha\psi$. Then, $\omega_R(.) := \langle\psi, .\ \psi\rangle$. Since a is not self-adjoint, α can take complex values.

Since $Y^t = e^{itA}Ye^{-itA}$, it follows from (4.28) that

$$Y^t = e^{itA}Ye^{-itA} = \begin{bmatrix} a & ze^{i\epsilon t} \\ \bar{z}e^{-i\epsilon t} & b \end{bmatrix} \tag{4.43}$$

and

$$[G(s), Y^t] = \begin{bmatrix} \bar{z}e^{i\epsilon(s-t)} - ze^{-i\epsilon(s-t)} & (b-a)e^{i\epsilon s} \\ (a-b)e^{-i\epsilon s} & ze^{-i\epsilon(s-t)} - \bar{z}e^{i\epsilon(s-t)} \end{bmatrix}, \tag{4.44}$$

and therefore, since in (4.63) we set $n = 1$,

$$\begin{aligned} \sum_{j=1}^{n} \omega_n([G_j(s), Y^t]) &= \omega_1([G(s), Y^t]) \\ &= \mathrm{tr}(\rho[G(s), Y^t]) \\ &= \bar{z}e^{i\epsilon(s-t)} - ze^{-i\epsilon(s-t)}. \end{aligned} \tag{4.45}$$

Note that, in (4.63), the lowest order term in λ, corresponding to $k = 0$ in $R_\lambda(s,t)$, is $\omega_R(B(s))$. Thus, we can write

$$\omega_{n,t}^{(1)}(Y) = \int_0^t ds\big[i\bar{z}e^{i\epsilon(s-t)} - ize^{-i\epsilon(s-t)}\big]\big[\omega_R(B(s)) + O(\lambda^2)\big]. \tag{4.46}$$

Since $a(t) = e^{-it}a$ and $a^*(t) = e^{it}a^*$, we have

$$\begin{aligned} \omega_R(B(s)) &= \omega_R(a^*(s) + a(s)) \\ &= \bar{\alpha}e^{is} + \alpha e^{-is}. \end{aligned} \tag{4.47}$$

Thus,

$$\begin{aligned} \omega_{n,t}^{(1)}(Y) &= \int_0^t \big[i\bar{z}e^{i\epsilon(s-t)} - ize^{-i\epsilon(s-t)}\big]\big[\bar{\alpha}e^{is} + \alpha e^{-is}\big]ds + O(\lambda^2) \\ &= \alpha\Big[\frac{\epsilon(z+\bar{z}) - (z-\bar{z})}{\epsilon^2 - 1}e^{-it} - \frac{\bar{z}}{\epsilon - 1}e^{-i\epsilon t} - \frac{z}{\epsilon + 1}e^{i\epsilon t}\Big] \\ &\quad + \text{h.c.} + O(\lambda^2), \end{aligned} \tag{4.48}$$

where 'h.c.' stands for the 'harmonic conjugation'.

4.5 Proof of Theorem 4.3.1

We use the following definition in the proof of Theorem 4.3.1.

Definition 4.5.1. Let $r \geq 1$. For any reservoir state ω_R, we define

$$\beta_r(t) := \sup_{t_1,\cdots,t_r\in[0,t]} \big|\omega_R\big(B(t_1)\cdots B(t_r)\big)\big|. \tag{4.49}$$

We can find a time-independent upper bound for $\beta_r(t)$ in the following cases.

Example 4.5.2. If B is a bounded operator, then $\beta_r(t) \leq \|B\|^r$. If $B = \varphi(f)$ is a Bosonic field operator and ω_R is the vacuum state, then by Theorem 3.2.5 of Wick,

$$\beta_r(t) \leq \frac{r!\|f\|^r}{2^{r/2}(r/2)!},$$

when r is even. For odd r, $\beta_r(t) = 0$.

Proof of Theorem 4.3.1. Let $Y \in \mathfrak{M}_{\leq n}$ be an n-particle observable. By the Dyson series expansion of the dynamics,

$$\omega(\tau^t_{\lambda,N}(Y)) = \omega_n(Y^t) + \sum_{r=1}^{\infty} i^r \int_0^t dt_1 \cdots \int_0^{t_{r-1}} dt_r\ \omega(P_{r,N}(Y^t)), \tag{4.50}$$

where

$$P_{r,N}(Y^t) = (\frac{\lambda}{\sqrt{N}})^r \sum_{j_1,j_2,\cdots,j_r=1}^{N} [G_{j_r}(t_r)\otimes B(t_r), [..., [G_{j_1}(t_1)\otimes B(t_1), Y^t]]...], \tag{4.51}$$

$Y^t := \tau^t_{0,n}(Y)$, and $B(t) := e^{itH_R}Be^{-itH_R}$.

We first prove in Proposition 4.5.3 that the limit of $\omega(\tau^t_{\lambda,N}(Y))$ as $N \to \infty$ exists and converges to free dynamics $\omega_n(Y^t)$. Next, in the Lemmas 4.5.4 and 4.5.6 in the following, we focus on deriving the precise formula of the first correction term $\omega^{(1)}_{n,t}(Y)$, defined in (4.63).

Proposition 4.5.3. *With the assumptions of Theorem 4.3.1, we have*

$$|\omega(\tau^t_{\lambda,N}(Y)) - \omega_n(Y^t)| \leq \frac{|\lambda|}{\sqrt{N}} C_{n,t}(Y), \tag{4.52}$$

where $C_{n,t}(Y)$ is a constant independent of N.

Proof of Proposition 4.5.3. Any tuple $(j_1, \cdots, j_r)$ determines a multi-commutator in (4.51) which corresponds to a term $T_t := T_t(p_1, \cdots, p_N)$ with $p_1 + \cdots + p_N = r$, where p_j counts the number of components in $(j_1, \cdots, j_r)$ which equal j. However, to any $T_t := T_t(p_1, \cdots, p_N)$, or equivalently, to any relevant tuple $(p_1, \cdots, p_N)$ there correspond $r!/(p_1! \cdots p_N!)$ tuples of the form $(j_1, \cdots, j_r)$. The well-known formula

$$\sum_{p_1+\cdots+p_N=r} \binom{r}{p_1, \ldots, p_N} = N^r$$

justifies the discussion, where $\binom{r}{p_1,\ldots,p_N} = r!/(p_1! \cdots p_N!)$ is the multinomial coefficient. Therefore, if we denote by $\mathcal{C}(p_1, \cdots, p_N)$ all possible $\binom{r}{p_1,\ldots,p_N}$ constellations $T_t = T_t(p_1, \cdots, p_N)$, then we have the following representation of (4.51) in terms of p_j's.

$$P_{r,N}(Y^t) \;=\; (\frac{\lambda}{\sqrt{N}})^r \sum_{p_1+\cdots+p_N=r} \;\sum_{T_t \in \mathcal{C}(p_1,\cdots,p_N)} T_t. \tag{4.53}$$

The first sum is over all $p_1, \cdots, p_N \in \mathbb{N} \cup \{0\}$ with the constraint $p_1 + \ldots + p_N = r$ (with r fixed). To apply the vanishing odd-moment condition (4.11), we use the Vandermonde identity

$$\binom{r+N-1}{r} = \sum_{p=0}^{r} \binom{n+r-p-1}{r-p} \binom{N-n+p-1}{p}$$

or in other words

$$\sum_{p_1+\cdots+p_N=r} \;=\; \sum_{p=0}^{r} \;\sum_{p_1+\cdots+p_n=r-p} \;\sum_{p_{n+1}+\cdots+p_N=p}$$

to split p_j's into two groups. Therefore,

$$P_{r,N}(Y^t) \;=\; (\frac{\lambda}{\sqrt{N}})^r \sum_{p=0}^{r} \;\sum_{p_1+\cdots+p_n=r-p} \;\sum_{p_{n+1}+\cdots+p_N=p} \;\sum_{T_t \in \mathcal{C}(p_1,\cdots,p_N)} T_t. \tag{4.54}$$

Note, however, that the case $p = r$ in (4.54) corresponds to a constellation T_t in which $p_j = 0$ for all $j \in \{1, \cdots, n\}$, which in turn corresponds to a term in (4.51) in which all $j_1, \cdots, j_r$ belong to $\{n+1, \cdots, N\}$. This term vanishes because $Y \in \mathfrak{M}_{\leq n}$ commutes with all involved G_j's. Thus, (4.54) takes the following form (we also act by ω on both sides)

$$\omega(P_{r,N}(Y^t)) \;=\; (\frac{\lambda}{\sqrt{N}})^r \sum_{p=0}^{r-1} \sum_{p_1+\cdots+p_n=r-p} \sum_{p_{n+1}+\cdots+p_N=p} \sum_{T_t \in \mathcal{C}(p_1,\cdots,p_N)} \omega(T_t). \quad (4.55)$$

Next, observe that each term $T_t = T_t(p_1, \cdots, p_N)$, introduced just after (4.52), can indeed be represented by 2^r terms of the form

$$\mathcal{O}_n(t) \otimes \mathcal{G}_{n+1}^{p_{n+1}} \otimes \cdots \otimes \mathcal{G}_N^{p_N} \otimes \mathcal{O}_R, \quad (4.56)$$

where $\mathcal{O}_n(t) := \mathcal{O}_n(Y^t; p_1, \cdots, p_n) \in \mathfrak{M}_{\leq n}$ is a product of operators $G_1, \cdots, G_n$ and Y^t; $\mathcal{O}_R \in \mathfrak{M}_R$ is a product of operators $B(t_\alpha)$'s. The operator $\mathcal{G}_j^{p_j}$ is defined by (4.10), where $j \in \{n+1, \cdots, N\}$. It follows from (4.51) that $|\omega(T_t)| \leq 2^r \|Y\| \|G\|^r \beta_r(t)$, where $\beta_r(t)$ is defined by (4.49). Now, the vanishing odd-moment condition (4.11) on ω ensures that all $p_{n+1}, \cdots, p_N$ and hence p must be even, see (4.55). Let $p = 2q$ and $p_j = 2q_j$ $(n+1 \leq j \leq N)$. Accordingly, (4.55) give rise to

$$|\omega(P_{r,N}(Y^t))| \;\leq\; \|Y\| \Big(\frac{2|\lambda|\|G\|}{\sqrt{N}}\Big)^r r!\; \beta_r(t) \sum_{q=0}^{\lfloor \frac{r-1}{2} \rfloor} \sum_{p_1+\cdots+p_n=r-2q} \frac{1}{p_1! \cdots p_n!} \sum_{q_{n+1}+\cdots+q_N=q} \frac{1}{(2q_{n+1})! \cdots (2q_N)!},$$

and if we apply the identity $\sum_{p_1+\cdots+p_N=r} \binom{r}{p_1,\ldots,p_N} = N^r$, we obtain

$$
\begin{aligned}
|\omega(P_{r,N}(Y^t))| &\leq \|Y\|\Big(\frac{2|\lambda|\|G\|}{\sqrt{N}}\Big)^r r!\beta_r(t)\sum_{q=0}^{\lfloor\frac{r-1}{2}\rfloor}\frac{n^{r-2q}}{(r-2q)!}\sum_{q_{n+1}+\cdots+q_N=q}\frac{1}{q_{n+1}!\cdots q_N!}\\
&= \|Y\|\Big(\frac{2|\lambda|\|G\|}{\sqrt{N}}\Big)^r r!\beta_r(t)\sum_{q=0}^{\lfloor\frac{r-1}{2}\rfloor}\frac{n^{r-2q}}{(r-2q)!}\frac{(N-n)^q}{q!}\\
&\leq \|Y\|(2|\lambda|\|G\|)^r r!\beta_r(t)\sum_{q=0}^{\lfloor\frac{r-1}{2}\rfloor}\frac{n^{r-2q}}{(r-2q)!q!}\frac{1}{N^{\frac{r}{2}-q}}\\
&\leq \frac{\|Y\|(2|\lambda|\|G\|)^r r!\beta_r(t)}{\sqrt{N}}\sum_{q=0}^{\lfloor\frac{r-1}{2}\rfloor}\frac{n^{r-2q}}{(r-2q)!q!}. \qquad (4.57)
\end{aligned}
$$

