AN ACCURATE CALCULATION OF ELECTRON COLLISION WITH ATOMIC HYDROGEN AT LOW ENERGY

HOA THI NGUYEN

AN ACCURATE CALCULATION OF ELECTRON COLLISION WITH ATOMIC HYDROGEN AT LOW ENERGY

by

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Abstract

The Harris-Nesbet variational method is used to carry out accurate calculations for electron collisions with hydrogen atoms at low energy below the first hydrogenic excitation threshold. Calculations are done with the employment of different coupling schemes which are composed of the atomic hydrogen states and pseudo states and a great number of correlation terms. Singlet and triplet phase shifts are obtained for the partial waves L=0, 1, 2, 3, 4, 5, 6 and 7. Phase shifts at the nine energies, where experimental data of differential cross section are available, are obtained with the partial waves L equal to up to 18, and then used to deduce the elastic differential and total cross sections for electron collisions with hydrogen atoms at these energies. The results of the present Harris-Nesbet calculations are compared with those made available in literature by other research groups. The differential cross sections obtained are compared with experimental data, and an excellent agreement is found between the two.

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Chapter 1

Introduction

1.1 Introduction

The field of electron-atom collision has been considered to be important in practice and of great scientific interest since the last few decades. This is due to the fact that the understanding of these fundamental collision processes plays a significant role not only in the study of the dynamics of many-particle quantum systems but also in many other fields such as astrophysics, quantum chemistry, laser physics, etc. For example, in the modeling of non-equilibrium plasmas, it is necessary to have sufficient knowledge of cross sections for elastic scattering, excitation, ionization and recombination in electron collision with neutral and/or ionized atomic species.

Collision of electrons with hydrogen atoms has been of a particular interest to atomic collision theorists working in this area. This is because the wave functions of the hydrogen atom are known exactly, and hence these collision processes should be the best testing ground for the various approximation methods developed for use in the studies of electron-atom collision. Throughout the years, a significant number of theoretical investigations have been carried out for electron collisions with hydrogen atoms. In particular, for electron collisions with hydrogen atoms at energies below the first excitation threshold of H, one may cite, for instance, the work by Schwartz (1961) [1] who considered the Kohn variational method with the employment of 50 Hylleraas-type trial wave functions in a calculation of the S–wave phase shifts. Sloan (1964) [2] studied elastic scattering of electrons from atomic hydrogen, using the method of polarized orbitals. Armstead (1967) [3] also considered the Kohn variational method in the calculation of the P–wave phase shifts, using 84 Hylleraas-type trial wave functions. Calculations of electron-hydrogen-atom collision at low energy were also carried out by Burke et al. (1969) [4] for the lowest (S, P, D and F) partial waves. These authors employed a modified close-coupling expansion of the wave function for their calculations. Matese and Oberoi (1971) [5] also did calculations for S– and P–wave elastic scattering of electrons from atomic hydrogen by using the same modified close-coupling method. Das and Rudge (1976) [6] investigated elastic scattering of electrons from hydrogen atom for P partial wave using a variational method. Callaway (1978) [7] considered the Harris-Nesbet variational method to study electron collision with atomic hydrogen for S–, P–, D– and F–partial waves. Scholz et al. (1988) [8] studied elastic scattering of electrons from atomic hydrogen for S, P and D partial waves, using the R-matrix method. In 1992, Botero and Shertzer [9] used a direct numerical method to perform calculations of electron-hydrogen collision for S–, P– and D–partial waves. Bhatia and Temkin (2001) [10] obtained S-wave elastic scattering of electrons from hydrogen atom, using the complex-correlation Kohn T-matrix (CCKT) method.

On the experimental side, a few measurements of differential and total cross sections for electron collisions with atomic hydrogen have been made available in the literature. In an early work, Gilbody et al. (1961) [11] measured the differential cross sections for elastic scattering of electrons from atomic hydrogen at energies of 3.8, 5.7, 7.1 and 9.4 eV. Williams (1975) [12] employed the method of crossed electron and modulated atom beams to perform measurement of absolute differential cross sections at energies from 3.8 to 8.7 eV.

In recent years, Gien and Gien et al. [13-33] have employed the Harris-Nesbet variational method to carry out the accurate calculations of electron and positron collisions with atoms and ions, considering a large coupling scheme for the calculations. In particular, Gien (1998, 2000) [26, 27, 29] also did calculations of electron collisions with hydrogen atoms at low energy, as well as determined the sequences of Feshbach resonances below the *n*=2 H excitation threshold for this scheme. A large scheme, the so-called 13-state scheme, was considered for these calculations (Gien 1998 [26]). This scheme is composed of the thirteen states and pseudo states and believed to represent well the interaction effects of the collision between electrons and hydrogen atoms at their ground states. As was discussed by Gien previously (Gien, 1997 [25]), another possible choice of large schemes which could also provide accurate results of calculation at low energy is to select a basic set of states and pseudo states which can reasonably take into account the various interaction effects of the collision system and then to add to the scheme a large number of correlation terms that are to improve both short-range and long-range interaction effects of the collision system. To some extent, the second scheme may be preferred over the first one as it has advantage of being able to improve the accuracy of the results of calculation by increasing the number of correlation terms to be added to the scheme. In practice, the number of correlation terms to be included may be increased gradually until the results of phase shift and cross section obtained no longer change significantly.

For the work of this thesis, we shall use the Harris-Nesbet variational method to obtain accurate results of phase shift, differential and total cross section at low energies below the first excitation threshold for elastic scattering of electrons from atomic hydrogen, considering the coupling schemes of the second kind. We shall use the so-called extended 4-state (E4S) coupling scheme, which is composed of the $\left(1s, 2s, 2p, \overline{3p}\right)$ H states (P. G. Burke et al. 1969 [4]) plus a great number of correlation terms for our calculations. The reason for the choice of this scheme has been expounded in detail elsewhere (Gien, 1997 [25], 2002 [32]). This scheme can account for both the short-range and long-range interaction effects of the collision system rather adequately. In order to show that our results of phase shift and cross section obtained already reach their convergent values and should, thereby, be very accurate, we also carry out calculations with the so-called extended 6-state (E6S) scheme, which is composed of the $\left(1s, 2s, 2p, \overline{3s}, \overline{3p}, \overline{3d}\right)$ H states and pseudo states (Geltman and Burke, 1970 [34]) plus a large number of correlation terms, and the so-called 3-state (E3S) scheme, which consists of the (1s, 2s, 2p) H states supplemented by a great number of correlation terms (Burke et al. 1966 [35]). Furthermore, for comparison and to show the significant effect of the correlation terms on the phase shifts (and cross sections) obtained, we also do calculations with the 3S, 4S and 6S coupling schemes which are composed of the (1s, 2s, 2p) H, $\left(1s, 2s, 2p, \overline{3p}\right)$ H and $\left(1s, 2s, 2p, \overline{3s}, \overline{3p}, \overline{3d}\right)$ H states respectively, without including the correlation terms. The results of our calculations will be compared with the theoretical values obtained by other groups who employ different numerical methods. They will also be compared with experimental data of differential cross section measured by Williams (1975) [12]. In view of the reliability of the Harris-Nesbet variational method in producing very accurate results for phase shifts and cross sections in electron and positron collisions with hydrogen atoms at low energy (Gien and Gien et al. [13-33]), our results may serve to double-check the accuracy of the results obtained by other authors for this process.

1.2 Outline of the thesis

The thesis will be organized as follow. In chapter 2, we shall describe the Harris-Nesbet variational method in electron (positron) collisions with atomic targets. We shall also briefly show how the method will be used for the special case of hydrogen atoms as targets. The method of calculation and numerical results of elastic electron-hydrogen collision below the first excitation threshold of H will be presented in Chapter 3 with discussion. We shall summarize the results of our work in chapter 4.

Chapter 2

The Harris-Nesbet Variational Method

The Hulthe′n - Kohn method (1944) [36], (1948) [37, 38] is a well-known variational method developed for collision problems. This method is based directly on the differential variational principles. One of the earliest applications of the Hulthe′n - Kohn method was done by Schwartz (1961) [1] to study S−wave elastic scattering of electrons from hydrogen atom, using 50 trial wave functions of Hylleraas type. Even though Schwartz obtained the results of phase shift below the first excitation threshold which are believed to be close to the exact values, he occasionally encountered large deviations (Schwartz (1961) [1, 39], Seiler et al. (1971) [40]) in his results. In order to avoid these fluctuations, Harris (1967) [41] proposed an expansion method for calculations of phase shift and cross section in atomic collision theory. The detail of this method which is, subsequently, known as the Harris variational method, will be discussed in the first section of this chapter.

2.1 Harris's expansion approach

For a single-channel scattering process with Hamiltonian H and wave function Ψ at energy E, the Schrödinger 's equation is

$$(H - E)\Psi = 0 \tag{2.1}$$

Following Harris (1967) [41], the total wave function Ψ can be expanded in the form

$$\Psi = \Phi + \alpha_0 S + \alpha_1 C , \tag{2.2}$$

S and C are asymptotic eigenfunctions of the Hamiltonian H at large distance r. The coefficients α_i in Eq. (2.2) ($i = 0,1$ corresponding to S and C functions respectively) characterize the scattering processes. They define the relative amplitude of the S and C functions, and thereby the phase shift of the scattering process.

The total wave function Ψ is to represent the electron-atom collision system at both short and long distance r. Since S and C in Eq. (2.2) only take care of the collisional state at large distance, it is necessary to include in Ψ a short-range wave function Φ to represent it at a short distance. The function Φ, which is known as the bound-part of Ψ, should be chosen in such a way that it is normalizable and does not affect the asymptotic behavior of Ψ at large distance. Thus, one starts by choosing a set of bound-state functions η_i, $i = 1,\ldots,n$ which can be canonically transformed into a basis that diagonalizes the Hamilltonian H in the subspace spanned by the functions η_i. This is equivalent to constructing and solving the finite matrix equation:

$$(\mathbf{H} - \mathbf{ES})\mathbf{X} = 0 , \tag{2.3}$$

where $H_{ij} = \langle \eta_i | H | \eta_j \rangle$ and $S_{ij} = \langle \eta_i | \eta_i \rangle$ are elements of the Hamiltonian matrix $\mathbf{H}$ and the overlap matrix $\mathbf{S}$, respectively. Solving Eq. (2.3), one obtains a set of the eigenfunctions $\varphi_i = X_i$ corresponding to a set of the eigenvalues E_i, $i = 1,\ldots,n$, that forms the basis mentioned above. The short-range function Φ can now be expanded in terms of this basis set

$$\Phi = \sum_{i=1}^{n} C_i \varphi_i \tag{2.4}$$

The coefficients C_i in Eq. (2.4) are determined by the (variational) conditions that the state $(H - E)\Psi$ has no components in the subspace spanned by the basis of eigenfunctions φ_i, i.e.

$$\langle \varphi_i | H - E | \Psi \rangle = 0 \text{, } i=1,\dots, n, \tag{2.5}$$

or

$$\sum_{j=1}^{n} \langle \varphi_i | H - E | \varphi_j \rangle C_j = -\langle \varphi_i | H - E | \alpha_0 S + \alpha_1 C \rangle \text{, } i=1,\dots, n. \tag{2.6}$$

The internal function Φ (bound part) and the external functions *S* and *C* are quadratically integrable and connected at the boundary. At energy $E=E_i$, Eq. (2.6) becomes

$$\alpha_0 \langle \varphi_i | H - E_i | S \rangle + \alpha_1 \langle \varphi_i | H - E_i | C \rangle = 0, \tag{2.7}$$

that can be solved for the ratio ${}^{\alpha_1}\!/_{\alpha_0}$. This ratio is nothing else but the tangent of the phase shift of the scattering process.

To summarize, the Harris's expansion approach consists of the following steps. First, one chooses a set of basis functions η_i, $i = 1,\dots,n$ and diagonalizes the Hamiltonian *H*. One then picks an eigenvalue E_i that corresponds to a relevant scattering solution X_i. Next, one defines the specific forms of the asymptotic functions *S* and *C* at this energy. Finally, one solves for α_1/α_0 from which one deduces the phase shift of the scattering process at energy E_i.

This method, however, has some limitation in obtaining the scattering information of a collision process. Indeed, it can provide the scattering information only at a discrete set of energies which are eigenvalues of H corresponding to the set of basis functions chosen. One can, of course, always adjust the parameters of the set of basis functions η_i to get a desired scattering energy, but this procedure would require a tremendous amount of time (and also computer time) to achieve. Nesbet (1968) [42] proposed a method, referred to as the Harris-Nesbet variational method, which is just an extension of the Harris one but allows for the calculation of phase shifts and cross sections at any arbitrary scattering energy. We shall describe this method in the subsequent section.

2.2 The Harris-Nesbet variational method

2.2.1 Single-channel scattering process

It is convenient to rewrite the total wave function Ψ in the form given by Schwartz (1961) [1, 39]

$$\Psi = \alpha_0(\Phi_S + S) + \alpha_1(\Phi_C + C), \tag{2.8}$$

in which the bound part Φ is divided into two parts Φ_S and Φ_C corresponding to the free functions S and C. The procedure used to construct the bound parts Φ_S and Φ_C is similar to the one of the Harris's expansion approach. Assuming that the numerical set of basis functions φ_i, $i=1,\ldots,n$ has already been found, the bound parts Φ_S and Φ_C can be written as

$$\Phi_S = \sum_{i=1}^{n} C_i^S \varphi_i, \tag{2.9}$$

$$\Phi_C = \sum_{i=1}^{n} C_i^C \varphi_i. \tag{2.10}$$

The conditions (2.5) that allow the determination of the coefficients C_i^S and C_i^C in this case are

$$\sum_{j=1}^{n} \langle \varphi_i | H - E | \alpha_0 \varphi_j \rangle C_j^S = -\langle \varphi_i | H - E | \alpha_0 S \rangle, \; i=1,\ldots, n, \tag{2.11}$$

$$\sum_{j=1}^{n} \langle \varphi_i | H - E | \alpha_1 \varphi_j \rangle C_j^C = -\langle \varphi_i | H - E | \alpha_1 C \rangle, \; i=1,\ldots, n \tag{2.12}$$

The free parts S and C are the so-called sin-like and cosine-like functions which have the asymptotic forms proportional to $\sin(kr - \frac{1}{2} l\pi)$ and $\cos(kr - \frac{1}{2} l\pi)$ respectively

$$S(r) \sim \sin(kr - \frac{1}{2} l\pi) \;, \tag{2.13}$$

$$C(r) \sim \cos(kr - \frac{1}{2} l\pi) \tag{2.14}$$

As usual, the variational functional Ξ for the case of one-channel scattering is

$$\Xi = \langle \Psi | H - E | \Psi \rangle \tag{2.15}$$

Substituting Eq. (2.8) into Eq. (2.15) and applying the conditions (2.11) and (2.12), one obtains the variational functional Ξ as

$$\Xi = m_{00}\alpha_0^2 + (m_{01} + m_{10})\alpha_0\alpha_1 + m_{11}\alpha_1^2, \tag{2.16}$$

where

$$m_{00} = (S|H - E|\Phi_S + S), \tag{2.17}$$

$$m_{11} = (C|H - E|\Phi_C + C), \tag{2.18}$$

$$m_{01} = (S|H - E|\Phi_C + C), \tag{2.19}$$

$$m_{10} = (C|H - E|\Phi_S + S), \tag{2.20}$$

m_{10} and m_{01} satisfy the following relation

$$m_{01} - m_{10}^{+} = \frac{1}{2}I, \tag{2.21}$$

where m_{10}^{+} is the Hermitian adjoint of m_{10}, and I is the unit 1×1 matrix.

Thus, the infinitesimal variation of the functional Ξ is

$$\delta\Xi = 2m_{00}\alpha_0\delta\alpha_0 + 2m_{11}\alpha_1\delta\alpha_1 + (m_{01} + m_{10})(\alpha_0\delta\alpha_1 + \alpha_1\delta\alpha_0). \tag{2.22}$$

In the Kohn variational method (Nesbet (1980) [43]), the matrices α_0 and α_1 are defined as

$$\alpha_0 = I, \qquad \alpha_1 = R, \tag{2.23}$$

and hence

$$\delta\alpha_0 = 0, \qquad \delta\alpha_1 = \delta R. \tag{2.24}$$

Applying Eqs (2.21), (2.23) and (2.24) into Eq. (2.22), one deduces that

$$\delta\Xi = 2(m_{10} + m_{11}R)\delta R + \frac{1}{2}\delta R. \tag{2.25}$$

One can choose a trial matrix $R_{(0)}$ such that

$$m_{10} + m_{11} R_{(0)} = 0\,, \tag{2.26}$$

or

$$R_{(0)} = -m_{11}^{-1} m_{10}\,. \tag{2.27}$$

With this choice, Eq. (2.25) reduces to

$$\delta\left(\Xi\left(R_{(0)}\right) - \frac{1}{2} R_{(0)} \right) = 0\,, \tag{2.28}$$

or

$$\delta[R] = 0. \tag{2.29}$$

Thus,

$$[R] = R_{(0)} - 2\Xi\left(R_{(0)}\right) \tag{2.30}$$

is the Kohn functional and is stationary. Using Eqs (2.16), (2.21), (2.23) and (2.27), one obtains

$$[R] = -2\left(m_{00} - m_{10}^{+} m_{11}^{-1} m_{10}\right). \tag{2.31}$$

Eq. (2.31) is known as the Kohn formula for a single-channel scattering process. Analogous formulas are also obtained in the inverse Kohn variational method. Here, the matrices α_0 and α_1 are defined as (Nesbet (1980) [43])

$$\alpha_0 = R^{-1}, \qquad \alpha_1 = I\,, \tag{2.32}$$

i.e.,

$$\delta\alpha_0 = \delta R^{-1}, \qquad \delta\alpha_1 = 0\,. \tag{2.33}$$

After substituting Eqs (2.32) and (2.33) into Eq. (2.22), one obtains the infinitesimal variation of the variational functional Ξ as

$$\delta\Xi = 2\left(m_{01} + m_{00}R^{-1}\right)\delta R^{-1} - \frac{1}{2}\delta R^{-1}. \tag{2.34}$$

In this case, $R_{(0)}^{-1}$ can be chosen such that

$$m_{01} + m_{00}R_{(0)}^{-1} = 0 \ , \tag{2.35}$$

or

$$R_{(0)}^{-1} = -m_{00}^{-1}m_{01}. \tag{2.36}$$

With this choice, Eq. (2.34) becomes

$$\delta\left(\Xi\left(R_{(0)}^{-1}\right) + \frac{1}{2}R_{(0)}^{-1} \right) = 0 \ , \tag{2.37}$$

or

$$\delta\left[R^{-1}\right] = 0 \ . \tag{2.38}$$

Thus,

$$\left[R^{-1}\right] = R_{(0)}^{-1} + 2\Xi_{\mu\nu}\left(R_{(0)}^{-1}\right) \tag{2.39}$$

is the inverse Kohn functional and is stationary. Using Eqs. (2.16), (2.21), (2.32) and (2.36), one arrives at the following formula for the inverse reactance matrix in the inverse Kohn variational method

$$\left[R^{-1}\right] = 2\left(m_{11} - m_{01}^{+}m_{00}^{-1}m_{01}\right). \tag{2.40}$$

2.2.2 Multi-channel scattering process

After succeeding in improving the Harris method to enable the calculations of the scattering parameters at any arbitrary energy for the case of single-channel scattering

(Nesbet 1968 [42]), Nesbet (1969) [44] extended his method to the multi-channel scattering case. Details of the Harris-Nesbet variational method for multi-channel scattering will be presented in this section.

