The Application of the Pseudostate-Close-Coupling Method Using a Non-Orthogonal Laguerre-$L^2$ Basis for Electron-Helium Scattering

Agus Kartono$^1$ and Mustafa Mamat$^2$

$^1$Laboratory for Theoretical and Computational Physics, Department of Physics, Faculty of Mathematical and Natural Sciences, Bogor Agricultural University, Kampus IPB Darmaga, Bogor 16680, Indonesia.

$^2$Department of Mathematics, Faculty of Sciences and Technology, Universiti Malaysia Terengganu, 21030 K. Terengganu, Malaysia.

Abstract. Differential and total cross sections for elastic and excitation from the ground state to $n \leq 2$ states of atomic helium by electrons are computed for incident energies in the range from 5 to 50 eV. The states excitation cross sections are calculated with the use of close-coupling expansion with a non-orthogonal Laguerre-$L^2$ basis function. Our method is a frozen-core model of the target in which one of the electrons is restricted to the $1s$ He$^+$ orbital, as has been used with great success recently. Generally good agreement with experiments and the other calculations is obtained with the available differential and total cross sections. On occasion, there is not good agreement with experiments, particularly at the forward and backward angles for projectile energy in the range 30 to 50 eV.

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1. Introduction

Helium is an ideal choice because of the central role that it has been used as the simple many electron atom in many different theoretical and experimental studies.
and the fact that it is widely used to normalize and calibrate results obtained from
more complex targets.

The energy range of interest in atomic physics has been divided into the low
(below ionization threshold), intermediate (between one and ten times the
ionization threshold) and high (more than ten times the ionization threshold)
regions. The ionization threshold of the helium atom is 24.58 eV.

At low and intermediate energies, the essential physics that must be
contained in any accurate calculation of electron excitation collision cross sections
is an adequate configuration interaction description of the target and a scattering
approximation that includes distortion of the target by the incident electron,
exchange symmetry between the scattered and orbital electrons, coupling to other
nearby states of the incident and final states, and correlation effects due to the
temporary formation of a compound state of the electron-plus-target system [1].

At low energies, the collision has many of the features of a bound state
problem. The wave functions describing the collision can be accurately
represented in terms of a sum of configurations in a similar way to the
configuration interaction expansion used for bound state calculations of atoms and
ions. This so-called close-coupling (CC) expansion was introduced by Massey
and Mohr in the 1930s [2] and developed by Seaton [3] and many others since.
The essential elements of the method, adapted to multi-channels scattering are still
in use today. Due to computational constraints approximations concentrated on
low and high incident energies, elastic scattering and excitation of just the lowest
few excited states. Since that time progress has been steady, with the major
handicap being the available computational resources. The 1990s saw a rapid
increase in the amount of computational power available in readily affordable
workstations and supercomputing facilities [4].

In terms of testing the basic assumptions of the pseudostate method and
understanding its theoretical justification the work of several groups deserves
mention. Early numerical calculations for the electron-atom problem utilizing
pseudostates were carried out by many literatures (Callaway [5], Bray and
Stelbovics [6], Fursa and Bray [7] and references therein). They demonstrated that
the inclusion of a few pseudostates significantly reduced the cross sections for
scattering, bringing them into better agreement overall with experiment. It was
soon realized that with pseudostates one often has the problem that spurious
resonance features are introduced into the model cross sections. The observation
that the effect of pseudoresonances decreased with increasing numbers of
pseudostates was a significant factor in the development of the CC method. Many
studies of the convergence properties of pseudostate sets have been undertaken
(see, e.g., Burke and Mitchell [8], Callaway [5], Bray and Stelbovics [6], Fursa
and Bray [7] and references therein). They considered the model of electron-
hydrogen and electron-helium scattering that treats states of zero and non-zero
orbital angular momentum.

