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A study of the pseudostate-close-coupling method using a non-orthogonal Laguerre-L^2 basis for electron-helium scattering

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Abstract. We present the pseudostate-close-coupling method using a non-orthogonal Laguerre-L^2 basis function for the calculations of electron-helium scattering. 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. We demonstrate its applicability at a range of projectile energies of 5 to 50 eV to scattering from the ground state to $n \leq 2$ states. 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.

PACS. 34.80.Bm Elastic scattering of electrons by atoms and molecules – 34.80.Dp Atomic excitation and ionization by electron impact

1 Introduction

Collision processes involving helium are important in plasmas, lasers, planetary atmospheres, interstellar space, and many other environments. The measurement of cross-sections for collisions with helium has been ongoing for over 40 years. 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].

For intermediate energies, in principle an infinite number of bound target states and also continuum states should be included in the expansion. One approach which has had some success is based on this expansion where some of the target states are replaced by suitably chosen pseudostates which are not eigenstates of the target Hamiltonian. Instead these pseudostates each represent an

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average in some sense over the complete set of target eigenstates. Another approach which uses expansions of the electron-plus-target system is the R-matrix method [5].

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 (see, e.g., Burke and Webb [6], Callaway [7], van Wyngaarden and Walters [8], Bray and Stelbovics [9], Fursa and Bray [10] 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 [11], Callaway [7], Bray and Stelbovics [9], Fursa and Bray [10] 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 CC method relies on the reformulation of the Schrödinger equation into an infinite set of coupled-channel equations by expanding over the complete set of target states. The key to the application of this method and the models it generates depends on the approximations we make to incorporate the "complete" set of target states. Since the complete set always includes an infinite number of discrete excited states as well as non-normalisable continuum states, approximations will always have to be made. The difficulty in applying this approach is that the continuum channels are known to be very important in the intermediate energy region and coupling to them must be included with little approximation. One of way approximate the continuum states is positive-energy pseudostates formed from the non-orthogonal Laguerre-L^2 basis function. Because there are an infinite number of discrete and continuum target states, methods must be devised in order to render the equations numerically soluble. One method which suggests itself is to replace the integration over continuum states of the CC equations by numerical quadrature. This may be achieved by using the non-orthogonal Laguerre-L^2 basis functions.

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-L^2 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 [12]. 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 computation of the electron-helium scattering previously by Stelbovics and Berge [13,14], Bray and Stelbovics [9], and Fursa and Bray [10].

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

$$(E-H)\left|\Psi\left(x_0,x_1,x_2\right)\right\rangle=0, \tag{1}$$

where the Hamiltonian

$$H=H_T+H_0+V_{01}+V_{02}, \tag{2}$$

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

$$\left|\Psi\left(x_0,x_1,x_2\right)\right\rangle= \left(1-P_{01}-P_{02}\right)\sum\int_n\left|\Phi_n\left(x_1,x_2\right)f_n\left(x_0\right)\right\rangle, \tag{3}$$

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

$$H_T\left|\Phi_n\right\rangle=\varepsilon_n\left|\Phi_n\right\rangle, \tag{4}$$

where the completeness relation for the states is expressed as

$$I = \sum \int_n |\Phi_n(x_1, x_2)\rangle \langle \Phi_n(x_1, x_2)|, \tag{5}$$

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

2.1 The close-coupling equations

The CC equations one gets upon inserting the eigenfunctions expansion are

$$\sum \int_n (K_0 \delta_{mn} + V_{mn}) f_n = (E - \varepsilon_m) f_m, \tag{6}$$

where

$$\begin{aligned} V_{mn} &= \langle \Phi_m | V | \Phi_n \rangle, \\ V &= V_0 + V_{01} + V_{02} + (E - H)(P_{01} + P_{02}). \end{aligned} \tag{7}$$

The CC equations may be written more compactly as

$$\left(G_0^{-1}(E) - V(E)\right) |f\rangle = 0, \tag{8}$$

where G_0 is the operator with matrix elements

$$(G_0(E))_{mn} = \delta_{mn} (E - \varepsilon_m - K_0)^{-1}, \tag{9}$$

and $|f\rangle$ is the column vector whose components are the f_n.