At a given system energy *E*, if the collision system has n_C open channels, the total wave function of the entrance channel μ, Ψ^{μ}, is expressed in terms of n_C open-channel wave functions as

$$\Psi^{\mu} = \sum_{p=1}^{n_C} \left\{ \alpha_{0p\mu} \left(\Phi_S^p + S_p \right) + \alpha_{1p\mu} \left(\Phi_C^p + C_p \right) \right\}. \tag{2.41}$$

Again, assuming that a set of basis functions $\varphi_{p,i}$, $i=1,\ldots,n$ has already been obtained by using the procedure of the Harris method, the bound functions Φ_S^P and Φ_C^P corresponding to the free functions S_p and C_p can be written as

$$\Phi_S^p = \sum_{i=1}^{n_p} C_{p,i}^S \varphi_{p,i} \ , \tag{2.42}$$

$$\Phi_C^p = \sum_{i=1}^{n_p} C_{p,i}^C \varphi_{p,i} \ . \tag{2.43}$$

Again, the coefficients $C_{p,i}^S$ and $C_{p,i}^C$ are determined by the (variational) conditions that $(H - E)\Psi^{\mu}$ have no component in the subspace spanned by the basis functions $\varphi_{p,i}$, i.e.

$$\left(\varphi_{p,i} \middle| H - E \middle| \Psi^{\mu} \right) = 0 \, , \tag{2.44}$$

or

$$\sum_{j=1}^{n_q} \sum_{q=1}^{n_c} \left(\varphi_{p,i} \middle| H - E \middle| \alpha_{0q\mu} \left(\Phi_S^q + S_q \right) \right) = 0 \, , \tag{2.45}$$

$$\sum_{j=1}^{n_q}\sum_{q=1}^{n_c}\left(\varphi_{p,i}\middle|H-E\middle|\alpha_{1q\mu}\left(\Phi_C^q+C_q\right)\right)=0\,. \tag{2.46}$$

In the case of multi-channel scattering, the variational functional involving the entrance channels of wave functions Ψ^{μ} and Ψ^{ν} is defined as

$$\Xi_{\mu\nu}=\left\langle\Psi^{\mu}\middle|H-E\middle|\Psi^{\nu}\right\rangle. \tag{2.47}$$

Substituting Eq. (2.41) into Eq. (2.47), one obtains

$$\Xi_{\mu\nu}=\sum_{p,q=1}^{n_C}\sum_{i,j=0}^{1}\alpha_{ip\mu}^{+}m_{ij}^{pq}\alpha_{jq\nu}\,, \tag{2.48}$$

where

$$m_{ij}^{pq}=M_{ij}^{pq}-\sum_{\mu}\sum_{\nu}M_{i}^{p\mu}\left(M^{-1}\right)_{\mu\nu}M_{j}^{\nu q}\,, \tag{2.49}$$

or

$$m_{ij}^{pq}=M_{ij}^{pq}-\sum_{k}M_{i}^{pk}\left(E-E_k\right)^{-1}M_{j}^{kq}\,. \tag{2.50}$$

Here, $i,\ j=0$ or 1 correspond to the free functions *S* or *C*. Thus, the explicit forms of the m-matrix elements (given by Eq. (2.50)) for the different cases of *S* and *C* functions are

$$m_{00}^{pq}=M_{SS}^{pq}-\sum_{k}M_{S}^{pk}\left(E-E_k\right)^{-1}M_{S}^{kq}\,, \tag{2.51}$$

$$m_{01}^{pq}=M_{SC}^{pq}-\sum_{k}M_{S}^{pk}\left(E-E_k\right)^{-1}M_{C}^{kq}\,, \tag{2.52}$$

$$m_{10}^{pq}=M_{CS}^{pq}-\sum_{k}M_{C}^{pk}\left(E-E_k\right)^{-1}M_{S}^{kq}\,, \tag{2.53}$$

$$m_{11}^{pq}=M_{CC}^{pq}-\sum_{k}M_{C}^{pk}\left(E-E_k\right)^{-1}M_{C}^{kq}\,. \tag{2.54}$$

The M matrices seen in Eqs. (2.50), (2.51), (2.52), (2.53) and (2.54) are the so-called bound-bound, bound-free and free-free ones. A bound-bound matrix element of *H-E* connects a bound state with a bound state

$$M_{\mu\nu} = \left(\Phi_{\mu}\middle|H-E\middle|\Phi_{\nu}\right), \tag{2.55}$$

while a bound-free matrix element connects a bound state with a free one such as

$$M_{S}^{pk} = \left\langle S_{q}\middle|H-E\middle|\Phi_{k}\right\rangle, \tag{2.56}$$

$$M_{C}^{pk} = \left\langle C_{p}\middle|H-E\middle|\Phi_{k}\right\rangle, \tag{2.57}$$

and a free-free matrix element of *H-E* connects a free state with a free state such as

$$M_{SS}^{pq} = \left\langle S_{p}\middle|H-E\middle|S_{q}\right\rangle, \tag{2.58}$$

$$M_{SC}^{pq} = \left\langle S_{p}\middle|H-E\middle|C_{q}\right\rangle, \tag{2.59}$$

$$M_{CS}^{pq} = \left\langle C_{p}\middle|H-E\middle|S_{q}\right\rangle, \tag{2.60}$$

$$M_{CC}^{pq} = \left\langle C_{p}\middle|H-E\middle|C_{q}\right\rangle. \tag{2.61}$$

More explicitly, the matrices α and m are written as

$$\alpha = \begin{pmatrix} \alpha_0 \\ \alpha_1 \end{pmatrix}, \tag{2.62}$$

$$\mathrm{m} = \begin{pmatrix} \mathrm{m}_{00} & \mathrm{m}_{01} \\ \mathrm{m}_{10} & \mathrm{m}_{11} \end{pmatrix}. \tag{2.63}$$

The matrices α_0 and α_1 in Eq. (2.62) are related to the reactance matrix R as

$$\mathrm{R} = \alpha_1 \alpha_0^{-1} \text{ if } \alpha_0 \text{ is not singular}$$

and to the inverse reactance matrix R^{-1} as

$$R^{-1} = \alpha_0 \alpha_1^{-1} \text{ if } \alpha_1 \text{ is not singular.}$$

If Ψ^{μ} is an exact solution of the Schrödinger equation

$$(H - E)\Psi^{\mu} = 0, \tag{2.64}$$

then

$$m\alpha = \begin{pmatrix} m_{00} & m_{01} \\ m_{10} & m_{11} \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \alpha_1 \end{pmatrix} = 0 \ , \tag{2.65}$$

where α_i and m_{ij} are $n_C \times n_C$ matrices (in the case when n_c scattering channels are open)

$$\alpha_i = \begin{pmatrix} \alpha_i^{11} & \dots & \alpha_i^{1n_C} \\ \dots & \dots & \dots \\ \alpha_i^{n_C 1} & \dots & \alpha_i^{n_C n_C} \end{pmatrix}, \tag{2.66}$$

$$m_{ij} = \begin{pmatrix} m_{ij}^{11} & \dots & m_{ij}^{1n_C} \\ \dots & \dots & \dots \\ m_{ij}^{n_C 1} & \dots & m_{ij}^{n_C n_C} \end{pmatrix}, \tag{2.67}$$

with $i, j = 0,1$.

It should be noted that m_{00} and m_{11} are Hermitian while m_{10} and m_{01} are not. They satisfy the following relation:

$$m_{01} - m_{10}^{+} = \frac{1}{2} I. \tag{2.68}$$

Here, m_{10}^{+} denotes the Hermitian adjoint of m_{10}, and I is the $n_C \times n_C$ unit matrix.

The variational functional $\Xi_{\mu\nu}$ (Eq. (2.48)) can be rewritten in matrix form as

$$\Xi_{\mu\nu} = \alpha^{+} m \alpha, \tag{2.69}$$

$$= \alpha_0^{+}(m_{00}\alpha_0 + m_{01}\alpha_1) + \alpha_1^{+}(m_{10}\alpha_0 + m_{11}\alpha_1). \tag{2.70}$$

Thus, the infinitesimal variation of $\Xi_{\mu\nu}$ is given by

$$\delta\Xi_{\mu\nu} = \delta\alpha^{+} m\alpha + (m\alpha)^{+}\delta\alpha + \alpha^{+}(m - m^{+})\delta\alpha . \tag{2.71}$$

Substituting Eqs. (2.62), (2.63) and (2.68) into Eq. (2.71) yields

$$\delta\Xi_{\mu\nu} = \delta\alpha^{+} m\alpha + (m\alpha)^{+}\delta\alpha + \frac{1}{2}\left(\alpha_0^{+}\delta\alpha_1 - \alpha_1^{+}\delta\alpha_0\right) . \tag{2.72}$$

In the Kohn variational method, the matrices α_0 and α_1 are defined as

$$\alpha_0 = I, \qquad \alpha_1 = R . \tag{2.73}$$

This implies

$$\delta\alpha_0 = 0, \qquad \delta\alpha_1 = \delta R . \tag{2.74}$$

The infinitesimal variation of the functional $\Xi_{\mu\nu}$ in the Kohn method can, therefore, be written as

$$\delta\Xi_{\mu\nu} = \delta R^{+}(m_{10} + m_{11}R) + (m_{10} + m_{11}R)^{+}\delta R + \frac{1}{2}\delta R . \tag{2.75}$$

Now, if one chooses a trial matrix $R_{(0)}$ such that

$$m_{10} + m_{11}R_{(0)} = 0 , \tag{2.76}$$

or

$$R_{(0)} = -m_{11}^{-1}m_{10} , \tag{2.77}$$

then Eq. (2.75) reduces to

$$\delta\left(\Xi_{\mu\nu}(R_{(0)}) - \frac{1}{2}R_{(0)}\right) = 0 , \tag{2.78}$$

or

$$\delta[R]=0. \tag{2.79}$$

Eqs. (2.78) and (2.79) imply that

$$[R]=R_{(0)}-2\Xi_{\mu\nu}\left(R_{(0)}\right) \tag{2.80}$$

is the Kohn variational functional and is stationary. Using Eqs. (2.70), (2.73) and (2.77), one arrives at

$$[R]=-2\left(m_{00}-m_{10}^{+}m_{11}^{-1}m_{10}\right) \tag{2.81}$$

Eq. (2.81), which gives the stationary reactance matrix R in the Kohn variational method, is the Kohn formula for the multi-channel scattering case.

In the inverse Kohn variational method, the matrices α_0 and α_1 are defined as (Nesbet (1980) [43])

$$\alpha_0=R^{-1}, \qquad \alpha_1=I. \tag{2.82}$$

This implies

$$\delta\alpha_0=\delta R^{-1}, \qquad \delta\alpha_1=0. \tag{2.83}$$

Substituting Eqs (2.82) and (2.83) into Eq. (2.72), one obtains the infinitesimal variation of the functional $\Xi_{\mu\nu}$ as

$$\delta\Xi_{\mu\nu}=\delta R^{-1+}\left(m_{01}+m_{00}R^{-1}\right)+\left(m_{01}+m_{00}R^{-1}\right)^{+}\delta R^{-1}-\frac{1}{2}\delta R^{-1}. \tag{2.84}$$

In this case, a trial inverse matrix $R_{(0)}^{-1}$ can be chosen for R^{-1} such that

$$m_{01}+m_{00}R_{(0)}^{-1}=0\ , \tag{2.85}$$

or

$$R_{(0)}^{-1}=-m_{00}^{-1}m_{01}. \tag{2.86}$$

With this choice, Eq. (2.84) becomes

$$\delta\left(\Xi_{\mu\nu}\left(\mathrm{R}_{(0)}^{-1}\right)+\frac{1}{2}\mathrm{R}_{(0)}^{-1} \right)=0 \ , \tag{2.87}$$

or

$$\delta\left[\mathrm{R}^{-1}\right]=0 \ . \tag{2.88}$$

The stationary value of the inverse Kohn functional $\left[\mathrm{R}^{-1}\right]$ is, therefore, given by

$$\left[\mathrm{R}^{-1}\right]=\mathrm{R}_{(0)}^{-1}+2\Xi_{\mu\nu}\left(\mathrm{R}_{(0)}^{-1}\right) . \tag{2.89}$$

Using Eqs. (2.70), (2.82) and (2.86), one arrives at

$$\left[\mathrm{R}^{-1}\right]=2\left(\mathrm{m}_{11}-\mathrm{m}_{01}^{+}\mathrm{m}_{00}^{-1}\mathrm{m}_{01}\right). \tag{2.90}$$

Eq. (2.90), which gives the inverse reactance matrix R^{-1} in the inverse Kohn variational method, is the so-called inverse Kohn formula for the multi-channel scattering case.

2.3 The Harris-Nesbet variational method for electron collisions with atomic hydrogen

In this section, we shall discuss the Harris-Nesbet variational method within the context of the collision of electrons with hydrogen atoms. As is well-known, the Hamiltonian of an electron-atomic-hydrogen collision system is

$$H=-\frac{1}{2}\vec{\nabla}_{r_1}^2-\frac{1}{2}\vec{\nabla}_{r_2}^2-\frac{1}{r_1}-\frac{1}{r_2}+\frac{1}{\left|\vec{r}_1-\vec{r}_2\right|} . \tag{2.91}$$

Atomic units (a.u.) are used throughout this section. $\vec{r}_1$ and $\vec{r}_2$ are the position vectors of the electron of the hydrogen atom and of the scattered electron respectively.

The total wave function of the electron-atomic-hydrogen system for a definite total angular momentum L and total spin S is written in a standard expansion form as (see for example, Gien, 1998 [26])

$$\Psi_{LS}(\vec{r}_1,\vec{r}_2)=\frac{1}{\sqrt{2}}\left[1\pm\hat{P}_{12}\right]\sum_{n_1,l_1,l_2}u_{n_1l_1}(r_1)F_{n_1l_1l_2}(r_2)\mathrm{Y}^{M_L}_{Ll_1l_2}(\hat{r}_1,\hat{r}_2), \tag{2.92}$$

l_1 and l_2 are the orbital angular quantum number of the hydrogenic electron and scattered electron respectively. S=0 or 1 corresponds to singlet or triplet scattering. $\hat{P}_{12}$ is the exchange operator which interchanges the coordinates of the hydrogenic and scattered electrons. A scattering channel is specified by $p=(n_1,l_1,l_2)$; n_1 is principal quantum number of the hydrogen atom, l_1 , its orbital angular momentum and l_2 , orbital angular momentum quantum number of the scattered electron. $u_{n_1l_1}(r_1)$ is a radial wave function of the hydrogen atom while $\mathrm{Y}^{M_L}_{Ll_1l_2}(\hat{r}_1,\hat{r}_2)$ is a bipolar spherical harmonic of the collision system and is as well known can be expressed in terms of the angular momentum wave function of the individual electrons as [45]

$$\mathrm{Y}^{M_L}_{Ll_1l_2}(\hat{r}_1,\hat{r}_2)=\sum_{m_1,m_1}C(l_1,l_2,L;m_1,m_2,M_L)\mathrm{Y}_{l_1,m_1}(\hat{r}_1)\mathrm{Y}_{l_2,m_2}(\hat{r}_2), \tag{2.93}$$

where $C(l_1,l_2,L;m_1,m_2,M_L)$ is the relevant Clebsch-Gordan coefficient.

An important part (see for instance, Gien, 1995 [18]) of the Harris-Nesbet variational method is to construct the scattering trial wave functions $F_{n_1l_1l_2}(r_2)$. $F_{n_1l_1l_2}(r_2)$, as was discussed in various sections above, is composed of two parts, a free part and a bound part. These scattered waves are, therefore, explicitly written as

$$F_p(r_2)=\Phi_p(r_2)+\alpha_{0p}S_p(r_2)+\alpha_{1p}C_p(r_2)\ . \tag{2.94}$$

The independent free wave functions S_p and C_p are for this case given by

$$S_p(r_2) = k_p j_{l_2}(k_p r_2) \quad , \tag{2.95}$$

and

$$C_p(r_2) = k_p \left(1 - e^{-\beta r_2}\right)^{2l_2+1} n_{l_2}(k_p r_2) \quad , \tag{2.96}$$

where k_p and l_2 are the momentum and angular momentum of the scattered electron, respectively. k_p is given by $E_p = E - \frac{1}{2}k_p^2$ where E_p is the energy of the electron of H. $j_{l_2}(k_p r_2)$ and $n_{l_2}(k_p r_2)$ are the spherical Bessel and spherical Neumann functions, respectively. The weight factor $\left(1 - e^{-\beta r_2}\right)^{2l_2+1}$ introduced is to force the spherical Neumann function to behave correctly in terms of r_2 (as $r_2^{l_2}$) near the coordinate origin. The weight factor is expressed in terms of the stability parameter β . The results of phase shift and cross section calculated do not depend on the value chosen for β. β may be varied to produce a good agreement between the Kohn and inverse Kohn results. An alternative approximate form which can be used to represent the free function $C_p(r_2)$ was introduced by Armstead (1968) [3]

$$C_p(r_2) = k_p G_{l_2}(k_p r_2), \tag{2.97}$$

$$G_{l_2}(k_p r_2) = j_{l_2+1}(k_p r_2) + \frac{l_2+1}{k_p r_2} j_{l_2+2}(k_p r_2) .$$

The Armstead form also provides correct asymptotic behaviors for the $C_p(r_2)$ function near the coordinate origin as well as at large distance r_2. The bound part $\Phi_p(r_2)$ is expanded in terms of a numerable set of the short-range square-integrable functions $\varphi_{p,i}(r_2)$

$$\Phi_p(r_2) = \sum_i C_{p,i}\varphi_{p,i}(r_2). \tag{2.98}$$

The functions $\varphi_{p,i}(r_2)$ have usually been chosen to be Slater-type functions,

$$\varphi_{p,i}(r_2) = \left(\frac{(2\alpha_{i2})^{2l_2+3}}{\Gamma(2l_2+3)}\right)^{1/2} r_2^{l_2} e^{-\alpha_{i2}r_2}. \tag{2.99}$$

In the case when correlation terms are added to the basis set, one can recast the expansion (2.92) as

$$\Psi_{LS}(\vec{r}_1,\vec{r}_2) = \frac{1}{\sqrt{2}}\left[1 \pm \hat{P}_{12}\right]\left\{\sum_{n_1,l_1,l_2} u_{n_1 l_1}(r_1) F_{n_1 l_1 l_2}(r_2) Y_{Ll_1l_2}^{M_L}(\hat{r}_1 \cdot \hat{r}_2) + \sum_i c_i \chi_i(r_1,r_2) Y_{Ll_1l_2}^{M_L}(\hat{r}_1,\hat{r}_2)\right\}, \tag{2.100}$$

where $\chi_i(r_1,r_2)$ is a correlation function.

Elements of the bound-bound matrix of *H-E* in the case of electron collisions with hydrogen atoms are, therefore, given, for example, by (see Gien (2002) [32])

$$M_{pq} = B_{i2}B_{j2} \times$$

$$\left\langle u_{n_{i1}l_{i1}}(r_1) r_2^{n_{i2}} e^{-\alpha_{i2}r_2} Y_{Ll_{i1}l_{i2}}^{M_L}(\hat{r}_1 \cdot \hat{r}_2) \right| \left(\hat{H} - E\right)\left(1 \pm \hat{P}_{12}\right) \left| u_{n_{j1}l_{j1}}(r_1) r_2^{n_{j2}} e^{-\alpha_{j2}r_2} Y_{Ll_{j1}l_{j2}}^{M_L}(\hat{r}_1,\hat{r}_2) \right\rangle, \tag{2.101}$$

where B_{i2} and B_{j2} are normalization constants.