The use of basis sets to solve the Schrödinger equation for electron
scattering from atomic has long history in atomic physics. Many types of basis set
have been tried in the past but we focus in the use of the non-orthogonal
Laguerre-L² basis function which is a relatively new development in two-electron
atom. The non-orthogonal Laguerre-$L^2$ basis function has the property of ‘complete’ with a relatively small number of basis set. It is therefore our further goal to apply these methods to the electron-helium atom scattering to complex atoms calculations. The primary purpose of this paper is to demonstrate the pseudostate-close-coupling (PSCC) method using a non-orthogonal Laguerre-$L^2$ basis function to the calculation of electron-helium scattering at low-to-intermediate-energy electron. We use here a detailed description of the helium target which was presented by Winata and Kartono [9]. The frozen-core approximation is used to calculate the helium states. This type of approximate description of the target should be good for scattering problems in which the dominant reaction mechanism is by one-particle excitations.

The PSCC method utilizes an expansion of the target in a complete set of non-orthogonal Laguerre-$L^2$ basis function which forms a basis for the underlying Hilbert space. The PSCC method is those calculations for which, in addition to the treatment of true discrete eigenstates, there are also a number of square-integrable states with positive energies. These so-called pseudostates are usually obtained by diagonalizing the Hamiltonian in a non-orthogonal Laguerre-$L^2$ basis function. We present here a detailed formalism of the PSCC method and apply it to the computation of the electron-helium scattering previously by Stelbovics and Berge [10], Bray and Stelbovics [6], and Fursa and Bray [7].

This paper is structured in the following way. In section 2 we give the elements of the formalism. Calculations based on the theory model are given in section 3. Differential and total cross sections for excitation of the ground state to $n \leq 2$ states are presented over an energy range of 5 to 50 eV. In section 4 we draw conclusions and future work for our research.

2. Pseudostate-close-coupling formalism

The time independent Schrödinger equation for electron scattering from atomic helium is

$$\langle E - H \rangle \Psi(x_0, x_1, x_2) = 0,$$

where the Hamiltonian

$$H = H_T + H_0 + V_{01} + V_{02},$$

and the subscript 0 is used to denote the projectile electron, with the subscripts 1 and 2 indices being used for the target electrons. The Hamiltonian target operator is $H_T$. The electron-electron potentials are $V_{01}$ and $V_{02}$. To solve this equation, we write $|\Psi\rangle$ as explicitly anti-symmetrized wave functions utilizing the multi-channel expansion

$$|\Psi(x_0, x_1, x_2)\rangle = (1 - P_{01} - P_{02}) \sum_n |\Phi_n(x_1, x_2) f_n(x_0)\rangle,$$

where $P_{01}$ and $P_{02}$ are the space (coordinate and spin) exchange operator. To derive the CC equations we obtain the (complete) set of target states by solving

$$H_T |\Phi_n\rangle = \varepsilon_n |\Phi_n\rangle,$$
where the completeness relation for the states is expressed as

\[ I = \sum_n \int |\Phi_n(x_1, x_2)\rangle \langle \Phi_n(x_1, x_2)|, \]

(5)

with the subscripts indicating the electron space. The index \( n \) is discrete for negative energies and continuous for positive energies.

The CC equations one gets upon inserting the eigenfunctions expansion are

\[ \sum_n \int (K_0 \delta_{mn} + V_{mn}) f_n = (E - \varepsilon_m) f_m, \]

(6)

where

\[ V_{mn} = \langle \Phi_m|V|\Phi_n\rangle, \quad V = V_0 + V_{01} + V_{02} + (E - H)(P_{01} + P_{02}). \]

(7)

The CC equations may be written more compactly as

\[ (G_0^{-1}(E) - V(E)) f = 0, \]

(8)

where \( G_0 \) is the operator with matrix elements

\[ (G_0(E))_{mn} = \delta_{mn}(E - \varepsilon_m - K_0)^{-1}, \]

(9)

and \( f' \) is the column vector whose components are the \( f_n \).