2.2 Lippmann-Schwinger forms

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

$$|f_n\rangle = |n\vec{k}_n\rangle + G_0(E^{(+)}) V |f_n\rangle, \tag{10}$$

and $|n\vec{k}_n\rangle_m \equiv \delta_{mn} \Phi_n |\vec{k}_n\rangle$ 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

$$|f_n\rangle = [1 + G_0(E^{(+)}) T(E^{(+)})] |n\vec{k}_n\rangle. \tag{11}$$

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

$$T(E^{(+)}) = V(E) + V(E) G_0(E^{(+)}) T(E^{(+)}). \tag{12}$$

The momentum-space matrix elements of the T-operator are

$$\langle m\vec{p}_m | T(E^{(+)}) | n\vec{p}_n \rangle = \langle \vec{p}_m | T_{mn}(E^{(+)}) | \vec{p}_n \rangle. \tag{13}$$

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

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 [13,14]. For larger target sets ($N > 15$) numerical instabilities begin to appear even for the on-shell amplitudes as the reciprocal condition numbers keep decreasing with the increasing number of homogeneous solutions. It is therefore important in large-scale models (such as Bray and Stelbovics [9]) 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

$$\langle \Phi_m \mid f_n \rangle = (-1)^S \langle \Phi_n \mid f_m \rangle, \quad n,\ m = 1, \ldots, N. \tag{14}$$

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 $\langle \Phi_m \mid f_n \rangle$ 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 [13,14].

2.3 Expansion of the helium target wave functions

We do not wish to repeat here most of the technical detail given earlier [12]. In this sub 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 ϕ_{nl} are taken to be the non-orthogonal Laguerre-L^2 basis

$$\phi_{nl}(r) = (\lambda_l r)^{l+1} \exp(-\lambda_l r/2) L_n^{2l+1}(\lambda_l r), \tag{15}$$

and where the $L_n^{2l+1}(\lambda_l r)$ are the associated Laguerre polynomials, λ_l 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

$$\langle \Phi_m | -\frac{1}{2}\nabla_1^2 - \frac{Z}{r_1} - \varepsilon_{n_\alpha} | \Phi_n \rangle = 0, \qquad (19)$$

in order to get a good description of the He^+ ion state, where ε_{n_α} is the energy associated with the $1s$ state of He^+ ion. The excitation states for $\Phi(x_1, x_2)$ can be obtained by solving the equation

$$\langle \Phi_m | -\frac{1}{2}\nabla_2^2 - \frac{Z}{r_2} + \frac{1}{r_{12}} - \varepsilon_{n_\beta} | \Phi_n \rangle = 0, \qquad (20)$$

where ε_{n_β} 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. [15]. 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 λ_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 λ_l. In order to get a good description of the ground and excitation states, we determine the interaction parameter λ_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^+ $1s$ 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 takes $\lambda_1 = 0.72$ (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

$$\left(C_{Ni}^{(\alpha\beta)}\right)^2 = \frac{2^{2l}}{\pi} \frac{\lambda_l}{\left(1 - X_{Ni}^{(\alpha\beta)}\right)} W_{Ni}^{(\alpha\beta)}, \qquad (21)$$

where the notations α and β 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

$$W_{Ni}^{(\alpha\beta)} = \frac{\pi \Gamma(N + 2l + 1)}{2^{2l}\Gamma(N + 1)} \frac{1}{P_{N-1}^{l+1}\left(X_{Ni}^{(\alpha\beta)}\right) \frac{d}{dx} P_N^l \left(X_{Ni}^{(\alpha\beta)}\right)}. \qquad (22)$$

2.4 Solving the coupled Lippmann-Schwinger equations

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

$$\lim_{r_0 \to \infty} \Psi(x_0, x_1, x_2) = \chi(\sigma) \exp\left(i\vec{k}_i \cdot \vec{r}_0\right) \Phi_i(x_1, x_2), \qquad (23)$$

where $\vec{k}_i$ is the incident projectile momentum and Φ_i is the initial target state. We define the coupled LS equation for the T-matrix is

$$\left\langle \vec{k}_f^{(-)} \Phi_f \middle| T \middle| \Phi_i \vec{k}_i^{(+)} \right\rangle = \left\langle \vec{k}_f^{(-)} \Phi_f \middle| V \middle| \Phi_i \vec{k}_i^{(+)} \right\rangle + \sum \int_n \int_k d^3k \frac{\left\langle \vec{k}_f^{(-)} \Phi_f \middle| V \middle| \Phi_n \vec{k} \right\rangle \left\langle \vec{k} \Phi_n \middle| T \middle| \Phi_i \vec{k}_i^{(+)} \right\rangle}{E^{(+)} - \varepsilon_n - \frac{1}{2}k^2}, \qquad (24)$$

where the projectile waves (discrete or continuous) $\left|\vec{k}^{(\pm)}\right\rangle$ satisfy

$$\left(\varepsilon_k^{(\pm)} - K_0\right) \left|\vec{k}^{(\pm)}\right\rangle = 0. \qquad (25)$$