The bound-free matrix elements for this collision process are given, for example, by

$$M_{pS} = B_{i2}k_{j2} \times$$

$$\left\langle u_{n_{i1}l_{i1}}(r_1) r_2^{n_{i2}} e^{-\alpha_{i2}r_2} Y_{Ll_{i1}l_{i2}}^{M_L}(\hat{r}_1 \cdot \hat{r}_2) \right| \left(\hat{H} - E\right)\left(1 \pm \hat{P}_{12}\right) \left| u_{n_{j1}l_{j1}}(r_1) j_{l_{j2}}(k_{j2}r_2) Y_{Ll_{j1}l_{j2}}^{M_L}(\hat{r}_1,\hat{r}_2) \right\rangle,$$

(2.102)

and

$$M_{pC}=B_{i2}\left\langle u_{n_{i1}l_{i1}}(r_1)r_2^{n_{i2}}e^{-\alpha_{i2}r_2}Y_{Ll_{i1}l_{i2}}^{M_L}(\hat{r}_1\cdot\hat{r}_2)\right|\left(\hat{H}-E\right)\left(1\pm\hat{P}_{12}\right)\left|u_{n_{j1}l_{j1}}(r_1)C_q(r_2)Y_{Ll_{j1}l_{j2}}^{M_L}(\hat{r}_1,\hat{r}_2)\right\rangle, \tag{2.103}$$

while the free-free matrix elements of *H-E* are given by

$$M_{SS}=k_{i2}k_{j2}\times$$

$$\left\langle u_{n_{i1}l_{i1}}(r_1)j_{l_{i2}}(k_{i2}r_2)Y_{Ll_{i1}l_{i2}}^{M_L}(\hat{r}_1\cdot\hat{r}_2)\right|\left(\hat{H}-E\right)\left(1\pm\hat{P}_{12}\right)\left|u_{n_{j1}l_{j1}}(r_1)j_{l_{j2}}(k_{j2}r_2)Y_{Ll_{j1}l_{j2}}^{M_L}(\hat{r}_1,\hat{r}_2)\right\rangle, \tag{2.104}$$

$$M_{CC}=\left\langle u_{n_{i1}l_{i1}}(r_1)C_p(r_2)Y_{Ll_{i1}l_{i2}}^{M_L}(\hat{r}_1\cdot\hat{r}_2)\right|\left(\hat{H}-E\right)\left(1\pm\hat{P}_{12}\right)\left|u_{n_{j1}l_{j1}}(r_1)C_q(r_2)Y_{Ll_{j1}l_{j2}}^{M_L}(\hat{r}_1,\hat{r}_2)\right\rangle, \tag{2.105}$$

$$M_{SC}=k_{i2}\left\langle u_{n_{i1}l_{i1}}(r_1)j_{l_{i2}}(k_{i2}r_2)Y_{Ll_{i1}l_{i2}}^{M_L}(\hat{r}_1\cdot\hat{r}_2)\right|\left(\hat{H}-E\right)\left(1\pm\hat{P}_{12}\right)\left|u_{n_{j1}l_{j1}}(r_1)C_q(r_2)Y_{Ll_{j1}l_{j2}}^{M_L}(\hat{r}_1,\hat{r}_2)\right\rangle, \tag{2.106}$$

$$M_{CS}=k_{j2}\left\langle u_{n_{i1}l_{i1}}(r_1)C_p(r_2)Y_{Ll_{i1}l_{i2}}^{M_L}(\hat{r}_1\cdot\hat{r}_2)\right|\left(\hat{H}-E\right)\left(1\pm\hat{P}_{12}\right)\left|u_{n_{j1}l_{j1}}(r_1)j_{l_{j2}}(k_{j2}r_2)Y_{Ll_{j1}l_{j2}}^{M_L}(\hat{r}_1,\hat{r}_2)\right\rangle. \tag{2.107}$$

The m-matrix elements can then be calculated in terms of these bound-bound, bound-free and free-free matrix elements through Eqs (2.49) to (2.54). Elements of the reactance matrix R and the inverse reactance matrix R^{-1} can then be deduced from their Kohn and inverse Kohn formulas (Eq. (2.81) and Eq. (2.90)). Once the R matrix or the inverse R matrix, R^{-1} , has been obtained, the cross sections can be calculated by using the well known relationship between the matrix R and the transition matrix T. The partial cross section Q_{pq} of a collision process in which the electron-hydrogen-atom system makes a transition from channel q to channel p is, therefore, given by

$$Q_{pq}=\frac{\pi}{k_q^2}\left|T_{pq}\right|^2=\frac{4\pi}{k_q^2}\left|\left(\frac{R}{1-iR}\right)_{pq}\right|^2. \tag{2.108}$$

At low energies below the first excitation threshold, only one scattering channel is open for any partial waves L. In this case, the reactance matrix R_L is nothing else but the tangent of the phase shift δ_L. Thus, in the Kohn variational method, δ_L is given by

$$\delta_L = \arctan\left(R_L\right), \tag{2.109}$$

while in the inverse Kohn method, by

$$\delta_L = arc\cot an\left(R_L^{-1}\right). \tag{2.110}$$

The elastic differential cross section $I(k,\theta)$ at a scattering angle θ for an electron of momentum k scattered from the hydrogen target is given in terms of the partial-wave phase shifts $\delta_L^{\pm}$ by

$$I(k,\theta) = \frac{3}{4}\left|f^{-}(k,\theta)\right|^2 + \frac{1}{4}\left|f^{+}(k,\theta)\right|^2, \tag{2.111}$$

where $f^{\pm}(k,\theta)$ are the scattering amplitudes,

$$f^{\pm}(k,\theta) = \frac{1}{2ik}\sum_{L}(2L+1)\left(e^{2i\delta_L^{\pm}} - 1\right)P_L(\cos\theta), \tag{2.112}$$

"$\pm$" refer to singlet and triplet scattering respectively.

Chapter 3

Accurate Calculation of e^- - H Scattering

3.1 Method of calculation

As was mentioned in chapter 2, the total wave function of the electron-hydrogen-atom system can be expanded in terms of the complete set of (discrete and continuum) states of hydrogen atom (Eq. (2.92)). In the well-known close-coupling approximation, the infinite series of Eq. (2.92) is, usually, truncated. Only a few lowest discrete states of the hydrogen atom are retained in the expansion, and one has, usually, used a number of pseudo states to represent the remainder hydrogenic states excluded from the expansion. In order to improve the accuracy of the truncated wave function, one may also add to the truncated expansion a number of correlation terms as shown in Eq. (2.100). It can be seen through Eq. (2.100) that a greater number of correlation terms added to the expansion of Ψ would likely provide a better accuracy for the truncated total wave function, and thereby a more accurate representation of the various interaction effects of the collision system. For convenience, we shall refer to the set of states and pseudo states (with or without the inclusion of correlation terms) that we consider for the expansion of the total wave function as a coupling scheme. For our present calculation of electron collision with hydrogen atom at energies below its first excitation threshold, we shall consider altogether six coupling schemes, the so-called four-state (4S), extended four-state (E4S), six-state (6S), extended six-state (E6S), three-state (3S) and extended three-state (E3S) ones.

(i) Four-state (4S) and extended four-state (E4S) schemes.

The four-state scheme is composed of the 1s, 2s, 2p states of the hydrogen atom and the $\overline{3p}$ pseudo state. The $\overline{3p}$ pseudo state was introduced by Burke et al. (1969) [4]. It is a linear combination of the 2p state and $\overline{2p}$ pseudo state derived by Damburg et al. (1967) [46]. Burke et al. (1969) [4] showed that the $\overline{3p}$ pseudo state together with the 2p state accounts for 100 percents of the dipole polarizability of the hydrogen atom in its ground state. Thus, an inclusion of the $\overline{3p}$ pseudo state to the coupling scheme will take good care of the long-range dipole interaction of the collision system. Explicit form for the normalized radial wave function of the $\overline{3p}$ pseudo state and its energy ε_{31} were given by Burke et al. (1969) [4].

The exponents α_i of the basis functions that are used to expand the bound part of the scattered wave ($\sim r_2^p e^{-\alpha_i r_2}$) were chosen over a wide range of values to speed up the convergence of the calculation. In the extended four-state scheme (E4S), a great number of correlation terms were added to the 4S scheme. The correlation terms that we use in our calculation were chosen to be in the form of a product of two Slater-type functions. The number of correlation terms was increased gradually until the results of the calculation no longer changed significantly, i.e., when these results were already approaching their convergent values. Again, the exponents a_{i1} and a_{i2} of the Slater-type functions were chosen over a wide range of values, and the power m_{i1} of the factor $r_1^{m_{i1}}$ has usually been taken to be equal to l_{i1}. Our experience indicates that it is not necessary to include the correlation terms with l_{i1} greater than 2 in order to reach the convergent values for our results at low energy. We also noticed that a higher number of basis functions and correlation terms were required for an accurate calculation of partial wave scattering of higher order. Usually, it has been quite time-consuming to find a suitable set of basis functions and correlation terms for our calculations in order to obtain accurate results for the phase shifts and/or cross sections. The principal criterion for choosing these sets of basis functions and correlation functions is to achieve the convergence values for the phase shifts as well as to speed up the convergence of the calculations.

The total number of basis functions used in the expansion of the bound part of the scattered wave functions are: 24 for L=0, 27 for L=1, 2 and 3, 30 for L=4 and 5, 33 for L=6, 7 and 8 and 36 for $L \geq 9$, respectively. The total number of correlation terms added to the expansion of Ψ are: 90 for L=0 triplet scattering, 108 for L=0 singlet scattering, 150 for L=1, 180 for L=2 triplet scattering, 270 for L=2 singlet scattering, 240 for L=3, 180 for L=4, 432 for L=5, 120 for L=6, 594 for L=7, 792 for L=8, 780 for L=9, 660 for L=10 and 780 for $L \geq 11$.

(ii) Six-state (6S) and extended six-state (E6S) schemes.

The 6S scheme consists of six atomic hydrogen states and pseudo states $1s, 2s, 2p, \overline{3s}, \overline{3p}, \overline{3d}$ (Geltman et al., 1970 [34]). The pseudo states $\overline{3s}$, $\overline{3p}$ and $\overline{3d}$ are those obtained by Damburg et al. (1968) [47] to provide 100% of polarizabilities for most of the open channels above the n=2 H excitation threshold. The normalized radial functions $u_{n_1 l_1}(r_1)$ of the $\overline{3\text{s}}$, $\overline{3\text{p}}$ and $\overline{3\text{d}}$ pseudo states and their effective energies $\varepsilon_{n_1 l_1}$ (in Rydbergs) (Damburg et al. (1968) [47]) are respectively given by

$$u_{30}(r_1) = \frac{3}{2}\left\{57 - \frac{2}{9}\left(\frac{4}{3}\right)^9\right\}^{-1/2}\left\{e^{-r_1/2}\left(1 - \frac{1}{2}r_1 - \frac{1}{2}r_1^2 + \frac{1}{12}r_1^3\right) + \frac{1}{2}\left(\frac{4}{3}\right)^6 e^{-r_1}\right\},$$

$$\varepsilon_{30} = \left\{3 + \frac{1}{9}\left(\frac{4}{3}\right)^8\right\}\left\{57 - \frac{2}{9}\left(\frac{4}{3}\right)^9\right\}^{-1} - \frac{1}{8}$$

$$u_{31}(r_1) = \frac{1}{2}\sqrt{\frac{5}{26}}\, r_1 e^{-r_1/2}\left(1 - \frac{1}{30}r_1^2\right), \qquad \varepsilon_{31} = -\frac{5}{104}$$

$$u_{32}(r_1) = \frac{1}{8\sqrt{55}}\, r_1^2 e^{-r_1/2}\left(1 + \frac{1}{6}r_1\right), \qquad \varepsilon_{32} = -\frac{9}{176}.$$

In the extended six-state (E6S) scheme, a large number of correlation terms is added to the scheme. The number of basis functions that is used to expand the bound part of the scattered wave functions is the same as in the case of the 4S and E4S schemes. The total number of correlation terms included to the E6S scheme are: 72 for L=0 triplet scattering, 90 for L=0 singlet scattering, 270 for L=1, 240 for L=2 singlet scattering, 588 for L=2 triplet scattering, 624 for L=3, 300 for L=4, 360 for L=5, 462 for L=6, 630 for L=7 and 8, 594 for $L \geq 9$.

(iii) Three-state (3S) and extended three-state (E3S) schemes.

The 3S scheme is composed of the 1s, 2s, 2p states of hydrogen atom. It is essentially the 4S scheme without the $\overline{3\text{p}}$ pseudo state. This scheme can account for approximately 65. 8% of the dipole polarizability of hydrogen atom in its ground state only (Castillejo et al., 1960 [48]). Thus, we had to add to the 3S scheme a great number of correlation terms so that the E3S scheme could yield convergent values for our results. The total number of correlation terms used are: 84 for L=0 singlet scattering, 90 for L=0 triplet scattering, 420 for L=1, 672 for L=2, 756 for L=3, 672 for L=4 singlet scattering, 546 for L=4 triplet scattering, 504 for L=5, 336 for L=6, 450 for L=7, 768 for L=8 and 780 for $L \geq 9$, respectively. The same number of basis functions as those of the 4S and E4S schemes were considered for the calculation.

We have employed a general computer code, which had been developed throughout the years by Gien (1995 [18], 1998 [26], 2001 [49], 2002 [32]) for the Harris-Nesbet variational calculations of electron (and positron) collisions with atomic targets, to obtain, with the consideration of the six coupling schemes described above, the phase shifts and cross sections for elastic scattering of electron from hydrogen atom at energies below its first excitation threshold. These results will be presented in the next section with discussion.

3.2 Numerical results and discussion

In tables 3.1 to 3.15, we display the results of our calculations of phase shift for both singlet and triplet scattering of electron from hydrogen atom at energies below the first excitation threshold of H and with the partial waves L=0, 1, 2, 3, 4, 5, 6 and 7. The calculations were done with the six coupling schemes described above, namely the three-state (3S), the four-state (4S), the six-state (6S), the extended three-state (E3S), the extended four-state (E4S) and the extended six-state (E6S). Theoretical values obtained by other researchers using other numerical methods, whenever available, are also shown in these tables for comparison. We also plot, as examples, the singlet and triplet S–wave phase shifts in figures 3.1 and 3.2, the singlet and triplet P–wave phase shifts in figures 3.3 and 3.4, the singlet and triplet D–wave phase shifts in figures 3.5 and 3.6 and the singlet and triplet F–wave phase shifts in figures 3.7 and 3.8 that were calculated with the 4S and E4S schemes. Samples of elastic differential cross sections obtained by us for electron-hydrogen collisions at the nine energies where experimental data have been available (*E*=0.582, 1.207, 1.597, 2.171, 3.009, 3.423, 4.889, 6.691 and 8.704 eV) (Williams (1975) [12]) are given in tables 3.16 to 3.24. We also present the results of elastic differential cross section calculated with the E4S scheme that we believe to be our most accurate ones in figures 3.9 to 3.17 for a visual comparison with experimental data by Williams. Table 3.25 displays our results of total cross section at these nine energies.

Tables 3.1 to 3.15 show that the phase shifts obtained with the 4S and 6S schemes are clearly greater than those with the 3S one. This fact indicates that the $\overline{3p}$ pseudo state and $\overline{3s}$, $\overline{3p}$ and $\overline{3d}$ pseudo states when added to the 3S scheme contribute significantly to the interaction effects of electron-hydrogen-atom collision system in the 4S and 6S schemes at both short and long distances. This is as expected since, as was discussed above, the $\overline{3p}$ pseudo state in the 4S scheme when combined with the 2p state accounts for 100 percents of the dipole polarizability of hydrogen atom in its ground state. The 4S scheme should, therefore, represent well the long-rang dipole interaction of the collision system. On the other hand, the $\overline{3s}$, $\overline{3p}$ and $\overline{3d}$ pseudo states, when added to the 3S coupling scheme to form the 6S one, improve the dipole as well as quadrupole interaction effects of the collision system.

The results of the singlet S−wave phase shifts, as shown in table 3.1, that we calculated with the E4S, E6S and E3S schemes in the Harris-Nesbet variational method, agree excellently with each other. They are also in excellent agreement with the phase shifts calculated by Gien (1998) [26] with the Harris-Nesbet method, using a 13-state scheme. The fact that these results calculated with completely different schemes agree excellently with each other indicates that our phase shifts obtained already are approaching their convergent values probably within a few percents at worst. They should, thereby, be very accurate. The results obtained with the employment of the direct numerical method by Botero et al. (1992) [9] and by Wang et al. (1994) [50] agree very well with ours within about 2%. The singlet S−wave phase shifts calculated by Schwartz (1961) [1] and Shimamura (1971) [51] with the Harris variational method also agree very well with ours within about 3%. Very good agreement is also found between our results and the ones calculated with the R-matrix method by Scholz et al. (1988) [8] and with the CCKT method by Bhatia et al. (2001) [10].

Our results of the singlet S−wave phase shifts calculated with the E4S and 4S schemes and displayed in table 3.1 and in figures 3.1 differ from each other noticeably. They show a significant improvement of the accuracy of the phase shifts when a great number of correlation terms are added to the scheme. We conclude that these correlation terms play a very important role in the acquirement of the accurate results for the phase

Table 3.1: Singlet *S*-wave phase shifts (in units of radian) of electron collision with hydrogen atom. The numbers in parentheses give the uncertainty in the last digit quoted.