In the last inequality, we use the fact that for all q, $\frac{r}{2}-q\geq\frac{r}{2}-\lfloor\frac{r-1}{2}\rfloor\geq\frac{1}{2}$. It can easily be shown that the finite sum in (4.57) is bounded by $\frac{n^2(1+n^2)^{r/2}}{\lfloor\frac{r}{2}\rfloor!}$. Indeed, by binomial expansion formula, we have

$$
\begin{aligned}
\sum_{q=0}^{\lfloor\frac{r-1}{2}\rfloor}\frac{n^{r-2q}}{(r-2q)!q!} &\leq \frac{1}{\lfloor\frac{r}{2}\rfloor!}\sum_{q=0}^{\lfloor\frac{r}{2}\rfloor}\frac{\lfloor\frac{r}{2}\rfloor!(n^2)^{\frac{r}{2}-q}}{(\lfloor\frac{r}{2}\rfloor-q)!q!}\\
&\leq \frac{1}{\lfloor\frac{r}{2}\rfloor!}\sum_{q=0}^{\lfloor\frac{r}{2}\rfloor}\binom{\lfloor\frac{r}{2}\rfloor}{q}(n^2)^{\frac{r}{2}-q}\\
&\leq \frac{n}{\lfloor\frac{r}{2}\rfloor!}\sum_{q=0}^{\lfloor\frac{r}{2}\rfloor}\binom{\lfloor\frac{r}{2}\rfloor}{q}(n^2)^{\lfloor\frac{r}{2}\rfloor-q}\\
&\leq \frac{n}{\lfloor\frac{r}{2}\rfloor!}(1+n^2)^{\lfloor\frac{r}{2}\rfloor}\leq\frac{n(1+n^2)^{r/2}}{\lfloor\frac{r}{2}\rfloor!}.
\end{aligned}
$$

Thus, we have

$$
|\omega(P_{r,N}(Y^t))| \leq \frac{n\|Y\|(2\sqrt{1+n^2}|\lambda|\|G\|)^r r!\ \beta_r(t)}{\sqrt{N}\lfloor\frac{r}{2}\rfloor!},
$$

and by (4.50)

$$\begin{aligned} |\omega(\tau^t_{\lambda,N}(Y)) - \omega_n(Y^t)| &\leq \sum_{r=1}^{\infty} \int_0^t dt_1 \cdots \int_0^{t_{r-1}} dt_r \ |\omega(P_{r,N}(Y^t))| \\ &\leq \frac{n\|Y\|}{\sqrt{N}} \sum_{r=1}^{\infty} \frac{(2\sqrt{n^2+1}|\lambda|\|G\|t)^r \beta_r(t)}{\lfloor \frac{r}{2} \rfloor !}. \end{aligned} \tag{4.58}$$

Now let t_0 be the largest time t such that the series in (4.58) converges on the time interval $[0, t_0)$. In particular, when B is a bounded operator, $t_0 = \infty$. This follows by the ratio test and example 4.5.2. In the case of a Bose field in the vacuum state,

$$t_0 = (2\|G\|\|f\|\sqrt{2(n^2+1)}|\lambda|)^{-1},$$

again by the ratio test and example 4.5.2. The proof of (4.52) is now complete if we set $C_{n,t}(Y) := n\|Y\| \sum_{r=1}^{\infty} |\lambda|^{r-1} \ (2\sqrt{n^2+1}\|G\|t)^r \beta_r(t)/\lfloor \frac{r}{2} \rfloor !$. ■

The first correction term. We derive the first correction term $\omega^{(1)}_{n,t}(Y)$ in the Lemma 4.5.6 in the following. As discussed after (4.54), $p < r$, which implies that at least one of the indices $j_1, \cdots, j_r$ must be $\leq n$. Referring to (4.51), observe that we must have $j_1 \leq n$. Note that, the less indices are $\leq n$, the highest order in N the multiple sum will be. Thus, in (4.51), we produce the highest order term in N when $j_1 \leq n$ and $j_2, \cdots, j_r \geq n+1$. This corresponds to $p = r-1$ in (4.55). Therefore, we can rewrite (4.50) and (4.51) as

$$\omega(\tau^t_{\lambda,N}(Y)) \ = \ \omega_n(\tau^t_{0,n}(Y)) + \frac{\lambda}{\sqrt{N}} \ \omega^{(1)}_{N,t}(Y) + \sum_{m=2}^{r} (\frac{\lambda}{\sqrt{N}})^m \omega^{(m)}_{N,t}(Y), \tag{4.59}$$

where

$$\begin{aligned} \frac{\lambda}{\sqrt{N}} \ \omega^{(1)}_{N,t}(Y) \ = \ & \sum_{r=1}^{\infty} (\frac{\lambda i}{\sqrt{N}})^r \int_0^t dt_1 \cdots \int_0^{t_{r-1}} dt_r \sum_{j_1=1}^{n} \sum_{j_2,\cdots,j_r=n+1}^{N} \omega([G_{j_r}(t_r) \otimes B(t_r), \\ & [..., [G_{j_2}(t_2) \otimes B(t_2), [G_{j_1}(t_1), Y^t] \otimes B(t_1)]...]]), \end{aligned} \tag{4.60}$$

and $\omega^{(m)}_{N,t}(Y)$ stands for all possibilities for indices $j_1, \cdots, j_r$ so that m of them are $\leq n$. Note that $\omega^{(m)}_{N,t}(Y)$ is uniformly bounded in N as it is a particular case of what we had in the proof of Proposition 4.5.3. [There, we had all possibilities for indices.] We estimate $\sum_{m\geq 2} (\frac{\lambda}{\sqrt{N}})^m \ \omega^{(m)}_{N,t}(Y)$ by $O(\frac{\lambda^2}{N})$ in the following.

Lemma 4.5.4. *We have*

$$\omega_{N,t}^{(1)}(Y) = \int_0^t i\ ds \sum_{j=1}^{n} \omega_n([G_j(s), Y^t])\Big(\omega_R(B(s)) + \sum_{k=1}^{N-n} (\frac{\lambda i}{\sqrt{N}})^{2k} \int_0^s dt_1 \cdots \int_0^{t_{2k-1}} dt_{2k} \sum_{\Lambda_k}^{*} \omega([G_{j_{2k}}(t_{2k}) \otimes B(t_{2k}), [\cdots, [G_{j_1}(t_1) \otimes B(t_1), B(s)] \cdots]])\Big), \tag{4.61}$$

where Λ_k is the set of all k-element pairings $\{j_{\alpha_1} = j_{\beta_1}, \cdots, j_{\alpha_k} = j_{\beta_k}\}$ of $2k$ indices $j_1, \cdots, j_{2k}$ with $n+1 \leq j_1, \cdots, j_{2k} \leq N$ and $\alpha_m < \beta_m, 1 \leq m \leq k$. Hence, $|\Lambda_k| = \frac{(2k)!}{k!2^k}$. Here,

$$\sum_{\Lambda_k}^{*} = \sum_{\Lambda_k} \sum_{j_{\alpha_1}=n+1}^{N} \cdots \sum_{j_{\alpha_k}=n+1}^{N}.$$

Example 4.5.5. When $k = 1$, $|\Lambda_1| = 1$ and we have only one possibility for pairing of indices j_1 and j_2, i.e. $\{j_1 = j_2\}$. Thus, in this case,

$$\sum_{\Lambda_1}^{*} = \sum_{j_1=j_2=n+1}^{N}.$$

When $k = 2$, $|\Lambda_2| = 3$ and we have three possibilities for pairing of indices j_1, j_2, j_3 and j_4, i.e. $\{j_1 = j_2, j_3 = j_4\}, \{j_1 = j_3, j_2 = j_4\}$,$\{j_1 = j_4, j_2 = j_3\}$. In this case,

$$\sum_{\Lambda_2}^{*} = \sum_{j_1=j_2=n+1}^{N} \sum_{j_3=j_4=n+1}^{N} + \sum_{j_1=j_3=n+1}^{N} \sum_{j_2=j_4=n+1}^{N} + \sum_{j_1=j_4=n+1}^{N} \sum_{j_2=j_3=n+1}^{N}.$$

Proof of Lemma 4.5.4. One may simplify (4.60) by writing

$$\begin{aligned}
\frac{\lambda}{\sqrt{N}}\,\omega^{(1)}_{N,t}(Y) &= \frac{\lambda i}{\sqrt{N}}\int_0^t dt_1 \sum_{j_1=1}^{n} \omega_n([G_{j_1}(t_1), Y^t])\;\omega_R(B(t_1)) \\
&+ \sum_{r=2}^{\infty}(\frac{\lambda i}{\sqrt{N}})^r \int_0^t dt_1 \cdots \int_0^{t_{r-1}} dt_r \sum_{j_1=1}^{n} \sum_{j_2,\cdots,j_r=n+1}^{N} \omega_n([G_{j_1}(t_1), Y^t]) \\
&\quad \omega([G_{j_r}(t_r)\otimes B(t_r), [..., [G_{j_2}(t_2)\otimes B(t_2), B(t_1)]...]]) \\
&= \frac{\lambda i}{\sqrt{N}}\int_0^t ds \sum_{j=1}^{n} \omega_n([G_j(s), Y^t])\;\omega_R(B(s)) + \frac{\lambda i}{\sqrt{N}}\int_0^t ds \sum_{j=1}^{n} \\
&\quad \omega_n([G_j(s), Y^t]) \sum_{r=2}^{\infty}(\frac{\lambda i}{\sqrt{N}})^{r-1} \int_0^s dt_2 \cdots \int_0^{t_{r-1}} dt_r \sum_{j_2,\cdots,j_r=n+1}^{N} \\
&\quad \omega([G_{j_r}(t_r)\otimes B(t_r), [..., [G_{j_2}(t_2)\otimes B(t_2), B(s)]...]]) \\
&= \frac{\lambda i}{\sqrt{N}}\int_0^t ds \sum_{j=1}^{n} \omega_n([G_j(s), Y^t])\;\omega_R(B(s)) + \frac{\lambda i}{\sqrt{N}}\int_0^t ds \sum_{j=1}^{n} \\
&\quad \omega_n([G_j(s), Y^t]) \sum_{r=1}^{\infty}(\frac{\lambda i}{\sqrt{N}})^{r} \int_0^s dt_1 \cdots \int_0^{t_{r-1}} dt_r \sum_{j_1,\cdots,j_r=n+1}^{N} \\
&\quad \omega([G_{j_r}(t_r)\otimes B(t_r), [..., [G_{j_1}(t_1)\otimes B(t_1), B(s)]...]]).
\end{aligned}$$

Therefore,

$$\begin{aligned}
\omega^{(1)}_{N,t}(Y) &= i\int_0^t ds \sum_{j=1}^{n} \omega_n([G_j(s), Y^t])\Big(\omega_R(B(s)) + \sum_{r=1}^{\infty}(\frac{\lambda i}{\sqrt{N}})^r \int_0^s dt_1 \cdots \int_0^{t_{r-1}} dt_r \\
&\quad \sum_{j_1,\cdots,j_r=n+1}^{N} \omega([G_{j_r}(t_r)\otimes B(t_r), [\cdots, [G_{j_1}(t_1)\otimes B(t_1), B(s)]\cdots]])\Big). \qquad (4.62)
\end{aligned}$$

Now, consider the series in (4.62). Due to the vanishing odd-moment condition on state ω, the number of system operators, r, must be even. Let $r = 2k$, $k \in \mathbb{N}$. Again by the vanishing odd-moment condition, the indices $j_1, \cdots, j_{2k}$ must be pairwise equal. We show that all terms with $r = 2k > 2(N-n)$ are of $O(\frac{\lambda^2}{N})$.