An alternative approach is to solve the coupled equations for the \( f_n \) in differential form is to use the integral form one derives by using the Green’s functions to obtain a Lippmann-Schwinger (LS) equation. The LS equation for the system is

\[ |f_n\rangle = |n\tilde{k}_n\rangle + G_0(E^{(+)})|V|f_n\rangle, \]

(10)

and \( |n\tilde{k}_n\rangle_m = \delta_{mn}\Phi_n|\tilde{k}_n\rangle \) is the incident-channel asymptotic state functions. We adopt the Green’s function \( G_0(E^{(+)}) \) which ensures outgoing spherical-wave boundary conditions. In practice, it is more useful to use a LS equation for the \( T \)-matrix operator which we formally define by

\[ |f_n\rangle = \left[ 1 + G_0(E^{(+)})T(E^{(+)}) \right] \langle n\tilde{k}_n\rangle. \]

(11)

It is easy to check that the LS equation for \( T \)-matrix becomes

\[ T(E^{(+)}) = V(E) + V(E)G_0(E^{(+)})T(E^{(+)}). \]

(12)

The momentum-space matrix elements of the \( T \)-operator are

\[ \langle m\tilde{p}_m|T(E^{(+)})|n\tilde{p}_n\rangle = \langle \tilde{p}_m|T_{mn}(E^{(+)})|\tilde{p}_n\rangle. \]

(13)

In order to solve the integral equation the momentum \( \tilde{p}_m, \tilde{p}_n \) are allowed to take on all possible values. The scattering amplitudes are derived from the on-shell amplitudes for which \( \tilde{p}_n = \tilde{k}_n \) and \( \varepsilon_n + \frac{1}{2}k_n^2 = \varepsilon_m + \frac{1}{2}k_m^2 = E \).

Though we have shown that one can compute reliable amplitudes for smallish target sets using the integral equation for the \( T \)-matrix it is annoying that the half-shell amplitudes diverge. This problem was illustrated for the helium target by Stelbovics and Berge [10]. For larger target sets \( (N > 15) \) numerical instabilities begin to appear even for the on-shell amplitudes as the reciprocal.
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Condition numbers keep decreasing with the increasing number of homogeneous solutions. It is therefore important in large-scale models to realize that one can formulate a set of integral equations which have no solutions to the homogeneous equation for scattering energies. The criterion to apply is the relation
\[
\langle \Phi_m | f_n \rangle = (-1)^S \langle \Phi_n | f_m \rangle, \quad n, m = 1, \ldots, N. \tag{14}
\]
This identity is a result of applying the symmetry property of the wave functions to its CC expansion. This relation is generally valid for finite target expansions, including those containing pseudostates. Its crucial importance in the scattering theory is that terms of the type \( \langle \Phi_m | f_n \rangle \) occur in the exchange part of the potential \( V \) defined in equation (7). Therefore we are at liberty to modify the CC equations with considerable generality. The result of applying the new symmetry condition liberally is to modify the form of the exchange potential to the extent that there are no homogeneous solutions in the new forms LS equations [10].

We do not wish to repeat here most of the technical detail given earlier [9]. In this section we summaries our method. Firstly, we must decide on the method of calculating structure of the helium target ground and excited states. We have written a general configuration interaction program which diagonalizes the helium Hamiltonian in the anti-symmetrized two-electron basis, where the radial part of the single-particle functions \( \phi_{nl} \) are taken to be the non-orthogonal Laguerre-L\(^2\) basis
\[
\phi_{nl}(r) = (\lambda_i r)^{l+1} \exp(-\lambda_i r/2) L_n^{2l+1}(\lambda_i r), \tag{15}
\]
and where the \( L_n^{2l+1}(\lambda_i r) \) are the associated Laguerre polynomials, \( \lambda_i \) is the interaction parameter and \( n \) ranges from 1 to the basis size \( N \).

The target Hamiltonian \( H_T \) is
\[
H_T = H_1 + H_2 + V_{12}, \tag{16}
\]
where
\[
H_i = K_i + V_i = -\frac{1}{2} \nabla_i^2 - \frac{Z}{r_i}, \tag{17}
\]
for \( i = 1, 2 \), is the one-electron Hamiltonian of the He\(^+\) ion \((Z = 2)\), and
\[
V_{12} = \frac{1}{r_{12}}, \tag{18}
\]
is the electron-electron potential. Atomic units (a.u.) are assumed throughout.