$k\left(a_0^{-1}\right)$	0.1	0.15	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.83	0.85	0.86
[a] HN 3S	2.492	2.215	1.976	1.595	1.310	1.093	0.930	0.817	0.773	0.873	0.642	0.716
[b] HN 4S	2.532	2.267	2.036	1.663	1.379	1.162	0.998	0.882	0.833	0.928	0.710	0.779
[c] HN 6S	2.520	2.252	2.018	1.640	1.352	1.130	0.964	0.848	0.802	0.904	0.688	0.754
[d] HN E3S	2.551	2.291	2.063	1.692	1.411	1.197	1.037	0.926	0.883	0.979	0.774	0.837
[e] HN E4S	2.551	2.291	2.063	1.692	1.411	1.196	1.036	0.926	0.883	0.979	0.774	0.837
[f] HN E6S	2.551	2.291	2.063	1.693	1.412	1.197	1.037	0.927	0.884	0.980	0.776	0.838
[g] HN 13S	2.550	2.290	2.062	1.692	1.410	1.196	1.035	0.9250	0.8814	0.9772	—	—
[h] DR I	2.553	—	2.066	1.695	1.414	1.200	1.040	0.930	0.887	—	—	—
[i] DR II	2.555	—	2.066	1.695	1.415	1.200	1.041	0.930	0.887	—	—	—
[j] R-matrix	2.550	—	2.062	1.691	1.410	1.196	1.035	0.925	—	—	—	—
[k] Variational	2.556	—	2.067	1.696	1.415	1.201	1.041	0.930	0.887	—	—	—
[l] Variational	2.553(1)	—	2.0673(9)	1.6964(5)	1.4146(4)	1.202(1)	1.041(1)	0.930(1)	0.886(1)	—	—	—
[m] CCKT	2.55358	—	2.06678	1.69816	1.41540	1.20094	1.04083	0.93111	0.88718	—	—	—

[a, b, c] present Harris-Nesbet calculation with 3S, 4S and 6S schemes respectively

[d, e, f] present Harris-Nesbet calculation with E3S, E4S and E6S schemes respectively

[g] Harris-Nesbet calculation, T.T.Gien (1998) [26]

[h] direct numerical method, J. Botero and J. Shertzer (1992) [9]

[i] direct numerical method, Y. D. Wang and J. Callaway (1994) [50]

[j] R-matrix method, T. Scholz, P. Scott and P. G. Burke (1988) [8]

[k] Variational method, I. Shimamura (1971) [51]

[l] Variational method, C. Schwartz (1961) [1]

[m] CCKT method, A. K Bhatia and A. Temkin (2001) [10]

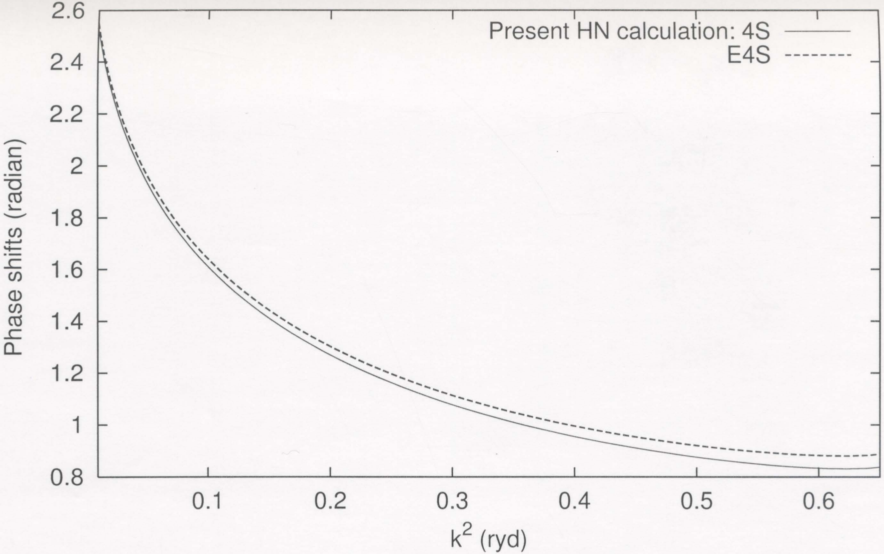

Figure 3.1: L = 0 phase shifts of e^--H singlet scattering

shifts and that the 4S scheme, by itself, cannot provide accurate results for the singlet S–wave phase shifts.

The triplet S–wave phase shifts calculated with the E4S, E6S and E3S schemes in the Harris-Nesbet variational method, as displayed in table 3.2, agree excellently with each other. They also agree excellently with the results obtained by Gien (1998) [26] in a Harris-Nesbet calculation using a 13-state scheme. Again, the excellent agreement of these phase shifts, which are obtained with completely different schemes, indicates that our results are already approaching their convergent values probably within a few percents at worst and should, thereby, be very accurate. They also agree excellently with the phase shifts calculated with the employment of other numerical methods, such as the direct numerical method by Botero et al. (1992) [9] and Wang et al. (1994) [50], the variational method by Shimamura (1971) [51] and Schwartz (1961) [1], the R-matrix method by Scholz et al. (1988) [8], and the CCKT method by Bhatia et al. (2001) [10] (within 0.01 percents, approximately).

The triplet S–wave phase shifts calculated with the 4S scheme and E4S one, where a great number of correlation terms are added, only differ minutely from each other. As a result, the 4S and E4S curves of phase shift that we display in figure 3.2 almost coincide with each other. This feature indicates that the 4S scheme by itself already represents very well the various collision effects of the electron-hydrogen-atom system in the case of S–wave triplet scattering at low energy. It also confirms that the phase shifts that we obtained with the E4S scheme are approaching their convergent

Table 3.2: Triplet S-wave phase shifts (in units of radian) of electron collision with hydrogen atom. The numbers in parentheses give the uncertainty in the last digit quoted.

$k\left(a_0^{-1}\right)$	0.1	0.15	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.83	0.85	0.86
[a] HN 3S	2.936	2.826	2.715	2.497	2.288	2.096	1.922	1.768	1.631	1.593	1.569	1.558
[b] HN 4S	2.938	2.827	2.716	2.498	2.292	2.103	1.931	1.777	1.641	1.604	1.580	1.568
[c] HN 6S	2.938	2.828	2.717	2.499	2.293	2.102	1.929	1.774	1.638	1.600	1.576	1.564
[d] HN E3S	2.938	2.828	2.717	2.500	2.294	2.104	1.933	1.779	1.644	1.606	1.582	1.571
[e] HN E4S	2.938	2.828	2.717	2.500	2.294	2.104	1.933	1.780	1.644	1.607	1.583	1.571
[f] HN E6S	2.938	2.828	2.717	2.500	2.294	2.104	1.933	1.779	1.644	1.606	1.682	1.571
[g] HN 13S	2.938	2.828	2.717	2.500	2.294	2.104	1.933	1.779	1.644	1.606	—	—
[h] DR I	2.938	—	2.717	2.500	2.294	2.104	1.933	1.780	1.645	—	—	—
[i] DR II	2.939	—	2.717	2.500	2.294	2.104	1.933	1.780	1.644	—	—	—
[j] R-matrix	2.939	—	2.717	2.500	2.294	2.105	1.933	1.780	—	—	—	—
[k] Variational	2.939	—	2.717	2.500	2.294	2.105	1.933	1.779	1.644	—	—	—
[l] Variational	2.9388(4)	—	2.7171(5)	2.4996(8)	2.2938(4)	2.1046(4)	1.9329(8)	1.7797(6)	1.643(3)	—	—	—
[m] CCKT	2.93853	—	2.71741	2.49975	2.29408	2.10454	1.93272	1.77950	1.64379	—	—	—

[a, b, c] present Harris-Nesbet calculation with 3S, 4S and 6S schemes respectively

[d, e, f] present Harris-Nesbet calculation with E3S, E4S and E6S schemes respectively

[g] Harris-Nesbet calculation, T.T.Gien (1998) [26]

[h] direct numerical method, J. Botero and J. Shertzer (1992) [9]

[i] direct numerical method, Y. D. Wang and J. Callaway (1994) [50]

[j] R-matrix method, T. Scholz, P. Scott and P. G. Burke (1988) [8]

[k] Variational method, I. Shimamura (1971) [51]

[l] Variational method, C. Schwartz (1961) [1]

[m] CCKT method, A. K Bhatia and A. Temkin (2001) [10]

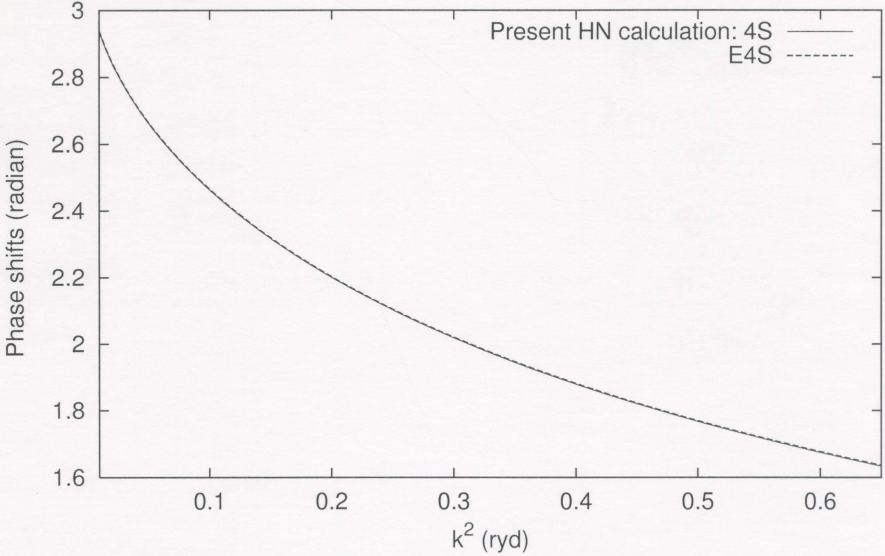

Figure 3.2: L = 0 phase shifts of e^--H triplet scattering

values, since the results of calculation almost do not change at all, despite an addition of a great number of correlation terms to the coupling scheme.

Again, the singlet P–wave phase shifts (see table 3.3) calculated with the E4S, E6S and E3S schemes agree excellently with each other. They also agree very well with those calculated with the Harris-Nesbet variational method by Gien (1998) [26], using however a 13-state coupling scheme. Again, this excellent agreement implies that the singlet P–wave phase shifts obtained are already approaching their convergent values within a few percents at worst and should, thereby, be very accurate. Our results also agree very well with those obtained with the direct numerical method by Botero et al. (1992) [9] and by Wang et al. (1994) [50] and those with the R-matrix method by Scholz et al. (1988) [8] within 2% to 5%. The variational phase shifts of Das et al. (1976) [6] and Armstead (1968) [3] deviate from ours about 2 to 10 percents. It is worth noting that the phase shifts of the calculation by Sloan (1964) [2], except at k=0.1 a.u., deviate considerably from ours, and hence from other theoretical calculations.

In figure 3.3, we display the singlet P–wave phase shifts that we obtained with the 4S and E4S schemes for a visual comparison. The E4S phase shifts lie considerably above those of the 4S. Thus, an inclusion of the correlation terms to the coupling scheme in the calculation improves the accuracy of the phase shifts considerably in this case, especially at higher scattering energies.

In table 3.4, our results of the triplet P–wave phase shift are given. The triplet P–wave phase shifts that we obtained in the present Harris-Nesbet calculations with the E4S, E6S and E3S schemes (shown in table 3.4) agree excellently with each other as well

Table 3.3: Singlet P-wave phase shifts (in units of radian) of electron collision with hydrogen atom.

$k\left(a_0^{-1}\right)$	0.1	0.15	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.83	0.85	0.86
[a] HN 3S	0.00399	0.00673	0.00823	0.00438	-0.00917	-0.0282	-0.0463	-0.0580	-0.0570	-0.0517	-0.0435	-0.0333
[b] HN 4S	0.00617	0.0107	0.0140	0.0143	0.00595	-0.00669	-0.0181	-0.0233	-0.0170	-0.0108	-0.0029	0.00643
[c] HN 6S	0.00586	0.0106	0.0141	0.0135	0.00277	-0.0133	-0.0289	-0.0385	-0.0362	-0.0308	-0.023	-0.0125
[d] HN E3S	0.00632	0.0111	0.0149	0.0162	0.00910	-0.00221	-0.0122	-0.0157	-0.00755	-0.00069	0.0078	0.0184
[e] HN E4S	0.00632	0.0111	0.0149	0.0161	0.00909	-0.00221	-0.0121	-0.0157	-0.00752	-0.00066	0.0079	0.0184
[f] HN E6S	0.00632	0.0111	0.0149	0.0161	0.00909	-0.00220	-0.0122	-0.0157	-0.00753	-0.00065	0.0079	0.0185
[g] HN 13S	0.0063	0.0111	0.0149	0.0162	0.0093	-0.0019	-0.0120	-0.0155	-0.0075	-0.00073	—	—
[h] DR I	0.006	—	0.0148	0.0160	0.0090	-0.0020	-0.0117	-0.0149	-0.0068	—	—	—
[i] DR II	0.006	—	0.016	0.017	0.010	-0.002	-0.012	-0.015	-0.007	—	—	—
[j] R-matrix	0.006	—	0.015	0.016	0.009	-0.002	-0.012	-0.016	—	—	—	—
[k] Variational	0.0062	—	0.0150	0.0165	0.0099	-0.0011	-0.0106	-0.014	-0.006	—	—	—
[l] Variational	0.007	—	0.0147	0.0170	0.0100	-0.0007	-0.009	-0.013	-0.004	—	—	—
[m] POM	0.0067	—	0.0171	0.0210	0.0163	-0.0064	-0.0039	-0.0100	-0.0095	—	—	—

[a, b, c] present Harris-Nesbet calculation with 3S, 4S and 6S schemes respectively

[d, e, f] present Harris-Nesbet calculation with E3S, E4S and E6S schemes respectively

[g] Harris-Nesbet calculation, T.T.Gien (1998) [26]

[h] direct numerical method, J. Botero and J. Shertzer (1992) [9]

[i] direct numerical method, Y. D. Wang and J. Callaway (1994) [50]

[j] R-matrix method, T. Scholz, P. Scott and P. G. Burke (1988) [8]

[k] Variational method, J. N. Das and M. R. H. Rudge (1976) [6]

[l] Variational method, R. L. Armstead (1968) [3]

[m] the polarized orbital method, I. H. Sloan (1964) [2]

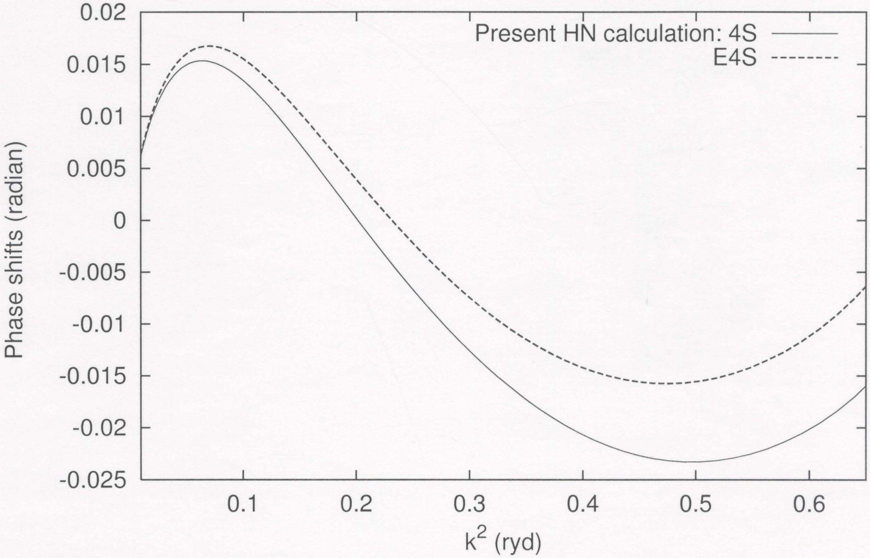

Figure 3.3: L = 1 phase shifts of e^--H singlet scattering

Table 3.4: Triplet P-wave phase shifts (in units of radian) of electron collision with hydrogen atom.

$k\left(a_0^{-1}\right)$	0.1	0.15	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.83	0.85	0.86
[a] HN 3S	0.00783	0.0194	0.0371	0.0906	0.162	0.236	0.302	0.353	0.391	0.407	0.339	0.396
[b] HN 4S	0.0102	0.0241	0.0446	0.105	0.184	0.265	0.335	0.386	0.421	0.434	0.394	0.425
[c] HN 6S	0.00986	0.0237	0.0441	0.103	0.177	0.255	0.321	0.371	0.407	0.421	0.380	0.412
[d] HN E3S	0.0104	0.0245	0.0453	0.107	0.187	0.270	0.341	0.392	0.427	0.440	0.406	0.432
[e] HN E4S	0.0104	0.0244	0.0453	0.107	0.187	0.270	0.341	0.392	0.427	0.440	0.406	0.432
[f] HN E6S	0.0104	0.0244	0.0453	0.107	0.187	0.270	0.341	0.392	0.427	0.440	0.406	0.432
[g] HN 13S	0.0103	0.0244	0.0452	0.1066	0.1869	0.2701	0.3408	0.3922	0.4269	0.4397	—	—
[h] DR I	0.0100	—	0.0452	0.1067	0.1873	0.2708	0.3417	0.3933	0.4283	—	—	—
[i] DR II	0.010	—	0.046	0.107	0.188	0.271	0.342	0.394	0.429	—	—	—
[j] R-matrix	0.010	—	0.045	0.107	0.187	0.270	0.341	0.392	—	—	—	—
[k] Variational	0.0103	—	0.0452	0.1067	0.1872	0.2705	0.3413	0.3927	0.4270	—	—	—
[l] Variational	0.0114	—	0.0450	0.1063	0.1872	0.2705	0.3412	0.3927	0.427	—	—	—
[m] POM	0.0109	—	0.0486	0.1151	0.2005	0.2867	0.3574	0.4063	0.4351	—	—	—

[a, b, c] present Harris-Nesbet calculation with 3S, 4S and 6S schemes respectively

[d, e, f] present Harris-Nesbet calculation with E3S, E4S and E6S schemes respectively

[g] Harris-Nesbet calculation, T.T.Gien (1998) [26]

[h] direct numerical method, J. Botero and J. Shertzer (1992) [9]

[i] direct numerical method, Y. D. Wang and J. Callaway (1994) [50]

[j] R-matrix method, T. Scholz, P. Scott and P. G. Burke (1988) [8]

[k] Variational method, J. N. Das and M. R. H. Rudge (1976) [6]

[l] Variational method, R. L. Armstead (1968) [3]

[m] the polarized orbital method, I. H. Sloan (1964) [2]

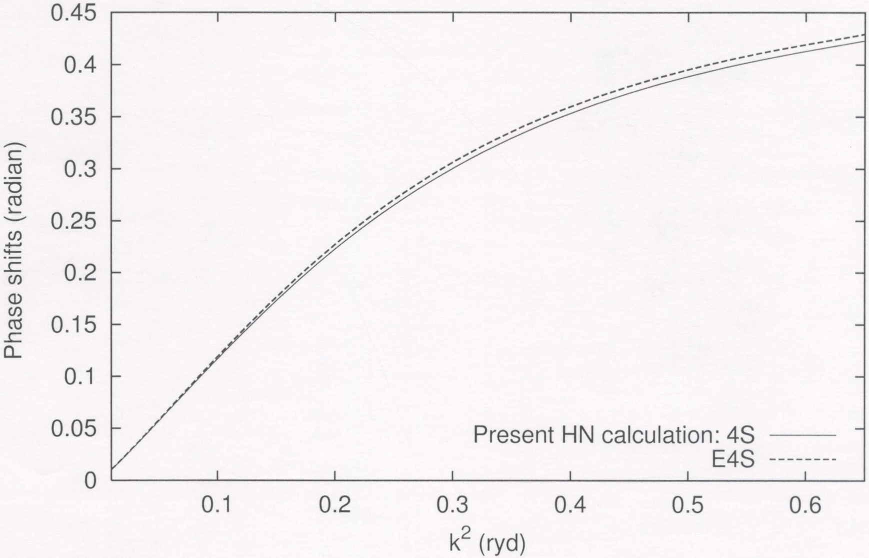

Figure 3.4: L = 1 phase shifts of e^--H triplet scattering

as with those calculated by Gien (1998) [26], employing the Harris-Nesbet method with a 13-state scheme instead. Our phase shifts also agree well with those calculated by Botero et al. (1992) [9], by Wang et al. (1994) [50], by Scholz et al. (1988) [8], by Das et al. (1976) [6], and by Armstead (1968) [3]. The maximum difference between ours and theirs is less than 4 percents. The present Harris-Nesbet results are approximately 5 percents smaller than the ones obtained by Sloan (1964) [2] who used the polarized orbital method for his calculation.

The triplet P–wave phase shifts calculated with the E4S and 4S schemes are displayed in figure 3.4 for a visual comparison. The phase shifts calculated with the E4S scheme are greater than those obtained with the 4S scheme, as expected. This reasserts the important role that correlation terms play in the acquirement of accurate values for the phase shifts.