Assume that $k > N-n$ and we have k pairs $j_{\alpha_1} = j_{\beta_1}$, ..., $j_{\alpha_k} = j_{\beta_k}$. Each of these pairs can take one of $N-n$ values $n+1, \cdots, N$ and therefore they cannot be all distinct pairs. Hence, the leading term in N is of $O(N^{k-1})$. Multiplying by the factor $(\frac{\lambda}{\sqrt{N}})^{2k}$ in (4.62), we produce terms of $O(\frac{\lambda^2}{N})$.

If $k \leq N-n$ then the leading term in N is exactly of $O(N^k)$ provided that all k pairs

are distinct. This is just the assignment of $N-n$ values $n+1,\cdots,N$ to k distinct pairs. Trivially, if the pairs are not distinct then the order of multiple sum is of order less than k and the leading term in N and all lower order terms are of $O(\frac{\lambda^2}{N})$. Therefore, the only cases in which we produce a sum of order k, a leading term in N, is when $k \leq N-n$ and indices $j_{\alpha_1} = j_{\beta_1}$, ..., $j_{\alpha_k} = j_{\beta_k}$ are distinct. The result follows if we denote the multiple sum of (4.62) by the multiple sum $\sum^*_{\Lambda_k}$ over Λ_k of all $\frac{(2k)!}{k!2^k}$ possibilities for forming pairings $\{j_{\alpha_1} = j_{\beta_1}, ..., j_{\alpha_k} = j_{\beta_k}\}$ with $\alpha_m < \beta_m$, $1 \leq m \leq k$, so that j_{α_m}'s are distinct and taking values from $\{n+1,\cdots,N\}$. That is,

$$\sum_{\Lambda_k}^{*} := \sum_{\Lambda_k} \sum_{j_{\alpha_1}=n+1}^{N} \cdots \sum_{j_{\alpha_k}=n+1}^{N}.$$

■

Using (4.61) in Lemma 4.5.4, we derive the first correction term as follows.

Lemma 4.5.6. *The first correction term $\omega^{(1)}_{n,t}(Y)$ is given by*

$$\omega^{(1)}_{n,t}(Y) := \int_0^t i\ ds\ \Big(\sum_{j=1}^{n} \omega_n([G_j(s), Y^t])\Big) R_\lambda(s,t), \tag{4.63}$$

where

$$R_\lambda(s,t) := \sum_{k=0}^{\infty} (\lambda i)^{2k} \int_0^s dt_1 \cdots \int_0^{t_{2k-1}} dt_{2k} \sum_{\Lambda_k} \sum^{2^{2k}} \prod_{m=1}^{k} \omega_1(G(t_{\alpha'_m}) G(t_{\beta'_m}))\ \omega_R(\mathcal{B}^{2k+1}(s))$$

is a function of λ analytic at $\lambda = 0$, $\sum_{\Lambda_k}$ is as in the Lemma 4.5.4, $(\alpha'_m, \beta'_m) = (\alpha_m, \beta_m)$ or $(\alpha'_m, \beta'_m) = (\beta_m, \alpha_m)$, and $\mathcal{B}^{2k+1}(s)$ is a product of $2k+1$ operators $B(t_1),\cdots,B(t_{2k})$, and $B(s)$. The sum $\sum^{2^{2k}}$ is the sum of 2^{2k} terms in the expansion of the multi-commutator in (4.61) which determines (α'_m, β'_m) and also the ordering of B's in $\mathcal{B}^{2k+1}(s)$. Note that the zeroth term of the series is $\omega_R(B(s))$.

Also, note that (4.63) and (4.61) are related by

$$\omega^{(1)}_{N,t}(Y) = \omega^{(1)}_{n,t}(Y) + O(\frac{\lambda^2}{N}), \quad N \geq 2(n-1), \tag{4.64}$$

as it can be seen from the proof of Lemma 4.5.6.

Example 4.5.7. We write the first term of $R_\lambda(s,t)$ in Lemma 4.5.6, the zeroth term being $\omega_R(B(s))$. For $k=1$, $|\Lambda_1|=1$ and we have one paring of indices j_1 and j_2, i.e. $\{j_1=j_2\}$. Then, for $k=1$,

$$\sum_{\Lambda_k}\sum^{2^{2k}}\prod_{m=1}^{k}\omega_1(G(t_{\alpha'_m})G(t_{\beta'_m}))\;\omega_R(\mathcal{B}^{2k+1}(s))=\sum^{2^2}\omega_1(G(t_{\alpha'_1})G(t_{\beta'_1}))\;\omega_R(\mathcal{B}^3(s)) \quad (4.65)$$

where on the right side, we have a sum of 2^2 terms obtained from the expansion of the multi-commutator in (4.61). Indeed, by expanding the commutators we obtain

$$\begin{aligned}\sum^{2^2}\omega_1(G(t_{\alpha'_1})G(t_{\beta'_1}))\;\omega_R(\mathcal{B}^3(s)) &= \omega_1(G(t_2)G(t_1))\;\omega_R(B(t_2)B(t_1)B(s))\\ &\quad -\omega_1(G(t_2)G(t_1))\;\omega_R(B(t_2)B(s)B(t_1))\\ &\quad +\omega_1(G(t_1)G(t_2))\;\omega_R(B(s)B(t_1)B(t_2))\\ &\quad -\omega_1(G(t_1)G(t_2))\;\omega_R(B(t_1)B(s)B(t_2)).\end{aligned} \quad (4.66)$$

Thus, the first term of $R_\lambda(s,t)$, corresponding to $k=1$, reads

$$\begin{aligned}(\lambda i)^2\int_0^s dt_1\int_0^{t_1}dt_2\;\Big[&\omega_1(G(t_2)G(t_1))\;\omega_R(B(t_2)B(t_1)B(s))\\ &-\omega_1(G(t_2)G(t_1))\;\omega_R(B(t_2)B(s)B(t_1))\\ &+\omega_1(G(t_1)G(t_2))\;\omega_R(B(s)B(t_1)B(t_2))\\ &-\omega_1(G(t_1)G(t_2))\;\omega_R(B(t_1)B(s)B(t_2))\Big].\end{aligned} \quad (4.67)$$

Proof of Lemma 4.5.6. For any given element $\{j_{\alpha_1}=j_{\beta_1},\cdots,j_{\alpha_k}=j_{\beta_k}\}$ of Λ_k, the expansion of the multi-commutator in (4.61) yields 2^{2k} different terms which are a product of operators $G_{j_\alpha}(t_\alpha)$, $G_{j_\beta}(t_\beta)$, $B(t_\alpha)$, $B(t_\beta)$, and $B(s)$ with different ordering. Since for fixed α and β, all $\omega_1(G_j(t_\alpha)G_j(t_\beta))$'s give the same value for any $j\in\{n+1,\cdots,N\}$, it is enough only to assign the lowest possible value to each index $j_\alpha=j_\beta$ and count the possibilities of each index arising from the corresponding sum $\sum_{j_\alpha=j_\beta=n+1}^{N}$. Therefore, because of distinctness of indices we may replace the sum $\sum_{j_{\alpha_1}=j_{\beta_1}=n+1}^{N}$ and its involved term $\omega_1(G_{j_{\alpha_1}}(t_{\alpha_1})G_{j_{\beta_1}}(t_{\beta_1}))$ by $(N-n)\;\omega_1(G(t_{\alpha_1})G(t_{\beta_1}))$, and the sum $\sum_{j_{\alpha_2}=j_{\beta_2}=n+1}^{N}$ and its involved term by $(N-n-1)\;\omega_1(G(t_{\alpha_2})G(t_{\beta_2}))$, etc. However, the expansion of mutli-commutator yields a reordering of (time) indices and hence we will also obtain terms of the form $\omega_1(G_{j_\beta}(t_\beta)G_{j_\alpha}(t_\alpha))$. Thus, we obtain product

of k terms of the form $\omega_1(G(t_{\alpha'})G(t_{\beta'}))$ such that $(\alpha',\beta') = (\alpha,\beta)$ or $(\alpha',\beta') = (\beta,\alpha)$. Hence, if we use the notation $\sum^{2^{2k}}$ for the sum of 2^{2k} terms in the expanded multi-commutator in (4.61), we have

$$\omega^{(1)}_{N,t}(Y) = \int_0^t i\ ds \sum_{j=1}^{n} \omega_n([G_j(s),Y^t])\ \Big(\omega_R(B(s)) + \sum_{k=1}^{N-n}(\lambda i)^{2k}\int_0^s dt_1\cdots\int_0^{t_{2k-1}} dt_{2k}$$
$$\sum_{\Lambda_k}\sum^{2^{2k}}\prod_{m=1}^{k}\frac{(N-n-m+1)}{N}\ \omega_1(G(t_{\alpha'_m})G(t_{\beta'_m}))\ \omega_R(\mathcal{B}^{2k+1}(s))\Big), \tag{4.68}$$

where $(\alpha'_m,\beta'_m) = (\alpha_m,\beta_m)$ or $(\alpha'_m,\beta'_m) = (\beta_m,\alpha_m)$, and $\mathcal{B}^{2k+1}(s)$ is a product of $2k+1$ operators $B(t_1),\cdots,B(t_{2k})$, and $B(s)$.

To remove the N-dependency and obtain $\omega^{(1)}_{n,t}(Y)$, we replace $\frac{N-n-m+1}{N}$ by 1 and $\sum_{k=1}^{N-n}$ by $\sum_{k=1}^{\infty}$, but then we have to show that the errors that we produce by these replacements are of $O(\frac{\lambda^2}{N})$. If we apply $\frac{N-n-m+1}{N} = 1 - \frac{n+m-1}{N}$ to (4.68), then it splits to two terms so that the first one is what we want (an N-independent term) and the second one is a term which is of $O(\frac{\lambda^2}{N})$. Hence, the first replacement of $\frac{N-n-m+1}{N}$ by 1 is justified.

For the second replacement, we use $\sum_{k=0}^{N-n} = \sum_{k=0}^{\infty} - \sum_{k>N-n}$, the zeroth term being $\omega_R(B(s))$. We show that the series converges and the error term corresponding to $\sum_{k>N-n}$ is of $O(\frac{\lambda^2}{N})$. Accordingly, the above replacements applied to (4.68) give the N-independent relation

$$\omega^{(1)}_{n,t}(Y) := \int_0^t i\ ds\ \Big(\sum_{j=1}^{n}\omega_n([G_j(s),Y^t])\Big)R_\lambda(s,t),$$

where

$$R_\lambda(s,t) := \sum_{k=0}^{\infty}(\lambda i)^{2k}\int_0^s dt_1\cdots\int_0^{t_{2k-1}} dt_{2k}\sum_{\Lambda_k}\sum^{2^{2k}}\prod_{m=1}^{k}\omega_1(G(t_{\alpha'_m})G(t_{\beta'_m}))\ \omega_R(\mathcal{B}^{2k+1}(s))$$

is an analytic function at $\lambda = 0$. This series is easily seen to converge for all times t. Indeed, when B is bounded, $|\omega_R(\mathcal{B}^{2k+1}(s))| \le \|B\|^{2k+1}$ and if we use the estimate

$$\Big|\sum_{\Lambda_k}\sum^{2^{2k}}\prod_{m=1}^{k}\omega_1(G(t_{\alpha'_m})G(t_{\beta'_m}))\Big| \le 2^{2k}\frac{(2k)!}{2^k k!}\|G\|^{2k},$$

we obtain

$$\begin{aligned} |R_\lambda(s,t)| &\leq \sum_{k=0}^{\infty} \frac{(\sqrt{2}\lambda t\|G\|)^{2k}\|B\|^{2k+1}}{k!} \\ &= \|B\| \sum_{k=0}^{\infty} \frac{(\sqrt{2}\lambda t\|G\|\|B\|)^{2k}}{k!}. \end{aligned} \tag{4.69}$$