Whereas the above Hamiltonian formalism is general and includes two-electron excitation, in practice we have found that it is sufficient to make the frozen-core approximation, where one of the electrons is in a fixed orbital while the second electron is described by a set of independent \( L^2 \) functions, thus permitting it to span the discrete and continuum excitations, in which all configurations have one of the electrons occupying the lowest orbital. The resulting target states \( \Phi(x_1, x_2) \), where \( x \) is used to denote both the spatial and spin coordinates, satisfy
\[
\langle \Phi_m | -\frac{1}{2} \nabla_1^2 - \frac{Z}{r_1} - E_n_{\alpha} | \Phi_n \rangle = 0, \tag{19}
\]
in order to get a good description of the He$^+$ ion state, where $\varepsilon_{n\alpha}$ is the energy associated with the 1$s$ state of He$^+$ ion. The excitation states for $\Phi(x_1, x_2)$ can be obtained by solving the equation

$$\langle \Phi_m | -\frac{1}{2} \nabla^2 + \frac{Z}{r_2} + \frac{1}{\eta_2} - \varepsilon_{n\beta} \rangle \Phi_n \rangle = 0,$$

where $\varepsilon_{n\beta}$ is the energy associated with the excitation states of the helium atom.

After diagonalization of the ground and excitation states Hamiltonian, equations (19) and (20) can be written as the resulting three-term recurrence relations are special case of the Pollaczek polynomials which are set of orthogonal polynomials having a non-empty continuous spectrum in addition to an infinite discrete spectrum. The three-term recurrence relations of the Pollaczek polynomials have complied with the positivity condition. These results, known as Favard’s theorem, can be found in Kartono et al [11]. The behavior of the non-orthogonal Laguerre-$L^2$ basis function in equation (15) is oscillations and dependent upon the number of basis size $N$ and interaction parameter $\lambda_l$. It is therefore the convergence of the resulting eigenvalues in equations (19) and (20) are dependent upon a number of the basis size $N$ and interaction parameter $\lambda_l$. In order to get a good description of the ground and excitation states, we determine the interaction parameter $\lambda_l$ from the positivity condition.

In our work we simplify the problem by using the frozen-core model, in which all configurations have one of the electrons occupying the lowest orbital. In order to get a good description of the ground states we take $\lambda_0 = 4$ for $n = 1$. This choice generates the He$^+$ 1$s$ orbital, which allows us to take into account short-range correlations in the ground state, as well as being suitable for obtaining an accurate representation of excited discrete and continuum states. To obtain good $nS$ excited states we take $\lambda_0 = 0.93$ (triplet and singlet) for $n > 1$. For $nP$ excited states we take $\lambda_1 = 0.72$ (triplet) and $\lambda_1 = 0.73$ (singlet), and for $nD$ excited states we take $\lambda_2 = 0.62$ (triplet) and $\lambda_2 = 0.63$ (singlet).

The configuration interaction coefficients $C_{Ni}^{(\alpha\beta)}$ are given by

$$\left(C_{Ni}^{(\alpha\beta)}\right)^2 = \frac{2^{2l}}{\pi} \frac{\lambda_l}{\left(1 - X^{(\alpha\beta)}_{Ni}\right)} W_{Ni}^{(\alpha\beta)},$$

where the notations $\alpha$ and $\beta$ are used to denote the first and second electron and $W_{Ni}$ are the associated quadrature weights of Gaussian quadrature based Pollaczek polynomials which are given by

$$W_{Ni}^{(\alpha\beta)} = \frac{\pi^{N+2l+1}}{2^{2l} \Gamma(N+1) p_{N}^{l+1}(x^{(\alpha\beta)}_{Ni})} \left(\frac{1}{d^l dx^l p_{N}^{l}(x^{(\alpha\beta)}_{Ni})}\right).$$
This rearrangement is such that the asymptotic (large $r_0$) Hamiltonian is $K_0 + H_T$, and this will be used to generate the Green’s functions and boundary conditions for the total wave functions
\[
\lim_{r_0 \to \infty} \Psi(x_0,x_1,x_2) = \chi(\sigma) \exp(i \vec{k}_i \cdot \vec{r}_0) \Phi_i(x_1,x_2),
\]
where $\vec{k}_i$ is the incident projectile momentum and $\Phi_i$ is the initial target state.