The singlet and triplet D–wave phase shifts calculated with the E4S, E6S and E3S schemes (see tables 3.5 and 3.6) in the Harris-Nesbet method agree excellently with each other. They also agree very well with the phase shifts obtained by Gien (1998) [26], using a 13-state scheme. A good agreement is found between our E4S results and those by Callaway (1978) [7] who also used the Harris-Nesbet method for his calculation, but with the consideration of an eleven-state coupling scheme and between our E4S results and those by Register et al. (1975) [52] who employed a basis set of 35 Hylleraas functions. In e^- - H collisions, one may choose to use the sets of basis functions in the form of a Hylleraas-type wave function to expand the wave function Ψ of the collision (two-electron) system. This choice should, in principle, be equivalent to ours, provided that the

Table 3.5: Singlet D-wave phase shifts (in units of radian) of electron collision with hydrogen atom.

$k\left(a_0^{-1}\right)$	0.1	0.15	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.83	0.85	0.86
[a] HN 3S	0.000863	0.00192	0.00336	0.00748	0.0133	0.0207	0.0297	0.0413	0.0609	0.0729	0.0906	0.130
[b] HN 4S	0.00132	0.00291	0.00505	0.0107	0.0179	0.0265	0.0369	0.0505	0.0723	0.0847	0.102	0.142
[c] HN 6S	0.00113	0.00255	0.00453	0.00989	0.0165	0.0243	0.0339	0.0468	0.0679	0.0803	0.0996	0.164
[d] HN E3S	0.00130	0.00293	0.00509	0.0110	0.0185	0.0276	0.0383	0.0524	0.0746	0.0872	0.1064	0.171
[e] HN E4S	0.00133	0.00294	0.00513	0.0110	0.0186	0.0276	0.0385	0.0526	0.0748	0.0874	0.107	0.171
[f] HN E6S	0.00132	0.00294	0.00512	0.0110	0.0185	0.0276	0.0385	0.0525	0.0747	0.0874	0.107	0.171
[g] HN 13S	0.00131	0.00292	0.00509	0.0110	0.0185	0.0276	0.0385	0.0526	0.0748	0.0873	—	—
[h] HN II	0.00120	—	0.00520	0.0108	0.0183	0.0274	0.0383	0.0523	0.0745	—	—	—
[i] HN III	0.0013	—	0.0051	0.0109	0.0184	0.0273	0.0381	0.0517	0.0739	—	—	—
[j] DR I	0.0007	—	0.0048	0.0105	0.0182	0.0271	0.0379	0.0518	0.0745	—	—	—
[k] DR II	0.0012	—	0.0056	0.011	0.018	0.027	0.038	0.052	0.075	—	—	—
[l] R-matrix	0.00132	—	0.00510	0.0109	0.0183	0.0272	0.0379	0.0518	—	—	—	—
[m] CCM	0.001	—	—	0.011	—	0.027	—	0.050	0.070	—	—	—

[a, b, c] present Harris-Nesbet calculation with 3S, 4S and 6S schemes respectively

[d, e, f] present Harris-Nesbet calculation with E3S, E4S and E6S schemes respectively

[g] Harris-Nesbet calculation, T.T.Gien (1998) [26]

[h] Harris-Nesbet calculation, D. Register and R. T. Poe (1975) [52]

[i] Harris-Nesbet calculation, J. Callaway (1978) [7]

[j] direct numerical method, J. Botero and J. Shertzer (1992) [9]

[k] direct numerical method, Y. D. Wang and J. Callaway (1994) [50]

[l] R-matrix method, T. Scholz, P. Scott and P. G. Burke (1988) [8]

[m] the close coupling method, P. G. Burke, D. F. Gallaher and S. Geltman (1969) [4]

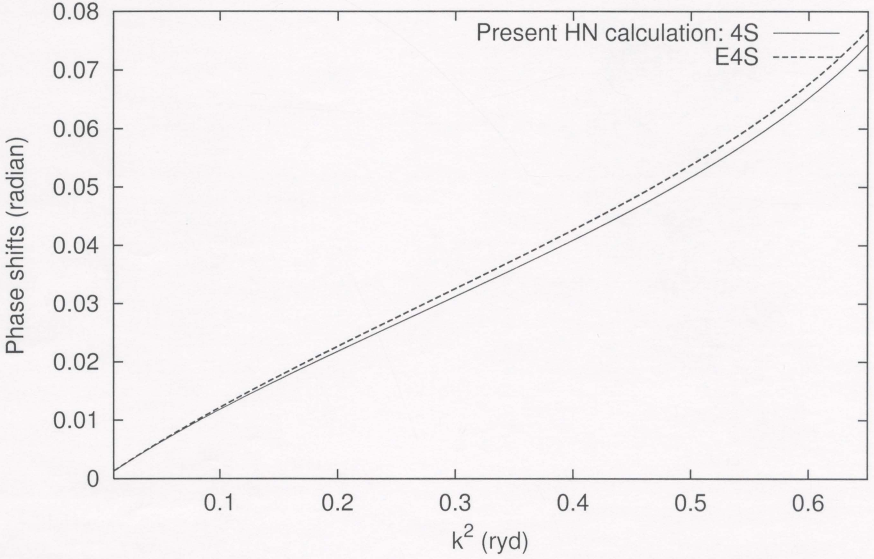

Figure 3.5: L = 2 phase shifts of e^--H singlet scattering

Table 3.6: Triplet D-wave phase shifts (in units of radian) of electron collision with hydrogen atom.

$k\left(a_0^{-1}\right)$	0.1	0.15	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.83	0.85	0.86
[a] HN 3S	0.000875	0.00200	0.00363	0.00857	0.0155	0.0239	0.0333	0.0436	0.0548	0.0585	0.0610	0.0623
[b] HN 4S	0.00132	0.00293	0.00513	0.0112	0.0195	0.0295	0.0410	0.0533	0.0662	0.0701	0.0728	0.0742
[c] HN 6S	0.00114	0.00259	0.00464	0.0103	0.0178	0.0272	0.0380	0.0498	0.0621	0.0659	0.0686	0.0699
[d] HN E3S	0.00131	0.00295	0.00516	0.0114	0.0198	0.0304	0.0424	0.0557	0.0697	0.0739	0.0768	0.0783
[e] HN E4S	0.00133	0.00296	0.00520	0.0115	0.0199	0.0304	0.0426	0.0559	0.0698	0.0741	0.0770	0.0785
[f] HN E6S	0.00130	0.00295	0.00518	0.0114	0.0199	0.0304	0.0424	0.0556	0.0696	0.0739	0.0768	0.0783
[g] HN 13S	0.00132	0.00294	0.00515	0.0114	0.0198	0.0302	0.0423	0.0555	0.0693	0.0736	—	—
[h] HN II	0.00130	—	0.00520	0.0114	0.0198	0.0304	0.0424	0.0559	0.0697	—	—	—
[i] HN III	0.0013	—	0.0052	0.0113	0.0197	0.0301	0.0421	0.0550	0.0688	—	—	—
[j] DR I	0.0007	—	0.0049	0.0110	0.0196	0.0300	0.0422	0.0554	0.0699	—	—	—
[k] DR II	0.0012	—	0.0057	0.011	0.020	0.030	0.042	0.055	0.070	—	—	—
[l] R-matrix	0.00132	—	0.00517	0.0114	0.0197	0.0301	0.0421	0.0553	—	—	—	—
[m] CCM	0.001	—	—	0.011	—	0.029	—	0.053	0.066	—	—	—

[a, b, c] present Harris-Nesbet calculation with 3S, 4S and 6S schemes respectively
[d, e, f] present Harris-Nesbet calculation with E3S, E4S and E6S schemes respectively
[g] Harris-Nesbet calculation, T.T.Gien (1998) [26]
[h] Harris-Nesbet calculation, D. Register and R. T. Poe (1975) [52]
[i] Harris-Nesbet calculation, J. Callaway (1978) [7]
[j] direct numerical method, J. Botero and J. Shertzer (1992) [9]
[k] direct numerical method, Y. D. Wang and J. Callaway (1994) [50]
[l] R-matrix method, T. Scholz, P. Scott and P. G. Burke (1988) [8]
[m] the close coupling method, P. G. Burke, D. F. Gallaher and S. Geltman (1969) [4]

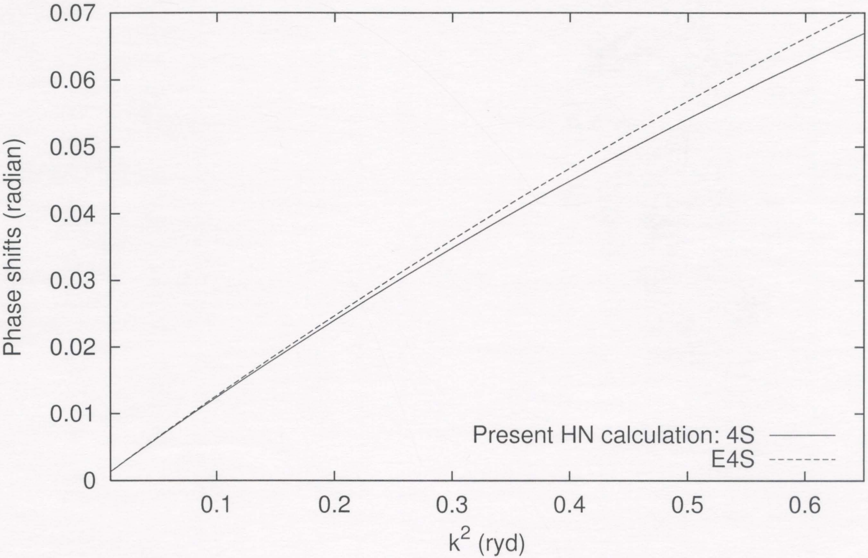

Figure 3.6: L = 2 phase shifts of e^--H triplet scattering

set of basis functions selected for each case are sufficient to represent Ψ accurately. Thus, we believe that the slight deviation sometimes seen to exist between our results and those calculated with the use of the Hylleraas-type wave functions originates, more or less, from the different numerical methods and/or the details of the numerical procedures (rather than from the type of the basis functions) that one considers for the calculations. As seen in tables 3.5 and 3.6, other sets of phase shifts obtained by Wang et al. (1994) [50], Scholz et al. (1988) [8] and Burke et al. (1969) [4] are also in good agreement with ours within a few percents approximately. The D–wave phase shifts of singlet and triplet scattering by Botero et al. (1992) [9] are about 5% smaller than ours.

Figures 3.5 and 3.6 show that both singlet and triplet D–wave phase shifts calculated with the E4S lie higher than their counterparts calculated with the 4S scheme. Once again, the inclusion of the correlation terms to the coupling scheme is seen to improve the accuracy of the phase shifts that we calculated.

Our results of singlet and triplet F–wave phase shifts that we calculated with the E6S, E4S and E3S schemes (see tables 3.7 and 3.8) again agree excellently with each other and with those calculated by Gien (1998) [26] with a 13-state scheme. The excellent agreement of these results which were obtained with completely different coupling schemes again indicates that our E4S, E6S and E3S phase shifts are already approaching their convergent values and should, thereby, be very accurate. Our phase shifts also agree well with those calculated by Callaway (1978) [7]. The phase shifts of the direct numerical method by Botero et al. (1992) [9] and by Wang et al. (1994) [50], and of the close coupling method by Burke et al. (1969) [4] also agree well with ours

Table 3.7: Singlet F-wave phase shifts (in units of radian) of electron collision with hydrogen atom.

$k\left(a_0^{-1}\right)$	0.1	0.15	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.83	0.85	0.86
[a] HN 3S	0.000288	0.000646	0.00114	0.00250	0.00435	0.00669	0.00953	0.0130	0.0173	0.0189	0.0201	0.0208
[b] HN 4S	0.000440	0.000985	0.00174	0.00384	0.00666	0.0102	0.0144	0.0194	0.0255	0.0277	0.0293	0.0302
[c] HN 6S	0.000374	0.000845	0.00151	0.00343	0.00609	0.00933	0.0131	0.0175	0.0230	0.0249	0.0264	0.0272
[d] HN E3S	0.000432	0.000980	0.00173	0.00387	0.00671	0.0104	0.0147	0.0198	0.0263	0.0285	0.0302	0.0311
[e] HN E4S	0.000441	0.000990	0.00175	0.00389	0.00680	0.0104	0.0148	0.0200	0.0264	0.0287	0.0303	0.0312
[f] HN E6S	0.000435	0.000989	0.00175	0.00388	0.00677	0.0104	0.0148	0.0200	0.0264	0.0286	0.0303	0.0312
[g] HN 13S	0.00043	0.00097	0.0017	0.0038	0.0067	0.0103	0.0146	0.0199	0.0262	0.0284	—	—
[h] HN III	—	—	—	0.0038	0.0066	0.0102	0.0145	0.0194	0.0259	—	—	—
[i] DR I	0.00000	—	0.0016	0.0037	0.0065	0.0101	0.0145	0.0199	0.0264	—	—	—
[j] DR II	0.00010	—	0.0015	0.0038	0.0064	0.010	0.015	0.020	0.026	—	—	—
[k] CCM	0.000	—	—	0.004	—	0.010	—	0.019	0.025	—	—	—

[a, b, c] present Harris-Nesbet calculation with 3S, 4S and 6S schemes respectively

[d, e, f] present Harris-Nesbet calculation with E3S, E4S and E6S schemes respectively

[g] Harris-Nesbet calculation, T.T.Gien (1998) [26]

[h] Harris-Nesbet calculation, J. Callaway (1978) [7]

[i] direct numerical method, J. Botero and J. Shertzer (1992) [9]

[j] direct numerical method, Y. D. Wang and J. Callaway (1994) [50]

[k] the close coupling method, P. G. Burke, D. F. Gallaher and S. Geltman (1969) [4]

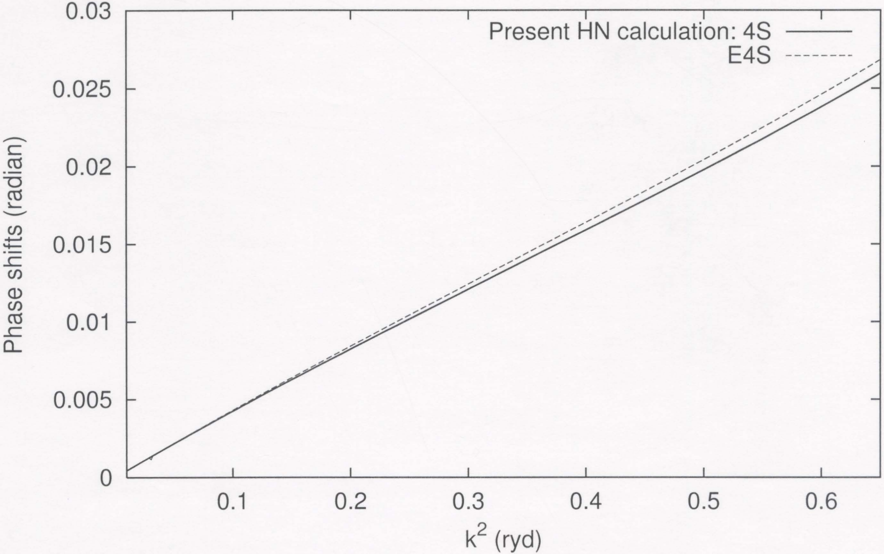

Figure 3.7: L = 3 phase shifts of e^-–H singlet scattering

Table 3.8: Triplet F-wave phase shifts (in units of radian) of electron collision with hydrogen atom.

$k\left(a_0^{-1}\right)$	0.1	0.15	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.83	0.85	0.86
[a] HN 3S	0.000288	0.000646	0.00114	0.00249	0.00429	0.00654	0.00930	0.0128	0.0174	0.0193	0.0208	0.0217
[b] HN 4S	0.000440	0.000985	0.00174	0.00385	0.00671	0.0103	0.0147	0.0198	0.0260	0.0281	0.0298	0.0307
[c] HN 6S	0.000374	0.000845	0.00151	0.00342	0.00612	0.00943	0.0132	0.0176	0.0229	0.0249	0.0264	0.0272
[d] HN E3S	0.000432	0.000980	0.00173	0.00388	0.00674	0.0105	0.0149	0.0202	0.0267	0.0290	0.0307	0.0317
[e] HN E4S	0.000441	0.000991	0.00175	0.00390	0.00683	0.0105	0.0151	0.0204	0.0269	0.0291	0.0308	0.0318
[f] HN E6S	0.000435	0.000989	0.00175	0.00389	0.00681	0.0105	0.0150	0.0204	0.0268	0.0291	0.0308	0.0317
[g] HN 13S	0.00043	0.00097	0.0017	0.0038	0.0067	0.0104	0.0148	0.0202	0.0266	0.0289	—	—
[h] HN III	—	—	—	0.0038	0.0067	0.0103	0.0147	0.0197	0.0263	—	—	—
[i] DR I	0.00000	—	0.0016	0.0037	0.0065	0.0102	0.0148	0.0204	0.0271	—	—	—
[j] DR II	0.00010	—	0.0015	0.0038	0.0064	0.010	0.015	0.020	0.026	—	—	—
[k] CCM	0.000	—	—	0.004	—	0.010	—	0.020	0.026	—	—	—

[a, b, c] present Harris-Nesbet calculation with 3S, 4S and 6S schemes respectively

[d, e, f] present Harris-Nesbet calculation with E3S, E4S and E6S schemes respectively

[g] Harris-Nesbet calculation, T.T.Gien (1998) [26]

[h] Harris-Nesbet calculation, J. Callaway (1978) [7]

[i] direct numerical method, J. Botero and J. Shertzer (1992) [9]

[j] direct numerical method, Y. D. Wang and J. Callaway (1994) [50]

[k] the close coupling method, P. G. Burke, D. F. Gallaher and S. Geltman (1969) [4]

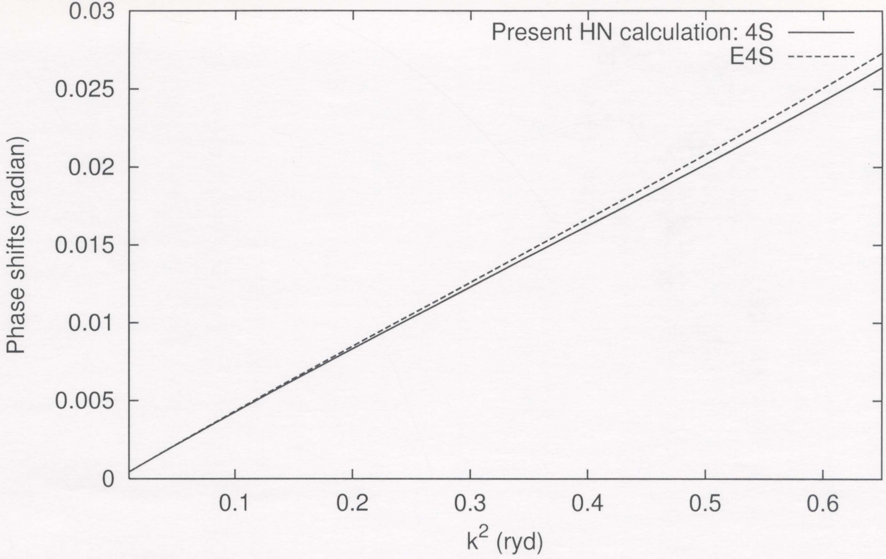

Figure 3.8: L = 3 phase shifts of e^--H triplet scattering

which were calculated with the extended schemes. They are about 2 to 8 percents smaller than ours at almost energies shown. However, at a small energy of 0.01 Ryd, as was noticed by Gien (1998) [26], the values obtained by these three research groups are quite small, compared with ours.