In the case of unbounded $B = \varphi(f)$, the Bosonic field operator, and a quasi-free state ω_R, $\omega_{n,t}^{(1)}(Y) = 0$, by Theorem 3.2.5 of Wick. We will discuss further on this case in the next paragraph. Finally, let us show that the error term corresponding to $\sum_{k>N-n}$ is of $O(\frac{\lambda^2}{N})$. It is enough to use the estimate (4.69) with $\sum_{k=0}^{\infty}$ replaced by $\sum_{k>N-n}$. Setting $x := (\sqrt{2}\lambda t\|G\|\|B\|)^2$,

$$\begin{aligned} \sum_{k>N-n} \frac{(\sqrt{2}\lambda t\|G\|\|B\|)^{2k}}{k!} &= \sum_{k=N-n+1}^{\infty} \frac{x x^{k-1}}{k(k-1)!} \\ &\leq \frac{x}{N-n+1} \sum_{k=N-n}^{\infty} \frac{x^k}{k!} \\ &< \frac{x e^x}{N-n+1} \\ &= \frac{x}{N} \frac{N}{N-n+1} e^x \\ &\leq \frac{2x}{N}\, e^x \\ &= O(\frac{\lambda^2}{N}). \end{aligned} \tag{4.70}$$

Here we use $\frac{N}{N-n+1} \leq 2$ which is valid if and only if $N \geq 2(n-1)$. ■

The proof of the Theorem 4.3.1 is now complete. ■

As we pointed out in the previous paragraph, if ω_R is a quasi-free Bose state, then $\omega_{n,t}^{(1)}(Y) = 0$, by Theorem 3.2.5 of Wick. Therefore, we would also like to find the next (non-trivial) correction term in this case, a second correction term in (4.52), which is the term $\omega_{N,t}^{(2)}(Y)$ defined in (4.59), which corresponds to $p = r-2$ in (4.55). This implies that for some $l \in \{2, \cdots, r\}$, $j_1, j_l \leq n$ and $j_m \geq n+1$, for all $m \in \{2, \cdots, r\} - \{l\}$. Moreover, r must be even by Wick's Theorem. Let $r = 2k$, $k \in \mathbb{N}$. Thus, we may rewrite (4.50) and

(4.51) as

$$\omega(\tau^t_{\lambda,N}(Y)) \;=\; \omega_n(\tau^t_{0,n}(Y)) + \frac{\lambda^2}{N}\,\omega^{(2)}_{N,t}(Y) + O(\frac{\lambda^4}{N^2}), \tag{4.71}$$

where

$$\begin{aligned}\omega^{(2)}_{N,t}(Y) \;:=\; & \sum_{k=1}^{\infty}(\frac{\lambda i}{\sqrt{N}})^{2k-2}\int_0^t dt_1\cdots\int_0^{t_{2k-1}} dt_{2k}\sum_{l=2}^{2k}\sum_{j_1,j_l=1}^{n}\sum_{\substack{j_m=n+1\\ m\in\{2,\cdots,2k\}-\{l\}}}^{N}\\ & \omega([G_{j_{2k}}(t_{2k})\otimes B(t_{2k}),[\cdots,[G_{j_1}(t_1)\otimes B(t_1),Y^t]...]]).\end{aligned} \tag{4.72}$$

Proposition 4.5.8. *Let ω_R be the vacuum state of a free Bose field, and let $\omega^{(2)}_{n,t}(Y)$ denote the second correction term in (4.52), an N-independent term obtained from (4.72). Then, with similar notation as in the Lemma 4.5.6,*

$$\begin{aligned}\omega^{(2)}_{N,t}(Y) \;:=\; & \sum_{k=1}^{N-n}(\frac{\lambda^2}{N})^{k-1}\int_0^t dt_1\cdots\int_0^{t_{2k-1}} dt_{2k}\sum_{l=2}^{2k}\sum_{j_1,j_l=1}^{n}\sum_{\Lambda_{k-1}}^{*}\\ & \omega([G_{j_{2k}}(t_{2k})\otimes B(t_{2k}),[\cdots,[G_{j_1}(t_1)\otimes B(t_1),Y^t]...]]),\end{aligned} \tag{4.73}$$

where Λ_{k-1} is the set of all $(k-1)$-element pairings $\{j_{\alpha_1}=j_{\beta_1},\cdots,j_{\alpha_{k-1}}=j_{\beta_{k-1}}\}$ of $2k-2$ indices j_α, and $\sum^*_{\Lambda_{k-1}}$ denotes the sum over Λ_{k-1} such that $n+1\le j_\alpha=j_\beta\le N$, with $\alpha,\beta\in\{2,\cdots,2k\}-\{l\}$. Moreover, the N-independent correction term reads

$$\begin{aligned}\omega^{(2)}_{n,t}(Y) \;:=\; & \sum_{k=1}^{\infty}(\lambda i)^{2k-2}\int_0^t dt_1\cdots\int_0^{t_{2k-1}} dt_{2k}\sum_{l=2}^{2k}\omega_S(Y^{(n)}_{1,l}(t))\sum_{\Lambda_{k-1}}\\ & \sum^{2^{2k-2}}\prod_{\substack{v=1\\ \alpha'_v\neq l\neq\beta'_v}}^{k-1}\omega_1(G(t_{\alpha'_v})G(t_{\beta'_v}))\;\omega_R(\mathcal{B}^{(2k)}).\end{aligned} \tag{4.74}$$

Here $Y^{(n)}_{1,l}(t)$ represents the two possibilities for the product of $\sum_{j_1=1}^n[G_{j_1}(t_1),Y^t]$ and $\sum_{j_l=1}^n G_{j_l}(t_l)$; and $\mathcal{B}^{(2k)}$ is a product of $2k$ Bosonic operators $B(t_1),\cdots,B(t_{2k})$. Also, $(\alpha'_v,\beta'_v)=(\alpha_v,\beta_v)$ or $(\alpha'_v,\beta'_v)=(\beta_v,\alpha_v)$. The sum $\sum^{2^{2k-2}}$ refers to the sum of terms in the expanded multi-commutator (4.73). Moreover, the series in (4.74) converges for all times $t<(2|\lambda|\|G\|\|f\|)^{-1}$.

The relation

$$\omega^{(2)}_{N,t}(Y) = \omega^{(2)}_{n,t}(Y) + O(\frac{\lambda^4}{N^2}), \tag{4.75}$$

holds between (4.73) and(4.74), as it can be seen from the proof of Proposition 4.5.8.

Example 4.5.9. When $k = 1$, we only have two indices j_1 and j_2. Referring to (4.73), we see that

$$\sum_{l=2}^{2k} \sum_{j_1,j_l=1}^{n} \sum_{\Lambda_{k-1}}^{*} = \sum_{j_1,j_2=1}^{n}$$

and the general term under these sums simplifies to

$$\omega([G_{j_2}(t_2) \otimes B(t_2), [G_{j_1}(t_1) \otimes B(t_1), Y^t]]).$$

Therefore, the first term of $\omega^{(2)}_{n,t}(Y)$, when in (4.74) we set $k = 1$, reads

$$\int_0^t dt_1 \int_0^{t_1} dt_2 \left(\omega_S\Big(\sum_{j_1,j_2=1}^{n} G_{j_2}(t_2)[G_{j_1}(t_1), Y^t] \Big)\ \omega_R(B(t_2)B(t_1)) \right.$$
$$\left. -\omega_S\Big(\sum_{j_1,j_2=1}^{n} [G_{j_1}(t_1), Y^t]G_{j_2}(t_2) \Big)\ \omega_R(B(t_1)B(t_2)) \right). \tag{4.76}$$

Proof of Proposition 4.5.8. In (4.72), $2k-2$ indices j_m with $m \in \{2, \cdots, 2k\} - \{l\}$ must form $k-1$ distinct pairs like $j_{\alpha_1} = j_{\beta_1}, \cdots, j_{\alpha_{k-1}} = j_{\beta_{k-1}}$ to produce the leading term in N. The same reasoning as in the proof of Lemma 4.5.4 shows in particular that $k \leq N-n$ and all other cases for k and indices j_α lead to terms which are of $O(\frac{\lambda^4}{N^2})$. Therefore, if we denote by Λ_{k-1} the set of all distinct pairings $j_{\alpha_1} = j_{\beta_1}, \cdots, j_{\alpha_{k-1}} = j_{\beta_{k-1}}$, and use the notation $\sum^*_{\Lambda_{k-1}}$ for sum over Λ_{k-1} such that $n+1 \leq j_\alpha = j_\beta \leq N$, with $\alpha, \beta \in \{2, \cdots, 2k\} - \{l\}$ we obtain 4.73. Note that this notation involves k sums, one on parings and the rest on j_α's.

Finally, a similar argument as in the proof of Lemma 4.5.6 results in the N-independent equation of (4.74), whose convergence for all times $t < (2|\lambda|\|G\|\|f\|)^{-1}$ can be seen by

noting that $|\omega_R(\mathcal{B}^{2k})| \leq \frac{(2k)!}{2^k k!}\|f\|^{2k}$ and

$$\Big|\sum_{l=2}^{2k}\omega_S(Y_{1,l}^{(n)}(t))\sum_{\Lambda_{k-1}}\sum^{2^{2k-2}}\prod_{\substack{v=1\\ \alpha'_v\neq l\neq\beta'_v}}^{k-1}\omega_1(G(t_{\alpha'_v})G(t_{\beta'_v}))\Big| \leq$$
$$(2k-1)4n^2\|G\|^2\|Y\|\frac{(2k-2)!}{(k-1)!2^{k-1}}2^{2k-2}\|G\|^{2k-4}. \tag{4.77}$$

■

4.6 Proof of Theorem 4.3.2

We use the following definition and lemma in the proof of Theorem 4.3.2.

Definition 4.6.1. Let $Z \in \mathfrak{M}_R$, and $Z(t) = e^{itH_R}Ze^{-itH_R}$. Define

$$\beta_r(t,Z) := \sup_{t_1,\cdots,t_r\in[0,t]}\max_{1\leq k\leq r}\big|\omega_R\big(B(t_1)\cdots\widehat{Z(t)}^{\,k}\cdots B(t_r)\big)\big|, \tag{4.78}$$

with $\widehat{Z(t)}^{\,k}$ used for $Z(t)$ in the k^{th} spot of the product of operators.

Lemma 4.6.2. *Assume that ω_R is the vacuum state, and B is the Bosonic field operator $\varphi(f)$. Then,*

$$\beta_r(t,Z) \leq (\sqrt{2}\ \|f\|)^r\|Z\|\sqrt{r!}. \tag{4.79}$$

Proof of Lemma 4.6.2. Let $\mathcal{N}$ be the number operator. For all $\psi \in D(\mathcal{N}^{1/2})$, by (3.12)

$$\|\varphi(f)\psi\| \leq \sqrt{2}\|f\|\|(\mathcal{N}+1)^{1/2}\psi\|, \tag{4.80}$$

and hence

$$\|\varphi(f)(\mathcal{N}+1)^{-1/2}\| \leq \sqrt{2}\|f\|.$$

If we denote by $P_{\mathcal{N}\leq\nu}$ the spectral projection on the eigenspace of the set of eigenvalues $\{0,1,\cdots,\nu\}$, then by rewriting $\|\varphi(f)^k\Omega\|$ as

$$\|\varphi(f)(\mathcal{N}+1)^{-1/2}(\mathcal{N}+1)^{1/2}P_{\mathcal{N}\leq k-1}\cdots\varphi(f)(\mathcal{N}+1)^{-1/2}(\mathcal{N}+1)^{1/2}P_{\mathcal{N}\leq 0}\Omega\|$$

and using $\|(\mathcal{N}+1)^{1/2}P_{\mathcal{N}\leq\nu}\| = \sqrt{\nu+1}$, we obtain the upper bound

$$\|\varphi(f)^k\Omega\| \leq (\sqrt{2}\|f\|)^k\sqrt{k!}.$$

The last inequality is still valid if we replace $\varphi(f)$ by $\varphi(t) := e^{itH_R}\varphi(f)e^{-itH_R}$, i.e.

$$\|\varphi(t_1)\cdots\varphi(t_k)\Omega\| \leq (\sqrt{2}\|f\|)^k\sqrt{k!}. \tag{4.81}$$

Thus,

$$\big|\omega_R\big(\varphi(t_1)\cdots\widehat{Z(t)}^k\cdots\varphi(t_r)\big)\big| \;=\; \big|\langle\Omega,\varphi(t_1)\cdots\widehat{Z(t)}^k\cdots\varphi(t_r)\Omega\rangle\big| \tag{4.82}$$

is bounded by

$$\|Z\|\|\varphi(t_{(k-1)})\cdots\varphi(t_1)\Omega\|\|\varphi(t_k)\cdots\varphi(t_r)\Omega\|,$$

and by the last inequality we obtain

$$\big|\langle\Omega,\varphi(t_1)\cdots\widehat{Z(t)}^k\cdots\varphi(t_r)\;\Omega\rangle\big| \leq \|Z\|(\sqrt{2}\|f\|)^r\sqrt{(k-1)!(r-k+1)!}.$$

Note that the maximum attains when $k=1$ or $k=r+1$, hence (4.79) follows. ■

Proof of Theorem 4.3.2. The proof is along the lines of the proof of Proposition 4.5.3, with some minor changes as follows.