We define the coupled LS equation for the $T$-matrix is
\[
\sum \int \int - \Phi \Phi = \Phi + \sum \int d^3 k \left( \vec{k} \Phi \right) \left( \vec{k} \Phi \right) + \sum \int d^3 k \left( \vec{k} \Phi \right) \left( \vec{k} \Phi \right)
\]
\[
E^{(s)} - \varepsilon_n - \vec{k}^2 = 0.
\]

where the projectile waves (discrete or continuous) $|\vec{k}(\pm)|$ satisfy
\[
\left( \varepsilon_k \pm K_0 \right) |\vec{k}(\pm)| = 0.
\]
The on-shell momenta $\varepsilon_k = k_n^2/2$ are obtained from
\[
E - \varepsilon_n - k_n^2/2 = 0,
\]
and exist only for open channels $n$ such that $E = \varepsilon_i - k_i^2/2 > \varepsilon_n$.

In practice no numerical method for solving the coupled $T$-matrix equations in the form (24) has yet been implemented. The difficulty is that in order to solve this integral equation it must be closed by allowing the index $i$ and $f$ to run over the same complete range as $n$, which leads to singular $V$-matrix elements whenever $i, f$ and $n$ are in the continuum.

The approach that is taken in this work is to diagonalize the helium target Hamiltonian in a set of non-orthogonal Laguerre-L^2 basis function which when extended to completeness form a basis for the target Hilbert space. The use of non-orthogonal Laguerre-L^2 basis function eliminates the problem of singular continuum-continuum $V$-matrix elements. Also most importantly, with a known basis the convergence of the expansions can be studied in a systematic manner with increasing number of basis functions.

We introduce a finite set of $N$ square-integrable states $|\Phi_n^N\rangle$ which satisfy
\[
\left\langle \Phi_m^N \right| H_T \left| \Phi_n^N \right\rangle = \varepsilon_n^N \delta_{mn},
\]
and have the property
\[
\sum \Phi_n(x_1,x_2) f_n(x_0) = \lim_{N \to \infty} \sum_{n=1}^N \Phi_n(x_1,x_2) f_n(x_0).
\]
With these definitions, the sum and integral in (5) and the LS equation (24) become a single sum over $N$, with the target states and energies being replaced by $|\Phi_n^N\rangle$ and $\varepsilon_n^N$, respectively. So instead of $I$, we define
\[ I = \sum_{n=1}^{N} \Phi_N^N(x_1, x_2) \Phi_N^N(x_1, x_2) \text{,} \tag{29} \]

and have

\[ \langle \tilde{k} \Phi_f^N \mid T \mid \Phi_i^N \tilde{k}^N(+)^N \rangle = \langle \tilde{k} \phi_f^N \mid V \mid \Phi_i^N \tilde{k}^N(+) \rangle + \sum_{n=1}^{N} \int d^3k E^{(+)} - \epsilon_n^N - k^2 \]

\[ \text{..........................(30)} \]

where for the physical \( T \)-matrix elements of interest we must have \( \Phi_f = \Phi_f^N \) and \( \Phi_i = \Phi_i^N \) to sufficiently high precision. With these definitions we have

\[ \langle \tilde{k} \Phi_f^N \mid T \tilde{k}^N(+)^N \rangle = \lim_{N \to \infty} \langle \tilde{k} \Phi_f^N \mid T \tilde{k}^N(+)^N \rangle \text{,} \tag{31} \]

for the physical \( T \)-matrix elements. The projection operator \( I \) is replaced by \( I^N \) in calculating the matrix elements of \( V \)-matrix.

It is a Gaussian-type quadrature and the underlying orthogonal polynomials are of the Pollaczek class. It can be shown that weights of the negative energy \( L^2 \) states converge to unity in equation (28) in the limit of large \( N \). This ensures that the limiting procedure (31) gives the correct \( T \)-matrix amplitudes (24) for the transitions to \( 1S, 2S \) and \( 2P \) levels.