Figures 3.7 and 3.8 display the singlet and triplet F–wave phase shifts calculated with the use of the E4S and 4S schemes, respectively. It can be seen clearly from figures 3.7 and 3.8 that the 4S phase shifts are smaller than the E4S ones. This reasserts the significant effects of correlation terms that we add to the coupling scheme on the singlet and triplet F–wave phase shifts, as expected.

Our singlet and triplet G–wave phase shifts calculated with the E4S, E6S and E3S schemes (shown in table 3.9) also agree excellently with each other and with those calculated with the same method by Gien (1998) [26], employing, however, a 13-state scheme. This again implies that our results of G–wave phase shifts that we calculated with the use of completely different extended coupling schemes are already approaching their convergent values, and should, thereby, be very accurate.

Tables 3.10 to 3.15 tabulate the singlet and triplet phase shifts that are obtained for higher partial-wave (L=5, 6, 7) elastic scattering of electrons from hydrogen atoms at energies below the first excitation threshold. These phase shifts that we calculated with the use of different schemes E4S, E6S and E3S also agree well with each other. We believe that these higher partial wave phase shifts are also approaching their convergent values, perhaps within a few percents.

The phase shifts at the nine energies of 0.582, 1.207, 1.597, 2.171, 3.009, 3.423, 4.889, 6.691 and 8.704 eV have been obtained for the partial waves L equal to up to 18 with the use of the 3S, 4S, 6S, E3S, E4S and E6S coupling schemes, and then used to deduce the elastic differential cross sections and total cross sections for electron collisions with hydrogen atoms at these energies.

Tables 3.16 to 3.24 display our results of elastic differential cross section at the nine energies of 0.582, 1.207, 1.597, 2.171, 3.009, 3.423, 4.889, 6.691 and 8.704 eV, respectively. They are also compared with experimental data available in the literature (Williams, 1975 [12]). The differential cross sections of our present Harris-Nesbet calculations with the use of the different coupling schemes E4S, E6S and E3S, as seen in these tables, agree excellently with each other. The maximum difference among these differential cross sections (DCS) for scattering angles between 10 and 150 degrees and for all nine energies is just 0.007 πa_0^2. The DCS results of the present Harris-Nesbet calculations also agree excellently with the ones calculated by Gien (2000) [29], using the same numerical method with a 13-state scheme however (see tables 3.16 to 3.24). For a visual comparison of our results with experimental data measured by Williams (1975) [12], we plotted, as example, in figures 3.9 to 3.17 our E4S elastic differential cross sections together with experimental data by Williams at these nine energies. Our theoretical differential cross sections (see figures 3.9 to 3.17) agree excellently with experimental data by Williams.

In table 3.25, we show the total cross sections of the present Harris-Nesbet calculations done with the 3S, 4S, 6S, E3S, E4S, and E6S schemes at the nine energies mentioned above. The total cross sections calculated with the E4S, E6S and E3S schemes agree very well with each other. The maximum difference between the cross sections calculated with these different schemes is less than 0.05%. Our results also agree excellently with those obtained by Gien (2000) [29], who used the same Harris-Nesbet method for his calculation, but with the consideration of a 13-state scheme instead (see table 3.25).

Table 3.9: G-wave phase shifts (in units of radian) of electron collision with hydrogen atom.

$k\left(a_0^{-1}\right)$	0.1	0.15	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.83	0.85	0.86
						Singlet						
[a] HN 3S	0.000129	0.000293	0.000520	0.00116	0.00202	0.00316	0.00450	0.00604	0.00795	0.00870	0.00938	0.0104
[b] HN 4S	0.000196	0.000447	0.000794	0.00177	0.00312	0.00493	0.00703	0.00934	0.0121	0.0133	0.0144	0.0167
[c] HN 6S	0.000167	0.000381	0.000677	0.00151	0.00266	0.00421	0.00602	0.00804	0.0105	0.0115	0.0125	0.0141
[d] HN E3S	0.000192	0.000423	0.000775	0.00175	0.00310	0.00487	0.00704	0.00954	0.0125	0.0137	0.0148	0.0167
[e] HN E4S	0.000197	0.000448	0.000797	0.00179	0.00317	0.00505	0.00723	0.00965	0.0126	0.0138	0.0150	0.0174
[f] HN E6S	0.000193	0.000433	0.000787	0.00177	0.00311	0.00488	0.00702	0.00954	0.0125	0.0137	0.0146	0.0154
[g] HN 13S	0.00019	0.00044	0.00078	0.0018	0.0031	0.0048	0.0069	0.0094	0.0124	0.0134	—	—
						Triplet						
[a] HN 3S	0.000129	0.000293	0.000520	0.00116	0.00202	0.00317	0.00450	0.00603	0.00796	0.00873	0.00945	0.0107
[b] HN 4S	0.000196	0.000447	0.000794	0.00177	0.00312	0.00497	0.00709	0.00942	0.0122	0.0135	0.0147	0.0176
[c] HN 6S	0.000167	0.000381	0.000677	0.00151	0.00267	0.00424	0.00604	0.00803	0.0105	0.0115	0.0124	0.0146
[d] HN E3S	0.000195	0.000442	0.000788	0.00177	0.00314	0.00502	0.00746	0.00972	0.0132	0.0136	0.0145	0.0152
[e] HN E4S	0.000197	0.000448	0.000797	0.00179	0.00317	0.00508	0.00728	0.00969	0.0126	0.0139	0.0151	0.0186
[f] HN E6S	0.000193	0.000433	0.000787	0.00177	0.00311	0.00488	0.00704	0.00958	0.0126	0.0137	0.0147	0.0156
[g] HN 13S	0.00019	0.00044	0.00078	0.0018	0.0031	0.0048	0.0069	0.0094	0.0124	0.0135	—	—

[a, b, c] present Harris-Nesbet calculation with 3S, 4S and 6S schemes respectively

[d, e, f] present Harris-Nesbet calculation with E3S, E4S and E6S schemes respectively

[g] Harris-Nesbet calculation, T.T.Gien (1998) [26]

Table 3.10: Singlet H-wave phase shifts (in units of radian) of electron collision with hydrogen atom. The number in [ ] indicates powers of ten.

$k\left(a_0^{-1}\right)$	[a]HN 3S	[b]HN 4S	[c]HN 6S	[d]HN E3S	[e]HN E4S	[f]HN E6S
0.1	0.682[-4]	0.104[-3]	0.883[-4]	0.102[-3]	0.107[-3]	0.102[-3]
0.15	0.156[-3]	0.238[-3]	0.203[-3]	0.231[-3]	0.243[-3]	0.236[-3]
0.2	0.279[-3]	0.425[-3]	0.362[-3]	0.416[-3]	0.432[-3]	0.424[-3]
0.3	0.625[-3]	0.954[-3]	0.813[-3]	0.942[-3]	0.969[-3]	0.957[-3]
0.4	0.110[-2]	0.169[-2]	0.144[-2]	0.168[-2]	0.171[-2]	0.169[-2]
0.5	0.171[-2]	0.263[-2]	0.224[-2]	0.263[-2]	0.266[-2]	0.264[-2]
0.6	0.244[-2]	0.377[-2]	0.322[-2]	0.387[-2]	0.383[-2]	0.380[-2]
0.7	0.330[-2]	0.510[-2]	0.437[-2]	0.523[-2]	0.522[-2]	0.519[-2]
0.8	0.433[-2]	0.666[-2]	0.573[-2]	0.686[-2]	0.686[-2]	0.685[-2]
0.83	0.471[-2]	0.725[-2]	0.623[-2]	0.719[-2]	0.746[-2]	0.718[-2]
0.85	0.500[-2]	0.772[-2]	0.622[-2]	0.766[-2]	0.792[-2]	0.776[-2]
0.86	0.521[-2]	0.810[-2]	0.694[-2]	0.788[-2]	0.822[-2]	0.798[-2]

Table 3.11: Triplet H-wave phase shifts (in units of radian) of electron collision with hydrogen atom. The number in [ ] indicates powers of ten.

$k\left(a_0^{-1}\right)$	[a]HN 3S	[b]HN 4S	[c]HN 6S	[d]HN E3S	[e]HN E4S	[f]HN E6S
0.1	0.681[-4]	0.104[-3]	0.883[-4]	0.102[-3]	0.107[-3]	0.102[-3]
0.15	0.156[-3]	0.238[-3]	0.203[-3]	0.231[-3]	0.243[-3]	0.236[-3]
0.2	0.279[-3]	0.425[-3]	0.362[-3]	0.416[-3]	0.432[-3]	0.424[-3]
0.3	0.625[-3]	0.954[-3]	0.813[-3]	0.942[-3]	0.969[-3]	0.957[-3]
0.4	0.110[-2]	0.169[-2]	0.144[-2]	0.168[-2]	0.171[-2]	0.169[-2]
0.5	0.171[-2]	0.263[-2]	0.224[-2]	0.263[-2]	0.266[-2]	0.264[-2]
0.6	0.244[-2]	0.377[-2]	0.322[-2]	0.387[-2]	0.383[-2]	0.380[-2]
0.7	0.330[-2]	0.511[-2]	0.437[-2]	0.524[-2]	0.522[-2]	0.519[-2]
0.8	0.434[-2]	0.669[-2]	0.573[-2]	0.686[-2]	0.687[-2]	0.685[-2]
0.83	0.472[-2]	0.728[-2]	0.622[-2]	0.719[-2]	0.747[-2]	0.717[-2]
0.85	0.502[-2]	0.774[-2]	0.661[-2]	0.767[-2]	0.792[-2]	0.777[-2]
0.86	0.522[-2]	0.812[-2]	0.691[-2]	0.788[-2]	0.820[-2]	0.799[-2]

[a, b, c] present Harris-Nesbet calculation with 3S, 4S and 6S schemes respectively
[d, e, f] present Harris-Nesbet calculation with E3S, E4S and E6S schemes respectively

Table 3.12: Singlet I-wave phase shifts (in units of radian) of electron collision with hydrogen atom. The number in [ ] indicates powers of ten.

$k\left(a_0^{-1}\right)$	[a]HN 3S	[b]HN 4S	[c]HN 6S	[d]HN E3S	[e]HN E4S	[f]HN E6S
0.1	0.401[-4]	0.609[-4]	0.519[-4]	0.559[-4]	0.609[-4]	0.574[-4]
0.15	0.924[-4]	0.141[-3]	0.120[-3]	0.135[-3]	0.141[-3]	0.135[-3]
0.2	0.166[-3]	0.252[-3]	0.215[-3]	0.245[-3]	0.253[-3]	0.246[-3]
0.3	0.374[-3]	0.570[-3]	0.486[-3]	0.557[-3]	0.572[-3]	0.562[-3]
0.4	0.661[-3]	0.101[-2]	0.862[-3]	0.996[-3]	0.102[-2]	0.100[-2]
0.5	0.103[-2]	0.159[-2]	0.136[-2]	0.157[-2]	0.161[-2]	0.160[-2]
0.6	0.157[-2]	0.250[-2]	0.245[-2]	0.229[-2]	0.310[-2]	0.309[-2]
0.7	0.201[-2]	0.310[-2]	0.266[-2]	0.310[-2]	0.316[-2]	0.314[-2]
0.8	0.263[-2]	0.405[-2]	0.348[-2]	0.408[-2]	0.414[-2]	0.412[-2]
0.83	0.288[-2]	0.447[-2]	0.386[-2]	0.447[-2]	0.460[-2]	0.460[-2]
0.85	0.295[-2]	0.451[-2]	0.389[-2]	0.453[-2]	0.462[-2]	0.460[-2]
0.86	0.304[-2]	0.466[-2]	0.401[-2]	0.470[-2]	0.477[-2]	0.475[-2]

Table 3.13: Triplet I-wave phase shifts (in units of radian) of electron collision with hydrogen atom. The number in [ ] indicates powers of ten.

$k\left(a_0^{-1}\right)$	[a]HN 3S	[b]HN 4S	[c]HN 6S	[d]HN E3S	[e]HN E4S	[f]HN E6S
0.1	0.401[-4]	0.609[-4]	0.519[-4]	0.559[-4]	0.609[-4]	0.574[-4]
0.15	0.924[-4]	0.141[-3]	0.120[-3]	0.135[-3]	0.141[-3]	0.135[-3]
0.2	0.166[-3]	0.252[-3]	0.215[-3]	0.245[-3]	0.253[-3]	0.246[-3]
0.3	0.374[-3]	0.570[-3]	0.486[-3]	0.557[-3]	0.572[-3]	0.562[-3]
0.4	0.662[-3]	0.101[-2]	0.862[-3]	0.996[-3]	0.102[-2]	0.100[-2]
0.5	0.104[-2]	0.159[-2]	0.136[-2]	0.157[-2]	0.161[-2]	0.159[-2]
0.6	0.155[-2]	0.245[-2]	0.216[-2]	0.228[-2]	0.271[-2]	0.261[-2]
0.7	0.201[-2]	0.311[-2]	0.265[-2]	0.310[-2]	0.316[-2]	0.314[-2]
0.8	0.264[-2]	0.405[-2]	0.347[-2]	0.408[-2]	0.414[-2]	0.412[-2]
0.83	0.289[-2]	0.446[-2]	0.383[-2]	0.447[-2]	0.459[-2]	0.457[-2]
0.85	0.296[-2]	0.451[-2]	0.389[-2]	0.452[-2]	0.462[-2]	0.460[-2]
0.86	0.305[-2]	0.466[-2]	0.401[-2]	0.469[-2]	0.477[-2]	0.475[-2]

[a, b, c] present Harris-Nesbet calculation with 3S, 4S and 6S schemes respectively

[d, e, f] present Harris-Nesbet calculation with E3S, E4S and E6S schemes respectively

Table 3.14: Singlet J-wave phase shifts (in units of radian) of electron collision with hydrogen. The number in [ ] indicates powers of ten.

$k\left(a_0^{-1}\right)$	[a]HN 3S	[b]HN 4S	[c]HN 6S	[d]HN E3S	[e]HN E4S	[f]HN E6S
0.1	0.253[-4]	0.384[-4]	0.328[-4]	0.301[-4]	0.389[-4]	0.383[-4]
0.15	0.587[-4]	0.893[-4]	0.761[-4]	0.836[-4]	0.911[-4]	0.862[-4]
0.2	0.106[-3]	0.161[-3]	0.137[-3]	0.153[-3]	0.164[-3]	0.158[-3]
0.3	0.240[-3]	0.365[-3]	0.312[-3]	0.355[-3]	0.371[-3]	0.363[-3]
0.4	0.427[-3]	0.651[-3]	0.556[-3]	0.634[-3]	0.662[-3]	0.649[-3]
0.5	0.668[-3]	0.102[-2]	0.872[-3]	0.980[-3]	0.103[-2]	0.102[-2]
0.6	0.967[-3]	0.149[-2]	0.127[-2]	0.144[-2]	0.149[-2]	0.147[-2]
0.7	0.131[-2]	0.200[-2]	0.172[-2]	0.197[-2]	0.204[-2]	0.201[-2]
0.8	0.171[-2]	0.263[-2]	0.225[-2]	0.250[-2]	0.269[-2]	0.265[-2]
0.83	0.188[-2]	0.290[-2]	0.249[-2]	0.283[-2]	0.291[-2]	0.287[-2]
0.85	0.194[-2]	0.294[-2]	0.255[-2]	0.300[-2]	0.305[-2]	0.307[-2]
0.86	0.200[-2]	0.303[-2]	0.265[-2]	0.309[-2]	0.313[-2]	0.338[-2]

Table 3.15: Triplet J-wave phase shifts (in units of radian) of electron collision with hydrogen atom. The number in [ ] indicates powers of ten.

$k\left(a_0^{-1}\right)$	[a]HN 3S	[b]HN 4S	[c]HN 6S	[d]HN E3S	[e]HN E4S	[f]HN E6S
0.1	0.246[-4]	0.385[-4]	0.323[-4]	0.295[-4]	0.393[-4]	0.383[-4]
0.15	0.587[-4]	0.893[-4]	0.761[-4]	0.836[-4]	0.911[-4]	0.858[-4]
0.2	0.106[-3]	0.161[-3]	0.137[-3]	0.153[-3]	0.164[-3]	0.158[-3]
0.3	0.239[-3]	0.365[-3]	0.311[-3]	0.354[-3]	0.371[-3]	0.361[-3]
0.4	0.423[-3]	0.652[-3]	0.551[-3]	0.630[-3]	0.661[-3]	0.648[-3]
0.5	0.658[-3]	0.102[-2]	0.861[-3]	0.973[-3]	0.103[-2]	0.101[-2]
0.6	0.955[-3]	0.149[-2]	0.125[-2]	0.144[-2]	0.149[-2]	0.146[-2]
0.7	0.130[-2]	0.201[-2]	0.171[-2]	0.197[-2]	0.203[-2]	0.201[-2]
0.8	0.171[-2]	0.264[-2]	0.225[-2]	0.250[-2]	0.267[-2]	0.264[-2]
0.83	0.187[-2]	0.286[-2]	0.246[-2]	0.283[-2]	0.290[-2]	0.286[-2]
0.85	0.192[-2]	0.292[-2]	0.252[-2]	0.298[-2]	0.305[-2]	0.301[-2]
0.86	0.198[-2]	0.300[-2]	0.259[-2]	0.306[-2]	0.313[-2]	0.309[-2]

[a, b, c] present Harris-Nesbet calculation with 3S, 4S and 6S schemes respectively

[d, e, f] present Harris-Nesbet calculation with E3S, E4S and E6S schemes respectively

Table 3.16: Differential cross sections (in units of πa_0^2 sr^{-1}) for the elastic scattering of electrons from atomic hydrogen at 0.582 eV. The numbers in parentheses are the maximum possible errors in the last significant digits and include both systematic and random errors.