Lemma 4.6.3. *Let $Z\in\mathfrak{M}_R$. We have*

$$\omega(\tau^t_{\lambda,N}(Z)) \;=\; \omega_R(Z(t)) + K_{\lambda,N}(Z(t)) + O(\frac{\lambda^2}{N}), \tag{4.83}$$

with

$$\begin{aligned} K_{\lambda,N}(Z(t)) \;:=\; & \sum_{k=1}^{N}(\frac{\lambda i}{\sqrt{N}})^{2k}\int_0^t dt_1\cdots\int_0^{t_{2k-1}}dt_{2k}\sum_{\Lambda_k}^{*} \\ & \omega([G_{j_{2k}}(t_{2k})\otimes B(t_{2k}),[\cdots,[G_{j_1}(t_1)\otimes B(t_1),Z(t)]\cdots]]), \end{aligned} \tag{4.84}$$

where $\sum^*$ is a multiple sum over Λ_k of all k-element pairings $\{j_{\alpha_1}=j_{\beta_1},\ \ldots,\ j_{\alpha_k}=j_{\beta_k}\}$ of $2k$ indices $1\leq j_1,\cdots,j_{2k}\leq N$ with $\alpha_m<\beta_m$, $1\leq m\leq k$, so that j_{α_m}'s are distinct and taking values from $\{1,\cdots,N\}$.

Proof of Lemma 4.6.3. The Dyson series expansion of the dynamics yields

$$\omega(\tau^t_{\lambda,N}(Z)) = \omega_R(Z(t)) + \sum_{r=1}^{\infty} i^r \int_0^t dt_1 \cdots \int_0^{t_{r-1}} dt_r \; \omega(P_{r,N}(Z(t))), \tag{4.85}$$

where

$$P_{r,N}(Z(t)) = (\frac{\lambda}{\sqrt{N}})^r \sum_{j_1,j_2,\cdots,j_r=1}^{N} [G_{j_r}(t_r) \otimes B(t_r), [..., [G_{j_1}(t_1) \otimes B(t_1), Z(t)]]...], \tag{4.86}$$

and $Z(t) = \tau^t_{0,N}(Z) = e^{itH_R} Z e^{-itH_R}$.

Due to the vanishing odd-moment condition (4.12) on the state ω, the number of system interaction operators, r, must be even. Let $r = 2k$, $k \in \mathbb{N}$. Again by the vanishing odd-moment condition, the indices $j_1, \cdots, j_{2k}$ must be pairwise equal. We show that all terms with $r = 2k > 2N$ are of $O(\frac{\lambda^2}{N})$.

If $k > N$ and we have k pairs $j_{\alpha_1} = j_{\beta_1}$, ..., $j_{\alpha_k} = j_{\beta_k}$, then each of these pairs can take one of N values $1, 2, \cdots, N$ and therefore they cannot be distinct pairs. Hence, the leading term is of $O(N^{k-1})$. Considering the factor $(\frac{\lambda}{\sqrt{N}})^{2k}$ in (4.86), we produce terms which are of $O(\frac{\lambda^2}{N})$.

If $k \leq N$ then the leading term in N is exactly of order k provided that all k pairs are distinct. This is just the assignment of N values $1, 2, \cdots, N$ to k distinct pairs. Trivially, if the pairs are not all distinct then the order of multiple sum is of order less than k and the leading term in N and all lower order terms are of $O(\frac{\lambda^2}{N})$. Therefore, the only cases in which we produce a sum of order k, a leading term in N, is when $k \leq N$ and indices $j_{\alpha_1} = j_{\beta_1}$, ..., $j_{\alpha_k} = j_{\beta_k}$ are distinct.

Thus, the multiple sum in (4.86) gives rise to a multiple sum $\sum^*$ over Λ_k of all $\frac{(2k)!}{k!2^k}$ possibilities for forming k-element pairings $\{j_{\alpha_1} = j_{\beta_1}, ..., j_{\alpha_k} = j_{\beta_k}\}$ of $2k$ indices $1 \leq j_1, \cdots, j_{2k} \leq N$ with $\alpha_m < \beta_m$, $1 \leq m \leq k$, so that j_{α_m}'s are distinct and taking values from $\{1, \cdots, N\}$. Note that the multiple sum $\sum^*$ over Λ_k also involves k sums of the form $\sum_{j_\alpha = j_\beta = 1}^{N}$. The proof is now complete. ■

Next, we show in the following that the finite sum on the right side of (4.84) yields an N-independent operator $K_\lambda(Z(t))$, which is a function of λ analytic at $\lambda = 0$.

For any given element $\{j_{\alpha_1} = j_{\beta_1}, \cdots, j_{\alpha_k} = j_{\beta_k}\}$ of Λ_k, the expansion of the multi-commutator in (4.84) yields 2^{2k} different terms which are a product of operators $G_{j_\alpha}(t_\alpha)$, $G_{j_\beta}(t_\beta)$, $B(t_\alpha)$, $B(t_\beta)$, and $Z(t)$ with different ordering. Since for fixed α and β,

all $\omega_1(G_j(t_\alpha)G_j(t_\beta))$'s give the same value for any $j \in \{1, \cdots, N\}$, it is enough only to assign the lowest possible value to each index $j_\alpha = j_\beta$ and count the possibilities of this index arising from the corresponding sum $\sum_{j_\alpha=j_\beta=1}^{N}$. Therefore, because of distinctness of indices we may replace the sum $\sum_{j_{\alpha_1}=j_{\beta_1}=1}^{N}$ and its involved term $\omega_1(G_{j_{\alpha_1}}(t_{\alpha_1})G_{j_{\beta_1}}(t_{\beta_1}))$ by $N\omega_1(G(t_{\alpha_1})G(t_{\beta_1}))$, and the sum $\sum_{j_{\alpha_2}=j_{\beta_2}=1}^{N}$ and its involved term by $(N-1)\omega_1(G(t_{\alpha_2})G(t_{\beta_2}))$, etc. However, the expansion of mutli-commutator yields a reordering of (time) indices and hence we will also obtain terms of the form $\omega_1(G_{j_\beta}(t_\beta)G_{j_\alpha}(t_\alpha))$. Thus, we obtain product of k terms of the form $\omega_1(G(t_{\alpha'})G(t_{\beta'}))$ such that $(\alpha', \beta') = (\alpha, \beta)$ or $(\alpha', \beta') = (\beta, \alpha)$. Hence, if we use the notation $\sum^{2^{2k}}$ for the sum of 2^{2k} terms in the expanded multi-commutator in (4.84), we have

$$\begin{aligned} K_{\lambda,N}(Z(t)) &= \omega_R(Z(t)) + \sum_{k=1}^{N}(\lambda i)^{2k}\int_0^t dt_1 \cdots \int_0^{t_{2k-1}} dt_{2k} \\ &\quad \sum_{\Lambda_k}\sum^{2^{2k}}\prod_{m=1}^{k}\frac{(N-m+1)}{N}\,\omega_1(G(t_{\alpha'_m})G(t_{\beta'_m}))\,\omega_R(\mathcal{B}^{2k}(Z(t))), \quad (4.87) \end{aligned}$$

where $(\alpha'_m, \beta'_m) = (\alpha_m, \beta_m)$ or $(\alpha'_m, \beta'_m) = (\beta_m, \alpha_m)$, and $\mathcal{B}^{2k}(Z(t))$ is a product of $2k+1$ operators $B(t_1), \cdots, B(t_{2k})$, and $Z(t)$.

To remove N-dependency of $K_{\lambda,N}(Z(t))$, we first replace $\frac{N-m+1}{N}$ by 1 and then show that the error that we produce by this replacement is of $O(\frac{\lambda^2}{N})$. If we use $\frac{N-m+1}{N} = 1 - \frac{m-1}{N}$ in (4.87), then it splits to two terms so that the first one is what we want (an N-independent term) and the second one is a term which is of $O(\frac{\lambda^2}{N})$. Hence, the replacement of $\frac{N-m+1}{N}$ by 1 is justified.

Next, we use $\sum_{k=0}^{N} = \sum_{k=0}^{\infty} - \sum_{k>N}$ to replace $\sum_{k=0}^{N}$ by $\sum_{k=0}^{\infty}$. We show that the series converges and the error term corresponding to $\sum_{k>N}$ is of $O(\frac{\lambda^2}{N})$. Thus, (4.87) yields the N-independent relation

$$\begin{aligned} K_\lambda(Z(t)) &:= \sum_{k=0}^{\infty}(\lambda i)^{2k}\int_0^t dt_1 \cdots \int_0^{t_{2k-1}} dt_{2k} \sum_{\Lambda_k}\sum^{2^{2k}}\prod_{m=1}^{k} \\ &\quad \omega_1(G(t_{\alpha'_m})G(t_{\beta'_m}))\omega_R(\mathcal{B}^{2k}(Z(t)) \quad (4.88) \end{aligned}$$

which is analytic at $\lambda = 0$. To see the convergence of the series, if B is bounded, we use

$\beta_{2k}(t,Z) \leq \|Z\|\|B\|^{2k}$ and

$$\Big|\sum_{\Lambda_k}\sum^{2^{2k}}\prod_{m=1}^{k}\omega_1(G(t_{\alpha'_m})G(t_{\beta'_m}))\Big| \leq 2^{2k}\frac{(2k)!}{2^k k!}\|G\|^{2k}, \tag{4.89}$$

to obtain

$$|K_\lambda(Z(t))| \;\leq\; \|Z\|\sum_{k=0}^{\infty}\frac{(\sqrt{2}\lambda t\|G\|\|B\|)^{2k}}{k!}, \tag{4.90}$$

which proves the convergence for (any given $\lambda > 0$ and) all times $t < s_0$ with $s_0 = \infty$. When $B = \varphi(f)$, the Bosonic field operator, we may assume that ω_R is the vacuum state and apply the estimate (4.79) in Lemma 4.6.2 to show that $s_0 = (2\sqrt{2}|\lambda|\|f\|\|G\|)^{-1}$.