The partial wave LS equation corresponding to (30) for the reduced \( T \)-matrix elements are

\[ \langle L_f k_f^N(-), \phi_f \mid L_s I^N_s \mid L_i k_i^N(+), \phi_i \rangle = \langle L_f k_f^N(-), \phi_f \mid V^{JN}_{I^N_s} \mid L_i k_i^N(+), \phi_i \rangle + \sum_{n=1}^{N} \sum_{L_k, \lambda} \int d^3k \left( \frac{L^N_{i^N_s} k_i^N(-), \phi_i \mid \tilde{L}^N k_f^N(-), \phi_f \mid T^{JN}_{I^N_s} \mid L_i k_i^N(+), \phi_i \rangle}{E^{(+)} - \epsilon_n^N - \epsilon_k} \right) \text{.} \tag{32} \]

The method of solution of this equation is identical to the CCC method for hydrogen target [9].

3. Numerical Results

In order to solve the fundamental system (32) one must approximate the integration over the electron momentum by a numerical integration and close the system by fixing all the momentum variables to be restricted to the quadrature. Continuation to other momentum may be effected by using an interpolation of the grid-point solution through the integral equation (32). The quadrature rule must be such that for an arbitrary function \( F(x) \), we may replace
where the weights \( W_j^N \) contain Gaussian-type weights as well as the Green's function. There are a number of suitable ways to choose the weights \( W_j^N \) and the corresponding knots \( k_j^N \). There are a number of difficulties that need to be addressed. The quadrature rule must be able to handle the singularity, which varies in position with channel. We do this taking an even number of Gaussian points in an interval which is symmetric about the singularity. This requires us to allow the \( W_j^N \) and \( k_j^N \) be different in each channel, as implied by the superscript \( n \). In practice we take \( N \) to be the same for each channel \( n \). To determine approximately how many quadrature points are necessary we check that the identity

\[
\int_0^\infty dk \frac{k^2 F(x)}{E - \varepsilon_n^N - \frac{1}{2}k^2} \approx \sum_{j=1}^N W_j^N F(k_j^N),
\]  

is satisfied for each \( n = 1 \) to the non-orthogonal Laguerre-L^2 basis size \( N \).

The target states cannot all be included in any practical implementation of the CC equations. A pragmatic way to approach a calculation is to include the effects of the target states which are liable to be most important, for example in the helium target to choose just the \( nS \) and \(nP \) \( (n = 1, 2) \) levels. Unfortunately it has been observed that such expansions are inadequate at all but the lowest energies; there is considerable evidence that the coupling to all open channels must be included in some way. Above ionization threshold this means that allowance for coupling to continuum channels must be made. It is therefore our tests of this approximation for low energy elastic scattering require few expansion states. We achieve convergence using a maximum of 80 channels and couples a total of 25 states consisting of 7 \( 1S \), 6 \( 3S \), 6 \( 1P \) and 6 \( 3P \), denoted by PSCC (25). To simplify convergence studies, in the most difficult intermediate energy region, we present at most two calculations, the PSCC (25) and PSCC (37). For intermediate, require many more states. Here we include a maximum of 120 channels and couples a total of 37 states consisting of 7 \( 1S \), 6 \( 3S \), 6 \( 1P \), 6 \( 3P \), 3 \( 1D \), 3 \( 3D \), 3 \( 1F \), and 3 \( 3F \), denoted by PSCC (37). For large bases used calculations are close to the limit of our desk-top workstation computational resources.

In this work it is our aim to demonstrate that the PSCC method is able to provide a relatively accurate description of electron-helium scattering at projectile energies ranging from low to intermediate. As discussed, we introduce the approximation of treating the helium target by the frozen-core model, where we restrict one of the electrons to be the \( 1s \) He \(^+\) orbital. The frozen-core model approximation reduces convergence studies to treating only one-electron excitation.
Figure 1. Elastic differential cross sections for electron-helium scattering at a projectile energy of 5 eV. The present calculation is denoted by PSCC, and is obtained using 25 states in the CC formalism. The calculations denoted by CCC are due to Fursa and Bray [7]. The measurements are due to Brunger et al [12] and Register et al [13].

Figure 2. Elastic differential cross sections for electron-helium scattering at a projectile energy of 12 eV. The present calculation is denoted by PSCC, and is obtained using 25 states in the CC formalism. The calculations denoted by variational method are due to Nesbet [14]. The measurements are due to Register et al [13].
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Figure 3. Elastic differential cross sections for electron-helium scattering at a projectile energy of 18 eV. The present calculation is denoted by PSCC, and is obtained using 25 states in the CC formalism. The calculations denoted by CCC are due to Fursa and Bray [7]. The measurements are due to Brunger et al [12] and Register et al [13].