Angle (deg)	[a]HN 3S	[b]HN 4S	[c]HN 6S	[d]HN E3S	[e]HN E4S	[f]HN E6S	[g]HN 13S	[h]Williams
10	2.036	1.812	1.864	1.756	1.754	1.754	1.759	—
15	2.069	1.855	1.902	1.798	1.798	1.796	1.800	—
20	2.102	1.898	1.941	1.841	1.841	1.839	1.843	1.79(24)
25	2.136	1.941	1.981	1.884	1.885	1.883	1.888	—
30	2.172	1.988	2.023	1.931	1.932	1.930	1.934	1.87(28)
35	2.210	2.036	2.068	1.980	1.981	1.979	1.982	—
40	2.248	2.085	2.114	2.030	2.030	2.029	2.031	1.95(28)
45	2.287	2.134	2.161	2.080	2.080	2.079	2.081	—
50	2.328	2.186	2.210	2.132	2.133	2.131	2.133	1.98(28)
55	2.370	2.238	2.260	2.185	2.186	2.185	2.186	—
60	2.412	2.290	2.311	2.239	2.240	2.238	2.239	2.20(17)
70	2.499	2.397	2.415	2.348	2.349	2.347	2.349	2.29(26)
80	2.587	2.505	2.521	2.458	2.459	2.457	2.459	2.44(24)
90	2.675	2.611	2.628	2.567	2.568	2.566	2.568	2.55(19)
100	2.760	2.715	2.731	2.673	2.673	2.672	2.674	2.70(19)
110	2.842	2.813	2.831	2.774	2.774	2.773	2.774	2.65(22)
120	2.917	2.904	2.922	2.867	2.867	2.866	2.868	2.85(16)
130	2.985	2.986	3.006	2.950	2.950	2.949	2.951	2.78(20)
140	3.043	3.055	3.076	3.022	3.021	3.020	3.022	2.84(27)
150	3.090	3.112	3.134	3.080	3.079	3.079	3.080	2.99(20)

[a, b, c] present Harris-Nesbet calculation with 3S, 4S and 6S schemes respectively
[d, e, f] present Harris-Nesbet calculation with E3S, E4S and E6S schemes respectively
[g] Harris-Nesbet calculation, T.T.Gien (2000) [29]
[h] experimental values, J. F. Williams (1975) [12]

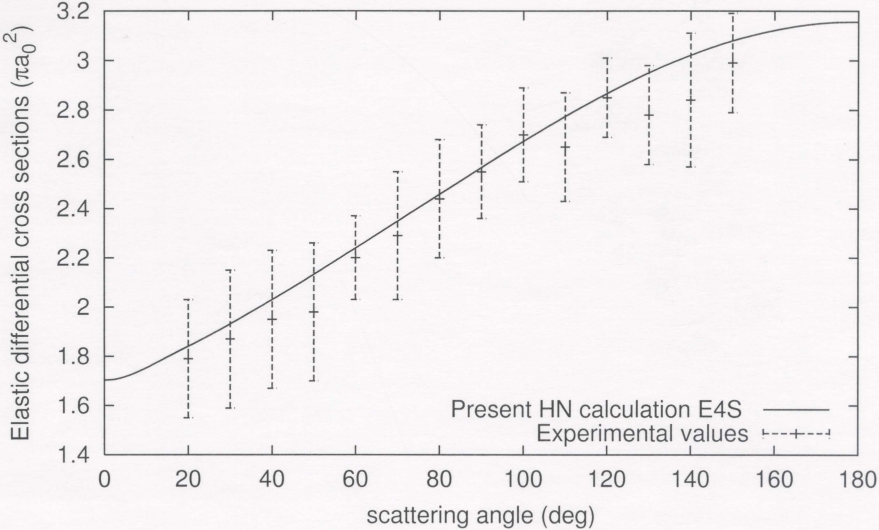

Figure 3.9: Differential cross sections for e^--H elastic scattering at 0.582 eV

Table 3.17: Differential cross sections (in units of πa_0^2 sr^{-1}) for the elastic scattering of electrons from atomic hydrogen at 1.207 eV. The numbers in parentheses are the maximum possible errors in the last significant digits and include both systematic and random errors.

Angle (deg)	[a]HN 3S	[b]HN 4S	[c]HN 6S	[d]HN E3S	[e]HN E4S	[f]HN E6S	[g]HN 13S	[h]Williams
10	1.341	1.300	1.311	1.284	1.284	1.284	1.285	—
15	1.355	1.309	1.321	1.293	1.293	1.293	1.294	—
20	1.371	1.323	1.334	1.306	1.306	1.306	1.307	1.38(24)
25	1.390	1.340	1.351	1.323	1.323	1.323	1.324	—
30	1.412	1.362	1.373	1.345	1.346	1.345	1.346	1.38(23)
35	1.438	1.389	1.398	1.372	1.373	1.372	1.373	—
40	1.466	1.419	1.427	1.403	1.403	1.403	1.404	1.56(27)
45	1.497	1.453	1.460	1.438	1.438	1.437	1.438	—
50	1.532	1.492	1.497	1.477	1.477	1.477	1.477	1.42(26)
55	1.570	1.534	1.538	1.520	1.520	1.520	1.519	—
60	1.611	1.579	1.582	1.566	1.566	1.566	1.565	1.77(23)
70	1.701	1.680	1.681	1.668	1.668	1.668	1.668	1.63(19)
80	1.800	1.791	1.790	1.781	1.781	1.781	1.781	1.94(17)
90	1.906	1.911	1.907	1.903	1.903	1.903	1.903	1.95(23)
100	2.014	2.034	2.028	2.028	2.029	2.029	2.029	2.02(24)
110	2.123	2.158	2.151	2.155	2.155	2.155	2.155	2.12(22)
120	2.227	2.277	2.269	2.277	2.277	2.277	2.277	2.24(23)
130	2.323	2.388	2.379	2.390	2.390	2.390	2.390	2.39(27)
140	2.406	2.486	2.476	2.490	2.489	2.489	2.490	2.58(24)
150	2.475	2.567	2.557	2.573	2.573	2.573	2.572	2.54(23)

[a, b, c] present Harris-Nesbet calculation with 3S, 4S and 6S schemes respectively
[d, e, f] present Harris-Nesbet calculation with E3S, E4S and E6S schemes respectively
[g] Harris-Nesbet calculation, T.T.Gien (2000) [29]
[h] experimental values, J. F. Williams (1975) [12]

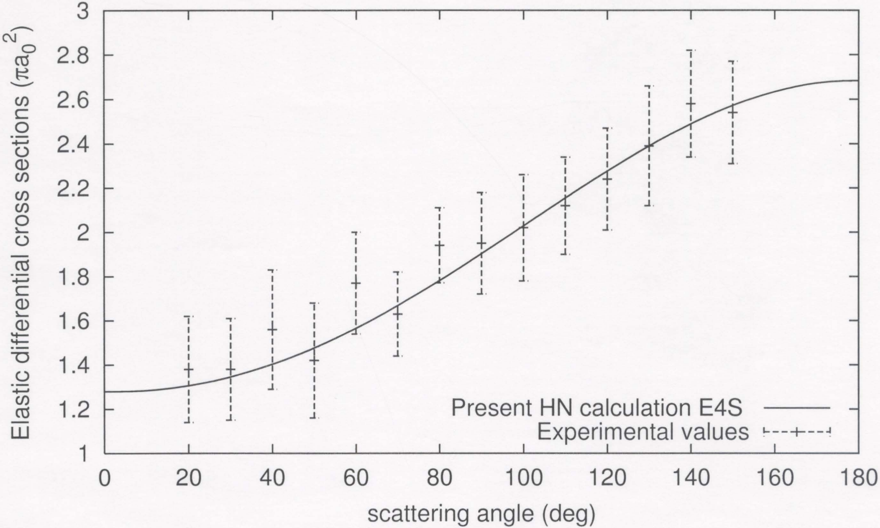

Figure 3.10: Differential cross sections for e^--H elastic scattering at 1.207 eV

Table 3.18: Differential cross sections (in units of πa_0^2 sr^{-1}) for the elastic scattering of electrons from atomic hydrogen at 1.597 eV. The numbers in parentheses are the maximum possible errors in the last significant digits and include both systematic and random errors.

Angle (deg)	[a]HN 3S	[b]HN 4S	[c]HN 6S	[d]HN E3S	[e]HN E4S	[f]HN E6S	[g]HN 13S	[h]Williams
10	1.189	1.231	1.217	1.228	1.230	1.230	1.229	—
15	1.188	1.215	1.207	1.213	1.214	1.214	1.214	—
20	1.191	1.207	1.202	1.205	1.205	1.205	1.205	1.17(11)
25	1.197	1.205	1.201	1.202	1.202	1.202	1.202	—
30	1.207	1.208	1.206	1.205	1.205	1.205	1.205	1.15(10)
35	1.221	1.218	1.217	1.213	1.213	1.214	1.214	—
40	1.239	1.232	1.232	1.227	1.228	1.228	1.228	1.18(12)
45	1.261	1.252	1.252	1.246	1.248	1.249	1.248	—
50	1.287	1.278	1.277	1.272	1.274	1.274	1.274	1.14(16)
55	1.318	1.309	1.308	1.303	1.305	1.305	1.305	—
60	1.352	1.345	1.343	1.339	1.341	1.341	1.341	1.26(7)
70	1.433	1.431	1.427	1.428	1.428	1.428	1.427	1.36(13)
80	1.527	1.533	1.528	1.534	1.532	1.532	1.531	1.45(14)
90	1.633	1.649	1.641	1.653	1.650	1.650	1.649	1.61(12)
100	1.746	1.774	1.763	1.778	1.776	1.776	1.775	1.69(9)
110	1.861	1.902	1.889	1.907	1.907	1.907	1.906	1.88(10)
120	1.973	2.029	2.013	2.032	2.035	2.036	2.036	2.01(12)
130	2.077	2.149	2.131	2.153	2.158	2.159	2.158	2.10(12)
140	2.169	2.256	2.237	2.263	2.267	2.268	2.268	2.20(12)
150	2.246	2.347	2.327	2.361	2.360	2.361	2.360	2.32(15)

[a, b, c] present Harris-Nesbet calculation with 3S, 4S and 6S schemes respectively

[d, e, f] present Harris-Nesbet calculation with E3S, E4S and E6S schemes respectively

[g] Harris-Nesbet calculation, T.T.Gien (2000) [29]

[h] experimental values, J. F. Williams (1975) [12]

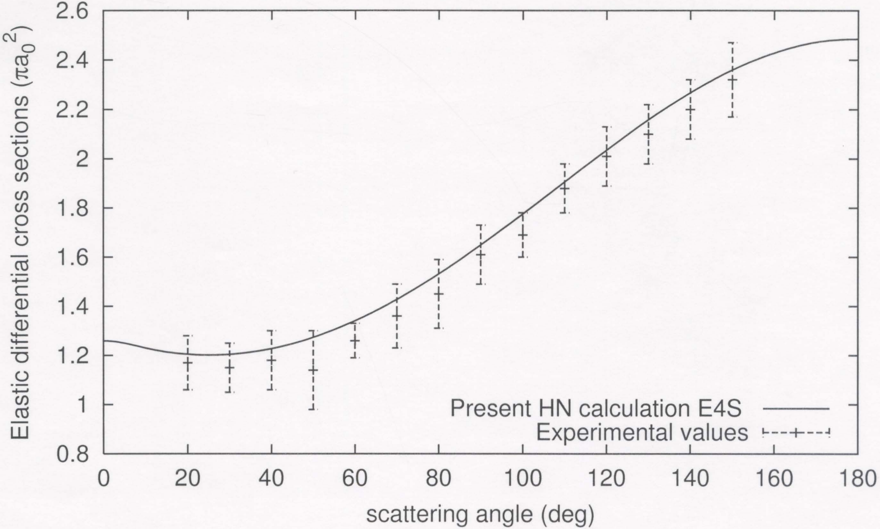

Figure 3.11: Differential cross sections for e^--H elastic scattering at 1.597 eV

Table 3.19: Differential cross sections (in units of πa_0^2 sr^{-1}) for the elastic scattering of electrons from atomic hydrogen at 2.171 eV. The numbers in parentheses are the maximum possible errors in the last significant digits and include both systematic and random errors.

Angle (deg)	[a]HN 3S	[b]HN 4S	[c]HN 6S	[d]HN E3S	[e]HN E4S	[f]HN E6S	[g]HN 13S	[h]Williams
10	1.138	1.278	1.229	1.294	1.297	1.296	1.292	—
15	1.115	1.227	1.189	1.243	1.243	1.243	1.243	—
20	1.098	1.188	1.157	1.201	1.202	1.202	1.201	1.17(10)
25	1.084	1.156	1.131	1.168	1.169	1.169	1.168	—
30	1.075	1.132	1.111	1.142	1.142	1.142	1.142	1.13(10)
35	1.070	1.115	1.099	1.124	1.124	1.124	1.124	—
40	1.071	1.106	1.092	1.113	1.113	1.113	1.113	1.12(10)
45	1.076	1.104	1.092	1.110	1.110	1.110	1.110	—
50	1.087	1.109	1.099	1.114	1.114	1.114	1.114	1.10(10)
55	1.103	1.121	1.112	1.125	1.125	1.126	1.125	—
60	1.124	1.140	1.131	1.144	1.144	1.144	1.143	1.13(10)
70	1.183	1.197	1.189	1.200	1.200	1.201	1.200	1.17(12)
80	1.262	1.277	1.268	1.281	1.281	1.282	1.281	1.22(8)
90	1.357	1.378	1.367	1.383	1.383	1.383	1.382	1.31(12)
100	1.465	1.493	1.479	1.500	1.500	1.500	1.500	1.44(13)
110	1.579	1.618	1.601	1.627	1.627	1.627	1.627	1.58(13)
120	1.693	1.745	1.725	1.757	1.756	1.757	1.757	1.74(12)
130	1.802	1.869	1.846	1.883	1.883	1.883	1.881	1.87(12)
140	1.899	1.981	1.957	1.997	1.997	1.997	1.997	1.98(12)
150	1.981	2.077	2.051	2.095	2.094	2.095	2.095	2.04(18)

[a, b, c] present Harris-Nesbet calculation with 3S, 4S and 6S schemes respectively

[d, e, f] present Harris-Nesbet calculation with E3S, E4S and E6S schemes respectively

[g] Harris-Nesbet calculation, T.T.Gien (2000) [29]

[h] experimental values, J. F. Williams (1975) [12]

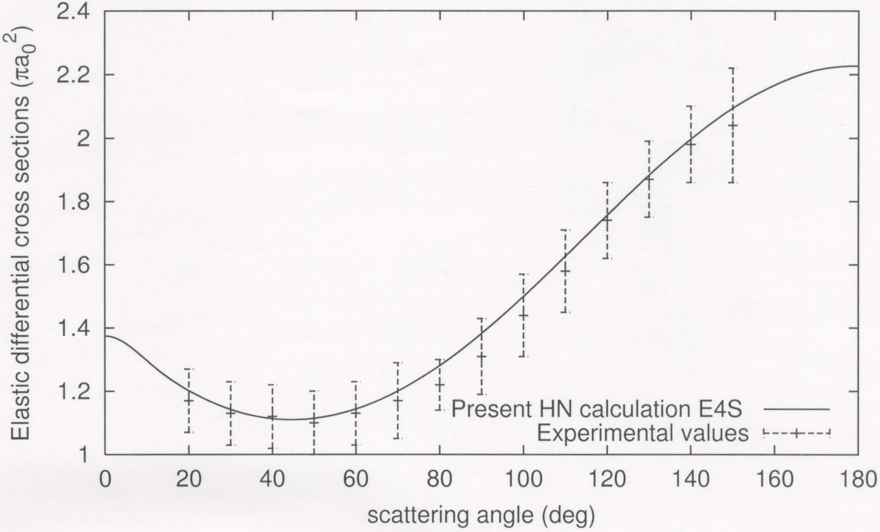

Figure 3.12: Differential cross sections for e^--H elastic scattering at 2.171 eV

Table 3.20: Differential cross sections (in units of πa_0^2 sr^{-1}) for the elastic scattering of electrons from atomic hydrogen at 3.009 eV. The numbers in parentheses are the maximum possible errors in the last significant digits and include both systematic and random errors.

Angle (deg)	[a]HN 3S	[b]HN 4S	[c]HN 6S	[d]HN E3S	[e]HN E4S	[f]HN E6S	[g]HN 13S	[h]Williams
10	1.223	1.474	1.376	1.510	1.513	1.511	1.504	—
15	1.171	1.375	1.297	1.410	1.410	1.411	1.409	—
20	1.125	1.294	1.229	1.325	1.325	1.326	1.325	1.15(12)
25	1.085	1.224	1.170	1.252	1.252	1.253	1.250	—
30	1.049	1.163	1.118	1.187	1.187	1.187	1.186	1.13(8)
35	1.018	1.110	1.073	1.131	1.131	1.132	1.131	—
40	0.993	1.068	1.037	1.087	1.087	1.087	1.086	1.04(11)
45	0.973	1.035	1.009	1.051	1.051	1.052	1.051	—
50	0.960	1.011	0.989	1.025	1.025	1.025	1.025	1.00(12)
55	0.954	0.996	0.977	1.008	1.008	1.008	1.008	—
60	0.954	0.989	0.973	1.000	1.000	1.000	0.999	1.01(7)
70	0.975	1.000	0.988	1.009	1.009	1.009	1.009	1.04(10)
80	1.021	1.042	1.031	1.050	1.050	1.050	1.049	1.08(11)
90	1.091	1.111	1.100	1.119	1.119	1.119	1.119	1.15(12)
100	1.179	1.201	1.189	1.210	1.210	1.210	1.210	1.29(10)
110	1.279	1.308	1.293	1.318	1.318	1.318	1.317	1.41(10)
120	1.383	1.422	1.403	1.434	1.434	1.434	1.434	1.47(14)
130	1.486	1.537	1.516	1.551	1.551	1.551	1.550	1.58(15)
140	1.580	1.644	1.620	1.660	1.659	1.659	1.659	1.72(9)
150	1.660	1.737	1.712	1.754	1.754	1.754	1.753	1.77(14)

[a, b, c] present Harris-Nesbet calculation with 3S, 4S and 6S schemes respectively

[d, e, f] present Harris-Nesbet calculation with E3S, E4S and E6S schemes respectively

[g] Harris-Nesbet calculation, T.T.Gien (2000) [29]

[h] experimental values, J. F. Williams (1975) [12]

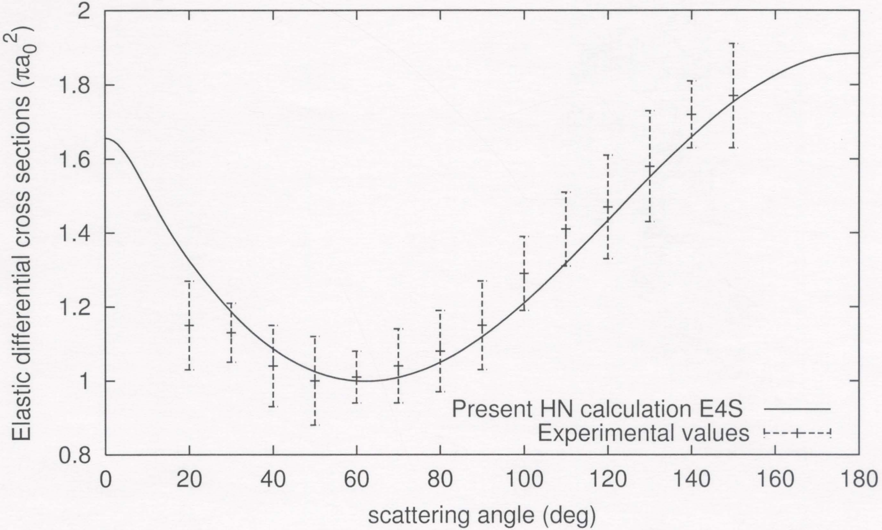

Figure 3.13: Differential cross sections for e^--H elastic scattering at 3.009 eV

Table 3.21: Differential cross sections (in units of πa_0^2 sr^{-1}) for the elastic scattering of electrons from atomic hydrogen at 3.423 eV. The numbers in parentheses are the maximum possible errors in the last significant digits and include both systematic and random errors.