We now show that the error term corresponding to $\sum_{k>N}$, discussed above, is of $O(\frac{\lambda^2}{N})$. When B is bounded, we set $x := (\sqrt{2}\lambda t\|G\|\|B\|)^2$ and use a similar argument as in (4.70) and write

$$\begin{aligned}\sum_{k>N}\frac{x^k}{k!} &\leq \frac{x}{N+1}\sum_{k=N+1}^{\infty}\frac{x^{k-1}}{(k-1)!}\\ &\leq \frac{x}{N}e^x\\ &= O(\frac{\lambda^2}{N}).\end{aligned} \tag{4.91}$$

In the case of $B = \varphi(f)$, the error term $\sum_{k>N}$ is of $O(\frac{\lambda^2}{N})$ for all $t < s_0$ with $s_0 = (2\sqrt{2}\lambda\|f\|\|G\|)^{-1}$. The proof of the Theorem 4.3.2 is now complete. ■

Chapter 5

Summary and Future Work

We consider a system of N identical quantum particles coupled to an environment. The coupling is scaled in the mean-field way, and the particles only interact indirectly through the environment. In this thesis, we prove that the mean-field limit does exist if the initial system states satisfy a suitable condition that we call *the vanishing odd-moment condition*. We show that the condition is satisfied in particular for spin $\frac{1}{2}$ (qubit) systems. Assuming this condition, we show that the dynamics of any system observable becomes free (uncoupled) in the mean-field limit $N \to \infty$. We find the first order correction (and the second order when the first one is zero) for large but finite N. We show that the particles have a collective effect on reservoir: the dynamics of reservoir observables is not free in the mean-field limit. We give examples to illustrate our results.

In general, without imposing any condition on the system states, the mean-field limit does not exist due to the appearance of large combinatorial sums in the calculations. One direction of research is to find the necessary and sufficient condition for the existence of the mean-field limit in the above model. Studying the mean-field limit in more complicated open models is another direction of research. Additionally, it is interesting to find the meaning of our vanishing odd-moment condition in closed models. Moreover, it is physically of interest to find the entanglement entropies of the correction terms of the limiting dynamics. Thus, another direction of research is to find the entanglement entropies of the correction terms in Theorem 4.3.1.

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Appendix A

Mathematical Preliminaries

The field of scalars in all spaces is the field $\mathbb{C}$ of the complex numbers, unless otherwise stated.

A.1 Linear operators on Hilbert spaces

A **norm** on a vector space V is a function $\|\cdot\| : V \to \mathbb{R}$ satisfying the following properties for all $\lambda \in \mathbb{C}$ and $x, y \in V$.

(a) $\|x\| \geq 0$, and $\|x\| = 0 \Leftrightarrow x = 0$;

(b) $\|\lambda x\| = |\lambda| \, \|x\|$;

(c) $\|x + y\| \leq \|x\| + \|y\|$.

A vector space equipped with a norm is called a **normed vector space** or simply a **normed space**.

Example A.1.1. The space $C_b(X)$ of all continuous bounded functions $f : X \to \mathbb{C}$ on $X \subseteq \mathbb{R}^n$ endowed with the p-norm

$$\|f\|_p := \begin{cases} \sup\{|f(x)| : x \in X\}, & p = \infty \\ (\int_X |f(x)|^p dx)^{1/p}, & p \geq 1 \end{cases} \tag{A.1}$$

is a norm space. Here, we take integral with respect to the Lebesgue measure on $\mathbb{R}^n$.

An **inner product** on a vector space V is a function $\langle \cdot, \cdot \rangle : V \times V \to \mathbb{C}$ satisfying the following properties for all $\lambda \in \mathbb{C}$ and $x, y, z \in V$.

(a) $\langle x, x\rangle \geq 0$, and $\langle x, x\rangle = 0 \Leftrightarrow x = 0$;

(b) $\langle x, \lambda y + z\rangle = \lambda\langle x, y\rangle + \langle x, z\rangle$;

(c) $\langle x, y\rangle = \overline{\langle y, x\rangle}$.

An **inner product space** is a vector space V equipped with an inner product. Note that the inner product that we defined is linear in the second and anti-linear in the first component.

Example A.1.2. (a) The **Hermitian space** $\mathbb{C}^n$ of all complex n-tuples with the inner product $\langle z, w\rangle = \sum \bar{z_j} w_j$ is an inner product space, where $z = (z_1, \cdots, z_n)$ and $w = (w_1, \cdots, w_n)$.

(b) The space $M_n(\mathbb{C})$ of all complex n-square matrices with the inner product $\langle A, B\rangle = \mathrm{tr}(A^* B)$ is an inner product space, where $A^* = \bar{A}^t$;

(c) The **Lebesgue space** $L^2(\mathbb{R}^n) = \{f : \mathbb{R}^n \to \mathbb{C} \mid \int_{\mathbb{R}^n} |f(x)|^2 dx < \infty\}$ of square-integrable functions (with respect to Lebesgue measure on $\mathbb{R}^n$) endowed with the inner product $\langle f, g\rangle = \int_{\mathbb{R}^n} \overline{f(x)} g(x) dx$ is an important example of an inner product space.

(d) The **Sobolev space** $H^d(\mathbb{R}^n)$ of order $d \in \mathbb{N}$ is an inner product space. Elements of the Sobolev space of order d are all elements of $L^2(\mathbb{R}^n)$ whose partial derivatives up to order d belong to $L^2(\mathbb{R}^n)$. The inner product in the case of $H^1(\mathbb{R}^n)$ is given by

$$\langle f, g\rangle_{H^1} = \langle f, g\rangle + \sum_{j=1}^{n} \langle \frac{\partial f}{\partial x_j}, \frac{\partial g}{\partial x_j}\rangle. \tag{A.2}$$

Note that the inner product on the right hand side is the inner product of L^2.

Any inner product space is a normed space whose norm, induced by the inner product, is defined by $\|x\| := \sqrt{\langle x, x\rangle}$. In an inner product space V, the relation of inner products of elements and their norms is given by the **Cauchy-Schwartz inequality**. It states that for all $x, y \in V$,

$$|\langle x, y\rangle| \leq \|x\|\|y\|. \tag{A.3}$$

A collection $\{x_j\}$ of vectors in an inner product space is called **orthonormal set** if $\langle x_i, x_j\rangle = \delta_{ij}$, the Kronecker delta function.

Example A.1.3. Let $V = L^2([-L, L])$ for some positive number $L > 0$. The collection $\{f_k\}$ defined by

$$f_k(x) = \frac{1}{\sqrt{2L}} e^{2\pi i k x/L}, \quad (k \in \mathbb{Z}) \tag{A.4}$$

forms an orthonormal set in V.

A complete normed vector space is called a **Banach space**. A Banach space with a countable dense subset is called a **separable Banach space**.

Definition A.1.4. *A **Hilbert space** is a complete inner product space.*

All inner product spaces in Example A.1.2 are Hilbert spaces. In particular, all finite-dimensional inner product spaces are Hilbert spaces. Note that Hilbert spaces are all Banach spaces, but the converse is not true.

An orthonormal set $\{x_j\}$ in a Hilbert spaces $\mathcal{H}$ is called a **complete orthonormal set** or **orthonormal basis** if the collection of all finite linear combinations of x_j's is dense in $\mathcal{H}$. A Hilbert space is said to be **separable** if it has a countable orthonormal basis. The collection $\{f_k\}$ in Example A.1.3 is an example of an orthonormal basis. Therefore, the Hilbert space $L^2([-L, L])$ is a separable Hilbert space.

Note that all Hilbert spaces that we deal with are assumed to be separable.

Definition A.1.5. Suppose that $\mathcal{H}_1$ and $\mathcal{H}_2$ are Hilbert spaces. The set $\mathcal{H}$ of pairs (x_1, x_2) with $x_1 \in \mathcal{H}_1$ and $x_2 \in \mathcal{H}_2$ forms a Hilbert space whose inner product is given by

$$\langle (x_1, x_2), (y_1, y_2) \rangle = \langle x_1, y_1 \rangle_{\mathcal{H}_1} + \langle x_2, y_2 \rangle_{\mathcal{H}_2}. \tag{A.5}$$

The Hilbert space $\mathcal{H}$ is then called the **direct sum** of $\mathcal{H}_1$ and $\mathcal{H}_2$ and is denoted by $\mathcal{H}_1 \oplus \mathcal{H}_2$. The elements of this new space are often denoted by $x_1 \oplus x_2$.

The direct sum of a countable family of Hilbert spaces is constructed in the following way. Suppose $\{\mathcal{H}_n\}_{n \in N}$ is a sequence of Hilbert spaces, and $\mathcal{H}$ is the set of all sequences $\{x_n\}_{n \in \mathbb{N}}$ with $x_n \in \mathcal{H}_n$, satisfying

$$\sum_{n \geq 1} \|x_n\|^2_{\mathcal{H}_n} < \infty. \tag{A.6}$$

The space $\mathcal{H}$ under the natural inner product

$$\langle \{x_n\}, \{y_n\} \rangle = \sum_{n \geq 1} \langle x_n, y_n \rangle_{\mathcal{H}_n} \tag{A.7}$$

forms a Hilbert space and is denoted by $\mathcal{H} = \bigoplus_{n\geq 1} \mathcal{H}_n$.

Definition A.1.6. Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be two Hilbert spaces, and $\mathcal{K}$ be the span or finite linear combinations of all bilinear forms $x_1 \otimes x_2 : \mathcal{H}_1 \times \mathcal{H}_2 \to \mathbb{C}$ with $x_1 \in \mathcal{H}_1$ and $x_2 \in \mathcal{H}_2$ defined by

$$(x_1 \otimes x_2)(y_1, y_2) = \langle x_1, y_1\rangle_{\mathcal{H}_1} \langle x_2, y_2\rangle_{\mathcal{H}_2}. \tag{A.8}$$

By defining the inner product

$$\langle x_1 \otimes x_2, y_1 \otimes y_2\rangle_{\mathcal{K}} = \langle x_1, y_1\rangle_{\mathcal{H}_1} \langle x_2, y_2\rangle_{\mathcal{H}_2} \tag{A.9}$$

(and extending by linearity), $\mathcal{K}$ becomes an inner product space. The **tensor product** of $\mathcal{H}_1$ and $\mathcal{H}_2$ is now defined as the completion of $\mathcal{K}$ under the inner product $\langle\cdot,\cdot\rangle_{\mathcal{K}}$ and is denoted by $\mathcal{H}_1 \otimes \mathcal{H}_2$.

The construction of tensor product of n Hilbert spaces is straightforward. It is a fact that if $\{x_m\}$ and $\{y_n\}$ are orthonormal bases for Hilbert spaces $\mathcal{X}$ and $\mathcal{Y}$ respectively, then $\{x_m \otimes y_n\}$ is an orthonormal basis for $\mathcal{X} \otimes \mathcal{Y}$. As a result, in finite dimensional spaces, we have $\dim(\mathcal{X} \otimes \mathcal{Y}) = \dim(\mathcal{X}) \dim(\mathcal{Y})$, which can be extended to n Hilbert spaces, by induction.

A map $A : \mathcal{H}_1 \to \mathcal{H}_2$ on Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ is called a **linear transformation** if $A(\lambda x + \mu y) = \lambda A(x) + \mu A(y)$, for all $x, y \in \mathcal{H}_1$ and $\lambda, \mu \in \mathbb{C}$. When $\mathcal{H}_1 = \mathcal{H}_2 = \mathcal{H}$, the linear transformation A is called a **linear operator** on $\mathcal{H}$. A linear map $f : \mathcal{H} \to \mathbb{C}$ is called a **linear functional** on Hilbert space $\mathcal{H}$.

Recall that an operator A on $\mathcal{H}$ is called a **bounded operator** if there exists a constant $M > 0$ satisfying $\|Ax\| \leq M\|x\|$ for all $x \in \mathcal{H}$. The set of all bounded operators on $\mathcal{H}$ is denoted by $\mathcal{B}(\mathcal{H})$. For example, all linear operators on finite-dimensional spaces are bounded. For $A \in \mathcal{B}(\mathcal{H})$, we define **the operator norm** $\|A\|$ by

$$\|A\| := \sup\big\{\|Ax\| \mid x \in \mathcal{H},\ \|x\| = 1\big\}. \tag{A.10}$$

A map $T : \mathcal{H}_1 \to \mathcal{H}_2$ between Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ is said to be an **isomorphism** between $\mathcal{H}_1$ and $\mathcal{H}_2$ if T is a surjective map that preserves the inner product structures, i.e.,

$$\langle T(f), T(g)\rangle_{\mathcal{H}_2} = \langle f, g\rangle_{\mathcal{H}_1}. \tag{A.11}$$

It can easily be shown that every surjective map that preserves inner products must be an injective linear operator. Such a linear operator is called a **unitary operator**. When there is a unitary operator between two Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$, we say that the Hilbert spaces are **isomorphic** and we use the notation $\mathcal{H}_1 \simeq \mathcal{H}_2$. Observe that if U is a unitary operator then $\|U\| = 1$, hence bounded.