Figure 4. Elastic differential cross sections for electron-helium scattering at a projectile energy of 20 eV. The present calculation is denoted by PSCC, and is obtained using 25 states in the CC formalism. The calculations denoted by CCC are due to Fursa and Bray [7]. The measurements are due to Brunger et al [12] and Register et al [13].
Figure 5. Elastic differential cross sections for electron-helium scattering at a projectile energy of 30 eV. The present calculation is denoted by PSCC, and is obtained using 25 and 37 states in the CC formalism. The calculations denoted by CCC are due to Fursa and Bray [7]. The measurements are due to Brunger et al [12] and Register et al [13].

Figure 6. Elastic differential cross sections for electron-helium scattering at a projectile energy of 40 eV. The present calculation is denoted by PSCC, and is obtained using 25 and 37 states in the CC formalism. The calculations denoted by CCC are due to Fursa and Bray [7]. The measurements are due to Brunger et al [12] and Register et al [13].
Figure 7. Elastic differential cross sections for electron-helium scattering at a projectile energy of 50 eV. The present calculation is denoted by PSCC, and is obtained using 25 and 37 states in the CC formalism. The calculations denoted by CCC are due to Fursa and Bray [7]. The measurements are due to Brunger et al [12] and Register et al [13].

Elastic electron-helium scattering is well understood experimentally and theoretically and has been used extensively for calibration purposes in various electron-scattering applications. Therefore, we begin the presentation of differential cross sections by starting with low to intermediate energy elastic cross sections. The reported data set of elastic differential and total cross sections given by Register et al [12] at an impact energy range of 5 to 200 eV are good agreement with the more recent study by Brunger et al [13] (1.5 to 50 eV). Therefore, the results of the experiments of Register et al [12] (± 5 to 7% error bars) and Brunger et al [13] (± 3.5 to 5% error bars) are presented for comparison in this work. For theory, the calculation results of Fursa and Bray [7] and Nesbet [14] are presented for comparison in this work. The CCC cross sections being chosen because of established accuracy of this technique over a wide range of states and energies. In the Figures 1 to 7, we present the elastic differential cross sections the $1^1S$ state calculated by the PSCC method for electron-helium scattering on the ground state at a range of projectile energies of 5 to 50 eV. These are compared with some of the available experiments and theories. From the figures, we see that there is essentially complete qualitative agreement between the PSCC calculations and experiments. The difference between the PSCC (37) and CCC calculations (5 to 15% error estimates) are predominantly due to the inclusion of the different basis size in the CC formalism. While the error estimates between PSCC (25) and PSCC (37) are 5 to 10%. The convergence of present calculations is not good agreement with experiments of Brunger et al [13] at an impact energy range of 30 to 50 eV, particularly at the forward angles.
Figure 8. The $2^1S$ differential cross sections for electron-helium scattering at a projectile energy of 30 eV. The present calculation is denoted by PSCC, and is obtained using 25 and 37 states in the CC formalism. The measurements are due to Trajmar et al [15]. The calculations denoted by CCC are due to Fursa and Bray [7].

Figure 9. The $2^3S$ differential cross sections for electron-helium scattering at a projectile energy of 30 eV. The present calculation is denoted by PSCC, and is obtained using 25 and 37 states in the CC formalism. The measurements are due to Trajmar et al [15]. The calculations denoted by CCC are due to Fursa and Bray [7].
Figure 10. The $2^1S$ differential cross sections for electron-helium scattering at a projectile energy of 40 eV. The present calculation is denoted by PSCC, and is obtained using 25 and 37 states in the CC formalism. The measurements are due to Trajmar et al [15]. The calculations denoted by CCC are due to Fursa and Bray [7].