Angle (deg)	[a]HN 3S	[b]HN 4S	[c]HN 6S	[d]HN E3S	[e]HN E4S	[f]HN E6S	[g]HN 13S	[h]Williams
10	1.290	1.585	1.467	1.628	1.634	1.628	1.616	1.66(10)
15	1.224	1.465	1.369	1.506	1.507	1.505	1.502	1.50(10)
20	1.166	1.364	1.285	1.401	1.402	1.401	1.400	1.33(10)
25	1.114	1.277	1.211	1.311	1.311	1.310	1.308	1.29(9)
30	1.065	1.198	1.144	1.228	1.228	1.228	1.227	1.19(8)
35	1.022	1.130	1.086	1.157	1.156	1.157	1.157	—
40	0.986	1.074	1.037	1.097	1.096	1.097	1.097	1.08(7)
45	0.956	1.028	0.997	1.048	1.047	1.048	1.048	—
50	0.932	0.991	0.965	1.008	1.008	1.009	1.008	1.03(6)
55	0.915	0.964	0.942	0.979	0.979	0.979	0.979	—
60	0.905	0.946	0.927	0.959	0.959	0.959	0.959	0.94(6)
70	0.908	0.936	0.922	0.946	0.946	0.947	0.946	0.91(7)
80	0.938	0.959	0.948	0.968	0.968	0.969	0.968	0.93(7)
90	0.993	1.011	1.002	1.020	1.020	1.021	1.020	1.01(8)
100	1.069	1.088	1.077	1.097	1.097	1.098	1.097	1.10(8)
110	1.160	1.184	1.170	1.194	1.194	1.194	1.193	1.19(7)
120	1.257	1.289	1.273	1.301	1.301	1.300	1.300	1.33(9)
130	1.354	1.389	1.378	1.411	1.411	1.409	1.409	1.42(8)
140	1.444	1.499	1.477	1.513	1.513	1.512	1.512	1.52(8)
150	1.520	1.587	1.563	1.602	1.602	1.603	1.601	1.58(8)

[a, b, c] present Harris-Nesbet calculation with 3S, 4S and 6S schemes respectively
[d, e, f] present Harris-Nesbet calculation with E3S, E4S and E6S schemes respectively
[g] Harris-Nesbet calculation, T.T.Gien (2000) [29]
[h] experimental values, J. F. Williams (1975) [12]

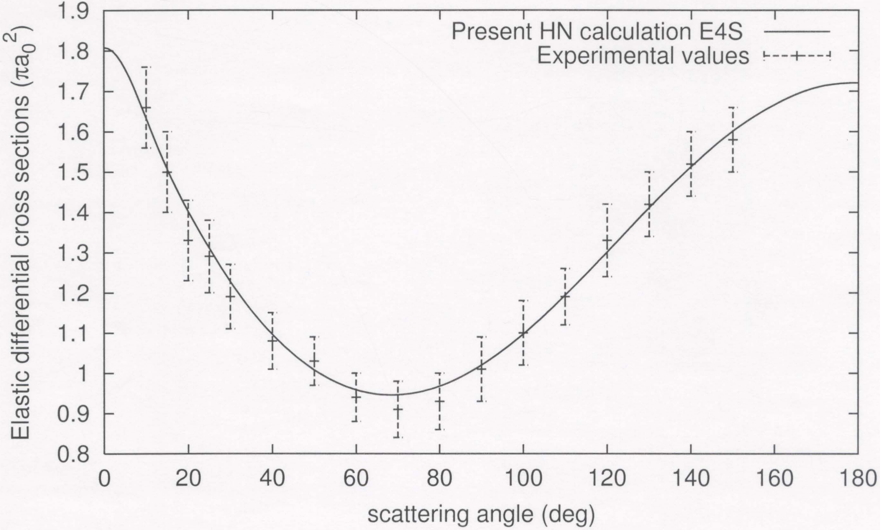

Figure 3.14: Differential cross sections for e^--H elastic scattering at 3.423 eV

Table 3.22: Differential cross sections (in units of πa_0^2 sr^{-1}) for the elastic scattering of electrons from atomic hydrogen at 4.889 eV. The numbers in parentheses are the maximum possible errors in the last significant digits and include both systematic and random errors.

Angle (deg)	[a]HN 3S	[b]HN 4S	[c]HN 6S	[d]HN E3S	[e]HN E4S	[f]HN E6S	[g]HN 13S	[h]Williams
10	1.509	1.903	1.737	1.966	1.972	1.965	1.949	2.04(10)
15	1.404	1.720	1.587	1.780	1.781	1.778	1.775	1.85(9)
20	1.311	1.567	1.459	1.620	1.620	1.619	1.618	1.62(8)
25	1.226	1.435	1.345	1.481	1.481	1.480	1.477	1.53(7)
30	1.144	1.312	1.239	1.352	1.352	1.352	1.351	1.37(7)
35	1.068	1.204	1.143	1.238	1.238	1.239	1.239	1.20(7)
40	1.001	1.111	1.061	1.140	1.140	1.141	1.141	1.17(7)
45	0.941	1.030	0.988	1.055	1.055	1.056	1.055	—
50	0.887	0.960	0.925	0.981	0.981	0.982	0.981	1.03(6)
55	0.841	0.901	0.872	0.919	0.919	0.920	0.919	—
60	0.804	0.853	0.829	0.869	0.868	0.869	0.868	0.88(4)
70	0.753	0.786	0.770	0.798	0.798	0.798	0.798	0.78(7)
80	0.735	0.756	0.746	0.766	0.766	0.766	0.766	0.75(7)
90	0.746	0.761	0.753	0.768	0.769	0.769	0.769	0.78(7)
100	0.782	0.793	0.787	0.801	0.801	0.801	0.801	0.83(8)
110	0.838	0.848	0.841	0.857	0.856	0.856	0.856	0.90(8)
120	0.905	0.918	0.910	0.927	0.926	0.926	0.926	0.94(7)
130	0.978	0.997	0.986	1.006	1.005	1.005	1.004	1.00(7)
140	1.047	1.073	1.061	1.083	1.082	1.083	1.081	1.07(6)
150	1.109	1.142	1.129	1.151	1.152	1.153	1.151	1.10(7)

[a, b, c] present Harris-Nesbet calculation with 3S, 4S and 6S schemes respectively

[d, e, f] present Harris-Nesbet calculation with E3S, E4S and E6S schemes respectively

[g] Harris-Nesbet calculation, T.T.Gien (2000) [29]

[h] experimental values, J. F. Williams (1975) [12]

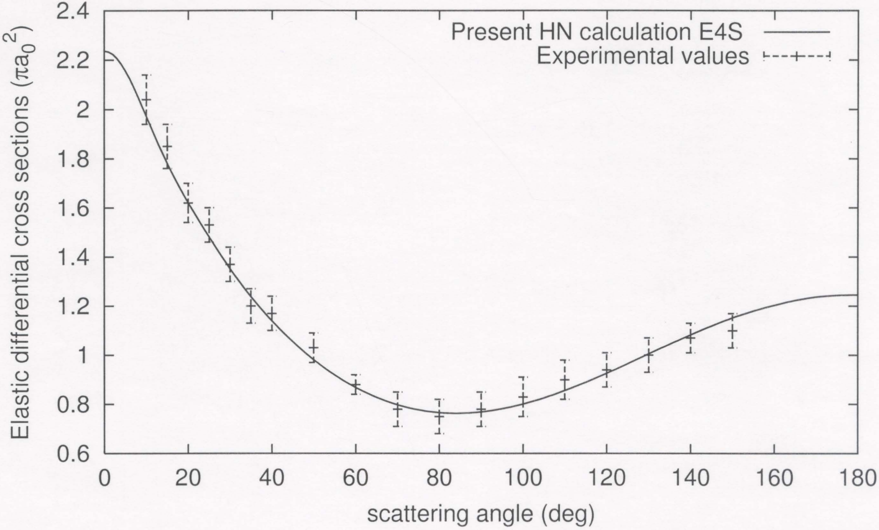

Figure 3.15: Differential cross sections for e^--H elastic scattering at 4.889 eV

Table 3.23: Differential cross sections (in units of πa_0^2 sr^{-1}) for the elastic scattering of electrons from atomic hydrogen at 6.691 eV. The numbers in parentheses are the maximum possible errors in the last significant digits and include both systematic and random errors.

Angle (deg)	[a]HN 3S	[b]HN 4S	[c]HN 6S	[d]HN E3S	[e]HN E4S	[f]HN E6S	[g]HN 13S	[h]Williams
10	1.668	2.113	1.921	2.189	2.195	2.189	2.174	2.23(10)
15	1.528	1.875	1.725	1.946	1.946	1.944	1.946	2.00(12)
20	1.405	1.680	1.560	1.741	1.741	1.740	1.742	1.66(13)
25	1.294	1.513	1.416	1.565	1.565	1.564	1.560	1.56(12)
30	1.187	1.359	1.281	1.402	1.403	1.403	1.401	1.37(10)
35	1.088	1.222	1.160	1.258	1.259	1.259	1.259	1.21(10)
40	0.998	1.104	1.054	1.135	1.135	1.135	1.135	1.15(8)
45	0.917	1.002	0.960	1.027	1.027	1.028	1.026	1.05(6)
50	0.843	0.910	0.876	0.932	0.931	0.932	0.931	0.97(6)
55	0.778	0.831	0.804	0.850	0.849	0.850	0.849	0.84(4)
60	0.722	0.765	0.742	0.780	0.780	0.780	0.780	0.82(5)
70	0.635	0.662	0.647	0.674	0.673	0.674	0.673	0.67(4)
80	0.580	0.598	0.589	0.607	0.607	0.607	0.606	0.63(5)
90	0.557	0.567	0.562	0.574	0.574	0.574	0.574	0.56(4)
100	0.559	0.564	0.561	0.571	0.571	0.571	0.570	0.57(5)
110	0.583	0.585	0.583	0.591	0.591	0.591	0.590	0.61(4)
120	0.621	0.622	0.620	0.628	0.628	0.628	0.628	0.64(6)
130	0.667	0.670	0.668	0.676	0.676	0.675	0.675	0.66(4)
140	0.715	0.721	0.717	0.725	0.725	0.726	0.726	0.70(5)
150	0.759	0.769	0.764	0.773	0.773	0.774	0.773	0.73(5)

[a, b, c] present Harris-Nesbet calculation with 3S, 4S and 6S schemes respectively

[d, e, f] present Harris-Nesbet calculation with E3S, E4S and E6S schemes respectively

[g] Harris-Nesbet calculation, T.T.Gien (2000) [29]

[h] experimental values, J. F. Williams (1975) [12]

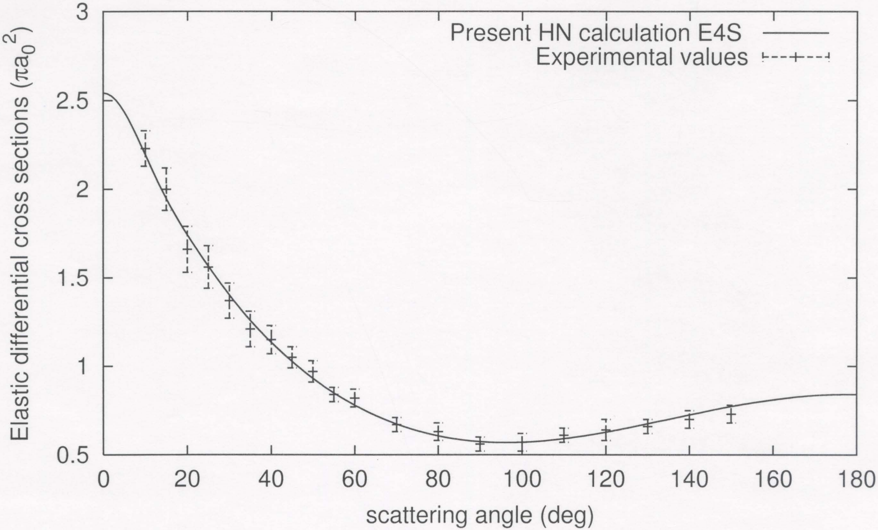

Figure 3.16: Differential cross sections for e^--H elastic scattering at 6.691 eV

Table 3.24: Differential cross sections (in units of πa_0^2 sr^{-1}) for the elastic scattering of electrons from atomic hydrogen at 8.704 eV. The numbers in parentheses are the maximum possible errors in the last significant digits and include both systematic and random errors.

Angle (deg)	[a]HN 3S	[b]HN 4S	[c]HN 6S	[d]HN E3S	[e]HN E4S	[f]HN E6S	[g]HN 13S	[h]Williams
10	1.762	2.225	2.022	2.314	2.317	2.312	2.283	2.24(14)
15	1.589	1.938	1.784	2.019	2.015	2.014	2.009	2.12(14)
20	1.440	1.707	1.588	1.774	1.771	1.771	1.771	1.83(12)
25	1.308	1.512	1.419	1.567	1.566	1.565	1.560	1.60(12)
30	1.181	1.335	1.264	1.379	1.379	1.379	1.378	1.33(10)
35	1.065	1.180	1.125	1.215	1.215	1.215	1.217	1.24(10)
40	0.962	1.049	1.006	1.076	1.077	1.077	1.078	1.11(10)
45	0.869	0.935	0.901	0.956	0.958	0.958	0.958	1.00(9)
50	0.784	0.834	0.807	0.852	0.853	0.853	0.852	0.92(6)
55	0.708	0.747	0.725	0.762	0.762	0.763	0.763	0.82(5)
60	0.643	0.674	0.656	0.686	0.686	0.686	0.686	0.73(4)
70	0.538	0.557	0.546	0.566	0.566	0.566	0.566	0.57(8)
80	0.465	0.477	0.470	0.484	0.484	0.484	0.484	0.47(8)
90	0.422	0.428	0.425	0.434	0.434	0.434	0.434	0.45(8)
100	0.404	0.406	0.405	0.411	0.411	0.411	0.411	0.41(9)
110	0.407	0.405	0.406	0.411	0.411	0.411	0.410	0.42(6)
120	0.425	0.422	0.423	0.427	0.426	0.426	0.426	0.45(7)
130	0.454	0.450	0.452	0.454	0.453	0.453	0.453	0.47(7)
140	0.487	0.483	0.485	0.486	0.485	0.485	0.486	0.48(3)
150	0.520	0.518	0.518	0.519	0.518	0.519	0.518	0.49(8)

[a, b, c] present Harris-Nesbet calculation with 3S, 4S and 6S schemes respectively

[d, e, f] present Harris-Nesbet calculation with E3S, E4S and E6S schemes respectively

[g] Harris-Nesbet calculation, T.T.Gien (2000) [29]

[h] experimental values, J. F. Williams (1975) [12]

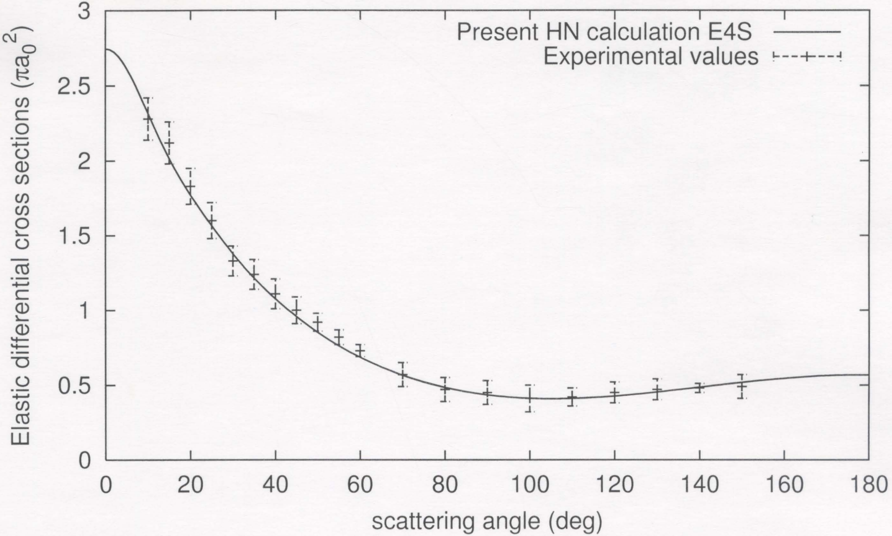

Figure 3.17: Differential cross sections for e^--H elastic scattering at 8.704 eV

Table 3.25: Total elastic cross sections for the scattering of electrons from atomic hydrogen in units of πa_o^2

Energy (eV)	[a]HN 3S	[b]HN 4S	[c]HN 6S	[d]HN E3S	[e]HN E4S	[f]HN E6S	[g]HN 13S
0.582	33.380	32.490	32.762	31.931	31.937	31.922	31.945
1.207	24.157	24.309	24.284	24.225	24.226	24.224	24.226
1.597	21.038	21.425	21.306	21.451	21.452	21.454	21.450
2.171	17.992	18.549	18.343	18.661	18.661	18.664	18.657
3.009	15.152	15.805	15.532	15.972	15.971	15.975	15.966
3.423	14.120	14.788	14.500	14.968	14.968	14.971	14.962
4.889	11.448	12.089	11.792	12.279	12.279	12.281	12.271
6.619	9.256	9.805	9.534	9.983	9.983	9.985	9.977
8.704	7.613	8.057	7.841	8.214	8.215	8.216	8.207

[a, b, c] present Harris-Nesbet calculation with 3S, 4S and 6S schemes respectively
[d, e, f] present Harris-Nesbet calculation with E3S, E4S and E6S schemes respectively
[g] Harris-Nesbet calculation, T.T.Gien (2000) [29]

Chapter4

Conclusions

In this thesis, we have carried out a very accurate calculation of the phase shifts for electron collisions with hydrogen atoms at low energy below the first hydrogenic excitation threshold, employing the Harris-Nesbet variational method. The phase shifts that we obtained for the partial waves *L*=0, 1, 2, 3, 4, 5, 6 and 7 with the use of the extended four-state (E4S) scheme appear to have reached their convergent values in both singlet and triplet scattering and should, thereby, be very accurate. The accuracy of these phase shifts has been double-checked by carrying out calculations with the use of different extended coupling schemes (the E6S and E3S ones), and the three sets of phase shifts calculated were found to agree excellently with each other. They also agreed excellently with the ones obtained by Gien (1998) [26], who employed the same Harris-Nesbet method for his calculation but with the 13-state scheme. The phase shifts of the present calculations for lower partial waves (S, P and D) also agree excellently with the ones that had been obtained by other research groups using different numerical methods. Accurate phase shifts at the nine energies, where experimental data of differential cross sections had been available in the literature, have been obtained for the partial waves *L* equal to up to 18, and then used to deduce the elastic differential and total cross sections for electron collisions with hydrogen atoms at these energies. The elastic differential and total cross sections that we obtained with the use of the E4S, E6S and E3S scheme have been found to agree excellently with each other as well as with those obtained earlier by Gien (2000) [29] with a 13-state scheme. An excellent agreement between our elastic differential cross sections and experimental data measured by Williams (1975) [12] has also been found.

We have also obtained the sets of phase shifts, elastic differential and total cross sections with the use of the coupling schemes 4S, 6S and 3S. A comparison of these results with those calculated with the use of the E4S, E6S and E3S schemes show a clear improvement of the latter as far as their accuracy is concerned. This reconfirms a significant effect of the correlation terms on the phase shifts and cross sections calculated, when these correlation terms are added to the coupling schemes.

In view of the reliability and accuracy of the Harris-Nesbet method that one has experienced with in the various calculations of electron and positron collisions with atomic targets (Gien and Gien et al. [13-33]), we believe that the phase shifts of our present Harris-Nesbet calculations are very accurate and may, thereby, serve to double-check the accuracy of the results obtained by other research groups who used different numerical methods for their calculations. With the success gained in this work, we hope to be able to determine again, with our present Harris-Nesbet calculations, the precise positions and widths of the sequences of S, P and D Feshbach resonances below the $n=2$ H excitation threshold in electron-hydrogen-atom scattering for comparison with those obtained by Gien (1998) [26] with the 13-state scheme.

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