Example A.1.7. The map $T : L^2(\mathbb{R}^m) \otimes L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^m \times \mathbb{R}^n)$ which sends $\phi_1 \otimes \phi_2$ to $T(\phi_1 \otimes \phi_2)$ and is given by

$$(T(\phi_1 \otimes \phi_2))(x, y) := \phi_1(x)\phi_2(y), \quad (x, y) \in \mathbb{R}^m \times \mathbb{R}^n, \tag{A.12}$$

defines an isomorphism between $L^2(\mathbb{R}^m) \otimes L^2(\mathbb{R}^n)$ and $L^2(\mathbb{R}^m \times \mathbb{R}^n) \simeq L^2(\mathbb{R}^{m+n})$. Thus, under this isomorphism, we regard an element $\phi_1 \otimes \phi_2 \in L^2(\mathbb{R}^m) \otimes L^2(\mathbb{R}^n)$ as an element of $L^2(\mathbb{R}^m \times \mathbb{R}^n)$ and often simplify the notation by writing $(\phi_1 \otimes \phi_2)(x, y) := \phi_1(x)\phi_2(y)$.

We review generalities of unbounded operators in the next section.

A.2 Unbounded self-adjoint operators

Technically, we only require the operators to be defined on a 'dense' domain $D(A) \subset \mathcal{H}$. Such an operator is called a **densely defined operator**. Indeed, most of the quantum mechanical operators, including the operators representing position, momentum, and energy, are not defined on the whole space, but only on a dense subspace of the relevant Hilbert space. For example, the **position operator** $X : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ given by

$$X\psi(x) = x\psi(x)$$

is only defined on the domain $D(X)$ of all functions $\psi \in L^2(\mathbb{R})$ for which $X\psi$ is still an element of $L^2(\mathbb{R})$. The domain $D(X)$ is indeed a dense subspace of $L^2(\mathbb{R})$.

Definition A.2.1. *A densely defined operator $A : D(A) \subset \mathcal{H} \to \mathcal{H}$ is said to be* ***unbounded*** *if it is not bounded.*

In the following example, all operators A act on $\mathcal{H} = L^2(\mathbb{R}^n)$. Their domain $D(A)$ can obviously be taken $D(A) = \{\psi \in L^2(\mathbb{R}^n) \mid A(\psi) \in L^2(\mathbb{R}^n)\}$. One can precisely calculate the domain of each operator when needed.

Example A.2.2. Let $\mathbf{x} = (x_1, \cdots, x_n) \in \mathbb{R}^n$.

(a) (**Potential operator**) The multiplication by a continuous function $v : \mathbb{R}^n \to \mathbb{C}$ is a linear operator $V : \psi \mapsto V\psi$ with

$$(V\psi)(\mathbf{x}) = v(\mathbf{x})\psi(\mathbf{x}).$$

(b) (**Position operator**) The multiplication by a coordinate $x_j \in \mathbb{R}$ is a linear operator $X_j : \psi \mapsto X_j\psi$, where

$$(X_j\psi)(\mathbf{x}) = x_j\psi(\mathbf{x}), \quad 1 \leq j \leq n.$$

This operator is indeed an special case of the potential operator, when $V(\mathbf{x}) = x_j$.

(c) (**Momentum operator**) The differentiation operator $P_j : \psi \mapsto P_j\psi$ is a linear operator, where

$$(P_j\psi)(\mathbf{x}) = -i\frac{\partial}{\partial x_j}\psi(\mathbf{x}), \quad 1 \leq j \leq n.$$

(d) (**Laplacian**) The operator $\Delta : \psi \mapsto \Delta\psi$ is a linear operator, where

$$(\Delta\psi)(\mathbf{x}) = \sum_{j=1}^{n} \frac{\partial^2}{\partial x_j^2}\psi(\mathbf{x}).$$

(e) (**Schrödinger operator**) The operator $H : \psi \mapsto (-\Delta + V)\psi$ is a linear operator, where Δ and V are as in part (b) and (e).

Assuming V is a locally bounded function, the domains of all operators in the above example are dense subspaces of $L^2(\mathbb{R}^n)$, because they contain the dense subset $C_0^\infty(\mathbb{R}^n)$ of infinitely differentiable functions on $\mathbb{R}^n$ with compact support

$$\text{supp}(f) := \overline{\{\mathbf{x} \in \mathbb{R}^n | f(\mathbf{x}) \neq 0\}}.$$

If the potential function V is bounded, then the largest domain on which the Schrödinger operator H is defined is the Sobolev space $H^2(\mathbb{R}^n)$ of order 2.

Recall that the adjoint operator A^* of a bounded operator A on $\mathcal{H}$ can be defined by using the **Riesz Representation Theorem**:

Theorem A.2.3 (Riesz)**.** *If $\eta : \mathcal{H} \to \mathbb{C}$ is a bounded linear functional, then there exists a unique element $x \in \mathcal{H}$ such that $\eta(y) = \langle x, y\rangle$ for all $y \in \mathcal{H}$.*

If $A \in \mathcal{B}(\mathcal{H})$, then for any $\phi \in \mathcal{H}$, the linear functional $\langle \phi, A\cdot \rangle$ is bounded. Thus, by the Riesz Theorem, there is a unique $\chi \in \mathcal{H}$ such that $\langle \phi, A\cdot \rangle = \langle \chi, \cdot \rangle$. Then, we define the adjoint A^* of A by $A^*\phi := \chi$. Thus, $\langle \phi, A\psi \rangle = \langle A^*\phi, \psi \rangle$, for all $\psi \in \mathcal{H}$. It can be easily shown that A^* is bounded operator and $\|A^*\| = \|A\|$. Moreover,

$$(AB)^* = B^*A^*, \quad (A^*)^* = A, \quad (A^*)^{-1} = (A^{-1})^*, \quad \|A^*A\| = \|A\|^2.$$

Also, if U is a unitary operator, then $U^{-1} = U^*$ and vice versa.

The operator $A \in \mathcal{B}(\mathcal{H})$ is called **self-adjoint** if $A^* = A$. For example, the matrix

$$\begin{bmatrix} \alpha & \gamma \\ \overline{\gamma} & \beta \end{bmatrix}, \quad (\alpha, \beta \in \mathbb{R}) \tag{A.13}$$

is a self-adjoint operator on $\mathbb{C}^2$.

If A is unbounded, then the linear functional $\langle \phi, A\cdot \rangle$ is not necessarily bounded, but may be bounded for some ϕ. Thus, A^* is not defined on the whole space $\mathcal{H}$.

Definition A.2.4. *Let A be an operator defined on a dense subspace $D(A) \subset \mathcal{H}$, and let $D(A^*)$ be the set of all $\phi \in \mathcal{H}$ for which the linear functional*

$$\psi \mapsto \langle \phi, A\psi \rangle, \quad \psi \in D(A)$$

is bounded. For $\phi \in D(A^*)$, define $A^*\phi$ to be the unique element such that

$$\langle \phi, A\psi \rangle = \langle A^*\phi, \psi \rangle,$$

*for all $\psi \in D(A)$. The operator A^* defined on $D(A^*)$ is linear (as in the case of bounded A) and called the **adjoint** of A.*

In general, the adjoint operator A^* of a densely defined operator A may not be densely defined, see [40]. However, for the operators of interest in many applications the adjoint is also a densely defined operator.

Definition A.2.5. *An unbounded operator A on $\mathcal{H}$ is **symmetric** if*

$$\langle \phi, A\psi \rangle = \langle A\phi, \psi \rangle,$$

for all $\psi, \phi \in D(A)$.

Definition A.2.6. *An unbounded operator A on $\mathcal{H}$ is called* ***self-adjoint*** *if $D(A) = D(A^*)$ and $A^*\phi = A\phi$ for all $\phi \in D(A)$.*

All operators defined in Example A.2.2 are self-adjoint operators on their domains. Unbounded self-adjoint operators cannot be defined on the entire Hilbert space. Indeed, by the **Hellinger-Toeplitz Theorem**, any operator satisfying $\langle Ax, y\rangle = \langle x, Ay\rangle$ for all $x, y \in \mathcal{H}$ must be bounded. In other words, a symmetric operator A with $D(A) = \mathcal{H}$ is bounded.

An unbounded operator A is called an **extension** of an unbounded operator B if $D(A) \supset D(B)$ and $A = B$ on $D(B)$. Then, it can be proved that an unbounded operator is symmetric if and only if A^* is an extension of A. Thus, every self-adjoint operator is symmetric, but there are many operators that are symmetric without being self-adjoint. However, one can say that a symmetric operator A is self-adjoint if and only if $D(A) = D(A^*)$.

Definition A.2.7. *Let $A : D(A) \subset \mathcal{H} \to \mathcal{H}$ be an unbounded operator.*

(a) A is called a ***closed operator*** *if the graph $\Gamma(A) := \{(x, Ax) | x \in D(A) \subset \mathcal{H}\}$ of A is a closed subset of $\mathcal{H} \times \mathcal{H}$.*

(b) A is called ***closable*** *if the closure of the graph $\Gamma(A)$ in $\mathcal{H} \times \mathcal{H}$ is the graph of an operator. The closure of a closable operator is denoted by $\overline{A}$. If A is closable, then the operator $\overline{A}$ is defined by $\Gamma(\overline{A}) = \overline{\Gamma(A)}$.*

(c) A is called ***essentially self-adjoint*** *if A is symmetric and colsable and $\overline{A}$ is self-adjoint.*

Some of the properties of closed and adjoint operators are the following:

Proposition A.2.8. *(a) If A is an unbounded operator on $\mathcal{H}$, then the graph of A^* is closed in $\mathcal{H} \times \mathcal{H}$.*

(b) A symmetric operator is always closable. As a result,

(c) If A is closable on $\mathcal{H}$, then the adjoint of $\overline{A}$ is A^*.

(d) If A is essentially self-adjoint, then $\overline{A}$ is the unique self-adjoint extension of A.

Recall that the **inverse** of an operator $A \in \mathcal{B}(\mathcal{H})$ is an operator $B \in \mathcal{B}(\mathcal{H})$ so that $AB = BA = \mathbb{1}$. The inverse operator is usually denoted by A^{-1}.

Let $A \in \mathcal{B}(\mathbb{C}^n)$. The complex number λ is an **eigenvalue** of A if $\det(\lambda\mathbb{1} - A) = 0$. The set of all (at most n) such λ is called the **spectrum** of A and is denoted by $\sigma(A)$. If $\lambda \notin \sigma(A)$, then $\det(\lambda\mathbb{1} - A) \neq 0$ and $\lambda\mathbb{1} - A$ has an inverse.

Let $A \in \mathcal{B}(\mathcal{H})$. The spectrum of A is defined by $\sigma(A) := \mathbb{C} \setminus \rho(A)$, where $\rho(A)$ is the **resolvent set** of A and is defined by

$$\rho(A) := \{\lambda \in \mathbb{C} \mid \lambda\mathbb{1} - A \text{ is a bijection}\}. \tag{A.14}$$

By the **Inverse Mapping Theorem**, also known as **Banach Theorem**, if $\lambda\mathbb{1} - A$ is a bijection, then it has a bounded inverse.