Figure 11. The $2^3S$ differential cross sections for electron-helium scattering at a projectile energy of 40 eV. The present calculation is denoted by PSCC, and is obtained using 25 and 37 states in the CC formalism. The measurements are due to Trajmar et al [15]. The calculations denoted by CCC are due to Fursa and Bray [7].
Figure 12. The $2^1S$ differential cross sections for electron-helium scattering at a projectile energy of 50 eV. The present calculation is denoted by PSCC, and is obtained using 25 and 37 states in the CC formalism. The measurements are due to Trajmar et al. [15]. The calculations denoted by CCC are due to Fursa and Bray [7].

Figure 13. The $2^3S$ differential cross sections for electron-helium scattering at a projectile energy of 50 eV. The present calculation is denoted by PSCC, and is obtained using 25 and 37 states in the CC formalism. The measurements are due to Trajmar et al. [15]. The calculations denoted by CCC are due to Fursa and Bray [7].
Figure 14. The $2^1P$ differential cross sections for electron-helium scattering at a projectile energy of 40 eV. The present calculation is denoted by PSCC, and is obtained using 25 and 37 states in the CC formalism. The measurements are due to Truhlar et al [16]. The calculations denoted by CCC are due to Fursa and Bray [7].

Figure 15. The $2^3P$ differential cross sections for electron-helium scattering at a projectile energy of 40 eV. The present calculation is denoted by PSCC, and is obtained using 25 and 37 states in the CC formalism. The measurements are due to Trajmar et al [15]. The calculations denoted by CCC are due to Fursa and Bray [7].
We next look at the $2^1S$ and $2^3S$ differential cross sections for 30 to 50 eV electron-impact excitation of helium. These are given in Figures 8 to 13. Once more convergence is very good and the PSCC (37) results are in good agreement with the experiments of Trajmar \textit{et al} [15] and Truhlar \textit{et al} [16] ($\pm$ 19 to 20% error bars), but the PSSC (25) results are not. We note one exception to this at the forward and backward angles for the $2^1S$ and $2^3S$ excitations, where the PSCC method is considerably below the measurements of Trajmar \textit{et al} [15] and Truhlar \textit{et al} [16]. To examine convergence studies in the PSCC method, we presented the differential cross sections for $2^1P$ and $2^3P$ at an impact energy range of 40 eV. These are given in Figures 14 and 15. Conclusions are much the same as for an impact energy range of 30 to 50 eV. In case of the $2^1S$ and $2^3S$ differential cross sections for 30 to 50 eV electron-impact excitation of helium, the discrepancy between the PSCC (37) and CCC calculations is 5 to 15% (error estimates). While the error estimates between PSCC (25) and PSCC (37) are 5 to 15%. The convergence of the differential cross sections is affected by the convergence of the target helium-atom spectrum for the $N$-dimensional subspace formed from the first $N$ non-orthogonal Laguerre-L$_2^2$ basis functions.

The total cross sections are given in Table 1. Upon examination of Table 1 we see generally good agreement with available measurements, though on occasion there are significant discrepancies. Most encouraging is the good agreement at all energies with the measurements of the total cross sections, where the error estimates are very small.

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4. Conclusions

We have demonstrated that the PSCC method using a non-orthogonal Laguerre-L$_2^2$ basis function for the calculations of electron-helium scattering is able to obtain
qualitative, and often quantitative, agreement with measurements of differential and total cross sections for projectile energies ranging from 5 to 50 eV.

We have established convergent differential and total cross sections for elastic and inelastic scattering to the \( nS \) and \( nP \) (\( n \leq 2 \)) levels over a range of projectile energies of 5 to 50 eV. As there is difference between the PSCC (37) and PSCC (25) calculations at the projectile energies of 30 to 50 eV for the differential cross sections, convergence is obtained by having \( 3^1D, 3^3D, 3^1F \) and \( 3^3F \) states in expansions. If we concentrate only on the elastic scattering at the projectile energies of 5 to 20 eV, then by dropping \( F \) and maybe most \( D \) states, we can probably provide more accurate elastic cross sections, still using our local computational facilities. There is not good agreement with experiments at an impact energy range of 30 to 50 eV, particularly at the forward and backward angles. As we found earlier for the target helium-atom states, once reasonable accuracy in the target wave functions is obtained, it becomes more important to treat accurately the scattering part of the calculation. It suggests that slightly large bases used calculations are necessary to get better accuracy.

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References


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