Let $A \in \mathcal{B}(\mathcal{H})$. A non-zero element $x \in \mathcal{H}$ is called the **eigenvector** of A if $Ax = \lambda x$ for some $\lambda \in \mathbb{C}$ which is called the corresponding **eigenvalue**. It is clear that the set of all eigenvalues of A is a subset of $\sigma(A)$. This subset is called the **point spectrum** of A. If λ is not an eigenvalue of A and the range of $\lambda\mathbb{1} - A$ is not dense, then λ is said to be in the **residual spectrum** of A. Note also that the spectrum is a nonempty (compact) set even for (bounded) operators on Banach spaces. Trivially, $\sigma(\mathbb{1}) = \{1\}$.

For unbounded operators, we have a similar definition for spectrum.

Definition A.2.9. *Let A be an unbounded operator on $\mathcal{H}$. A number $\lambda \in \mathbb{C}$ belongs to the **resolvent set** of A if there exists a bounded operator B such that:*

(a) for all $\psi \in \mathcal{H}$, $B\psi$ belongs to the domain $D(A)$ of A and $(A - \lambda\mathbb{1})B\psi = \psi$,

(b) for all $\psi \in D(A)$, $B(A - \lambda\mathbb{1})\psi = \psi$.

*If no such bounded operator B exists, then λ belongs to the **spectrum** of A.*

As in the bounded case, even if A is self-adjoint, the points λ in the spectrum of an unbounded operator A are not necessarily eigenvalues. That is, there does not necessarily exist a non-zero $\psi \in D(A)$ with $A\psi = \lambda\psi$. However, if A is self-adjoint, then A has no residual spectrum and $\sigma(A)$ is a closed subset of $\mathbb{R}$. If, in addition, $A \in \mathcal{B}(\mathcal{H})$, then $\sigma(A) \subseteq [-\|A\|, \|A\|]$ and $\sigma(A)$ includes at least one of $\|A\|$ or $-\|A\|$.

Referring to Example A.2.2, the spectrum of the multiplication and differential operators is $\mathbb{R}$, the spectrum of the potential operator V is the closure of the range of v, and $\sigma(-\Delta) = [0, \infty)$.

An operator $P \in \mathcal{B}(\mathcal{H})$ is called a **projection** if $P^2 = P$. If in addition $P^* = P$, then P is called an **orthogonal projection**. A **finite-rank operator** is an operator

$A \in \mathcal{B}(\mathcal{H})$ whose range is finite dimensional. As an example, for any $\psi \in \mathcal{H}$ with $\|\psi\| = 1$, the operator $P_\psi : \mathcal{H} \to \mathcal{H}$ defined by

$$P_\psi(f) = \langle \psi, f \rangle \psi \tag{A.15}$$

is a rank 1 orthogonal projection. In general, if $\{\psi_j\}_{j=1}^N$ is an orthonormal set in $\mathcal{H}$, then the operator $P : \mathcal{H} \to \mathcal{H}$ defined by

$$P(f) = \sum_{j=1}^{N} \langle \psi_j, f \rangle \psi_j \tag{A.16}$$

is a rank N orthogonal projection.

Definition A.2.10. *An operator A is called **non-negative**, denoted by $A \geq 0$, if $\langle \psi, A\psi \rangle \geq 0$ for all $\psi \in D(A) \subset \mathcal{H}$. More generally, A is **bounded below** by $c \in \mathbb{R}$ if $\langle \psi, A\psi \rangle \geq c\|\psi\|^2$ for all $\psi \in D(A)$.*

Any non-negative bounded operator A is self-adjoint. (This result is not valid for real Hilbert spaces.) If $A \in \mathcal{B}(\mathcal{H})$, then A^*A is non-negative and hence self-adjoint. One can easily show that every orthogonal projection P is non-negative, $\sigma(P) = \{0, 1\}$, and $\|P\| = 1$. The unbounded operator $-\Delta$ in Example A.2.2 (e) is non-negative.

The spectrum of any non-negative unbounded self-adjoint operator is contained in $[0, \infty)$. More generally, if A is bounded below by c, then the spectrum of A is contained in $[c, \infty)$. Applying the spectral theorem for unbounded self-adjoint operators, that we shall discuss in the following, one can prove that the converse of the last two statements are also valid. In other words, one can prove, for instance, that if the spectrum of an unbounded self-adjoint operator A is contained in $[c, \infty)$, then A is bounded below by c. For details, see [40], for example.

Suppose A is a self-adjoint operator on a Hilbert space $\mathcal{H}$. If A is bounded, we can define the **exponential** of A by the norm-convergent series

$$e^{itA} := \sum_{n=0}^{\infty} \frac{(it)^n A^n}{n!}. \tag{A.17}$$

However, if A is unbounded and self-adjoint, we cannot define the exponential of A directly by power series. The best way to define the exponential of an unbounded self-adjoint operator A is to diagonalize A, using the **Spectral Theorem**.

In finite dimensions, the Spectral Theorem states that any self-adjoint matrix has an orthonormal basis of eigenvectors. There are three equivalent versions which are the different extensions of the finite-dimensional Spectral Theorem. We present less precise statements here. For precise statements of these three forms of the Spectral Theorem, their variants and proofs, see [61], for instance.

(1) Projection-valued measure. If $\lambda_1, \cdots, \lambda_J$ are the distinct eigenvalues of A, a finite-dimensional self-adjoint matrix, and E_j is the orthogonal projection onto $\{\psi \mid A\psi = \lambda_j\psi\}$, then the spectral theorem is equivalent to

$$A = \sum_{j=1}^{J} \lambda_j E_j. \tag{A.18}$$

Define a projection-valued measure $dE_\lambda = \sum_{j=1}^{J} \delta(\lambda - \lambda_j)E_j$. Then, (A.18) becomes

$$A = \int \lambda \, dE_\lambda, \tag{A.19}$$

where E_λ is a Stieltjes measure. This form does generalize if we allow measures beyond the finite pure point measure of the finite-dimensional case.

(2) Functional calculus. For any Banach space X, if $A \in \mathcal{L}(X)$, we can define $P(A)$ for any polynomial P or even we can define $f(A)$ for certain analytic functions f. In the finite-dimensional self-adjoint case, (A.18) allows us to define

$$f(A) = \sum_{j=1}^{J} f(\lambda_j)E_j \tag{A.20}$$

for any continuous function f, a definition that agrees with $P(A)$ if P is a polynomial. We can show that not only does the spectral theorem in the infinite-dimensional case allow one to define $f(A)$, one can go backwards from the functional calculus to the other forms.

(3) Multiplication operator. Suppose A is a finite-dimensional self-adjoint operator and suppose that the spectrum $\sigma(A)$ is simple, i.e., each E_j is one-dimensional. Let μ be the point probability measure

$$d\mu(x) = \frac{1}{n} \sum_{j=1}^{n} \delta(x - \lambda_j) \tag{A.21}$$

on $\mathbb{R}$. It can be proved that if $B : L^2(\mathbb{R}, d\mu) \to L^2(\mathbb{R}, d\mu)$ is the multiplication operator

$$(Bf)(x) = xf(x), \tag{A.22}$$

then A and B are unitarily equivalent. More precisely, there is a unitary transformation $U : \mathbb{C}^n \to L^2(\mathbb{R}, d\mu)$ such that $UAU^{-1} = B$. To accommodate degenerate eigenvalues, we need to allow direct sums of multiplication operators. Then, one form of the finite-dimensional spectral theorem is that A is unitarily equivalent to a direct sum of multiplications on $L^2(\mathbb{R}, d\mu_k)$ where μ_k is a pure point measure with only finitely many pure points. The corresponding form of the general spectral theorem is to say this is true in the infinite-dimensional case if we allow a general measure supported on $[-\|A\|, \|A\|]$.

We can use functional calculus to define the exponential e^{itA} of an unbounded self-adjoint operator A. Then, we can prove that $U : \mathbb{R} \to \mathcal{L}(\mathcal{H})$, defined by

$$U(t) := e^{itA}, \tag{A.23}$$

has the following properties:

$$U(t+s) = U(t)U(s), \qquad U(0) = \mathbb{1}, \qquad U(t)^* = U(-t), \tag{A.24}$$

and the mapping $t \mapsto U(t)\psi$ is continuous for all $\psi \in \mathcal{H}$. In other words, $U(t)$ is a one-parameter unitary group, or more precisely, a **strongly continuous one-parameter unitary group**.

An important application of the Spectral Theorem is Stone's Theorem which states that every unitary operator on a Hilbert space can be written as an exponential operator of the form e^{iA} for some self-adjoint operator A. More precisely,

Theorem A.2.11 (**Stone's Theorem**). *Let $t \in \mathbb{R}$. For any strongly continuous one-parameter unitary group $U(t)$, there exists a unique (not necessarily bounded) self-adjoint operator A on a Hilbert space $\mathcal{H}$ such that*

$$U(t) = e^{itA}. \tag{A.25}$$

Conversely, for any (not necessarily bounded) self-adjoint operator A on a Hilbert space $\mathcal{H}$, by the Spectral Theorem the one-parameter family $U(t)$ of the unitary operators defined

by

$$U(t) := e^{itA} \tag{A.26}$$

is a strongly continuous one-parameter group.

We finish the appendix by a brief review of definitions of trace and partial trace.

Definition A.2.12. *Let A be a non-negative operator on a Hilbert space $\mathcal{H}$ and $\{\psi_j\}$ be an orthonormal basis for $\mathcal{H}$. The **trace** of A is denoted by $\mathrm{tr}(A)$ and is defined by*

$$\mathrm{tr}(A) = \sum_j \langle \psi_j, A\psi_j \rangle.$$

*If $\mathrm{tr}(A) < \infty$, then A is called a **trace-class operator**. A general operator $A \in \mathcal{B}(\mathcal{H})$ is called **trace class** if the non-negative self-adjoint operator $\sqrt{A^*A}$ is a trace-class operator.*

Note that if A is a non-negative operator, then there exist a unique non-negative operator B satisfying $B^2 = A$, see [57]. Such an operator B is called the **square root** of A and is denoted by $\sqrt{A}$.

As a simple example for trace, one can easily show that for a rank N orthogonal projection P, $\mathrm{tr}(P) = N$.

Proposition A.2.13. *Let $A \in \mathcal{B}(\mathcal{H})$ be a trace-class operator. Then,*

(a) For any orthonormal basis $\{\psi_j\}$, the sum $\sum_j \langle \psi_j, A\psi_j \rangle$ is absolutely convergent, and the value of the sum is independent of the choice of the chosen orthonormal basis.

(b) If A is trace class, then so is A^* and $\mathrm{tr}(A^*) = \overline{\mathrm{tr}(A)}$.

(c) If $B \in \mathcal{B}(\mathcal{H})$, the operators AB and BA are also trace class and $\mathrm{tr}(AB) = \mathrm{tr}(BA)$.

Suppose that A is a trace-class operator and set $|A| := \sqrt{A^*A}$. Then, $\mathrm{tr}\,|A| < \infty$. The **trace norm** $\|A\|_1$ of A is defined by

$$\|A\|_1 := \mathrm{tr}\,|A|. \tag{A.27}$$

The relation

$$\|A\| \leq \|A\|_1 \tag{A.28}$$

holds between operator and trace norms. Thus, the **trace-norm topology** is weaker than the operator-norm topology.

Definition A.2.14. Let T be a linear operator on the Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$. The **partial trace** of T over $\mathcal{H}_A$ is the linear transformation $\mathrm{tr}_A : \mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B) \to \mathcal{L}(\mathcal{H}_B)$ defined by

$$\mathrm{tr}_A := \mathrm{tr} \otimes \mathbb{1}_B, \tag{A.29}$$

where tr is the trace functional on $\mathcal{L}(\mathcal{H}_A)$ and $\mathbb{1}_B$ is the identity operator in $\mathcal{L}(\mathcal{H}_B)$.

The transformation tr_B can be defined similarly. The partial trace commutes with the operation of taking the adjoint.