The on-shell momenta $\varepsilon_k = k_n^2/2$ are obtained from

$$E - \varepsilon_n - k_n^2/2 = 0, \qquad (26)$$

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, in Section 2.3, a finite set of N square-integrable states $\left|\Phi_n^N\right\rangle$ which satisfy

$$\left\langle\Phi_m^N\right| H_T \left|\Phi_n^N\right\rangle = \varepsilon_{_n}^N \delta_{mn}, \tag{27}$$

and have the property

$$\sum\int_n \Phi_n\left(x_1,x_2\right) f_n\left(x_0\right) = \lim_{N\to\infty} \sum_{n=1}^{N} \Phi_n^N\left(x_1,x_2\right) f_n^N\left(x_0\right). \tag{28}$$

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 $\left|\Phi_n^N\right\rangle$ and ε_n^N, respectively. So instead of I, we define

$$I = \sum_{n=1}^{N} \left|\Phi_n^N\left(x_1,x_2\right)\right\rangle \left\langle\Phi_n^N\left(x_1,x_2\right)\right|, \tag{29}$$

and have

$$\left\langle \vec{k}_f^{(-)}\Phi_{_f}^N \right| T \left| \Phi_{_i}^N \vec{k}_i^{(+)} \right\rangle = \left\langle \vec{k}_f^{(-)}\Phi_{_f}^N \right| V \left| \Phi_{_i}^N \vec{k}_i^{(+)} \right\rangle + \sum_{n=1}^{N} \int_k d^3k \frac{\left\langle \vec{k}_f^{(-)}\Phi_{_f}^N \right| V \left| \Phi_{_n}^N \vec{k} \right\rangle \left\langle \vec{k}\Phi_{_n}^N \right| T \left| \Phi_{_i}^N \vec{k}_i^{(+)} \right\rangle}{E^{(+)} - \varepsilon_{_n}^N - \frac{1}{2}k^2}, \tag{30}$$

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

$$\left\langle \vec{k}\Phi_f \right| T \left| \vec{k}_i^{(+)}\Phi_i \right\rangle = \lim_{N\to\infty} \left\langle \vec{k}\Phi_f^N \right| T \left| \vec{k}_i^{(+)}\Phi_i^N \right\rangle, \tag{31}$$

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 convergence 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

$$\begin{aligned} &\left\langle L_f k_f^{(-)}, f\pi_f l_f s_f \right\| \left| T_{\Pi S}^{JN} \right\| \left| L_i k_i^{(+)}, i\pi_i l_i s_i \right\rangle \\ &\quad = \left\langle L_f k_f^{(-)}, f\pi_f l_f s_f \right\| \left| V_{\Pi S}^{JN} \right\| \left| L_i k_i^{(+)}, i\pi_i l_i s_i \right\rangle \\ &\quad + \sum_{n=1}^{N} \sum_{l,L} \sum_{k} \int \left\langle L_f k_f^{(-)}, f\pi_f l_f s_f \right\| \left| V_{\Pi S}^{JN} \right\| \left| L k^{(-)}, n\pi l s \right\rangle \\ &\quad \times \frac{\left\langle L k^{(-)}, n\pi l s \right\| \left| T_{\Pi S}^{JN} \right\| \left| L_i k_i^{(+)}, i\pi_i l_i s_i \right\rangle}{E^{(+)} - \varepsilon_n^N - \frac{1}{2}k^2}. \end{aligned} \tag{32}$$

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

3 Numerical results

In this work, two sources of uncertainty occur in our systematic numerical problems, arising respectively from (i) inherent approximations in the numerical methods used, often called *truncation errors*, and (ii) approximations in the machine evaluation of the results due to the limited accuracy with which numbers are stored and manipulated by computer, known as *round-off errors*. Both sources of error can be minimized by using careful numerical techniques. Accordingly, we determined the target helium-atom spectrum from the roots of the three-term recurrence relation of the Pollaczek polynomials by synthetic division method with the Newton-Raphson method to get a new approximation from an initial guess. The new approximation is repeated, to get a still better approximation to the root. This continues until successive values of the approximate root differ by less than a prescribed small epsilon ($\varepsilon \approx 10^{-8}$) which controls the allowable error in the root or until the Pollaczek polynomials becomes less than some prescribed small value ($\approx 10^{-8}$).

The convergence of the associated quadrature weights of the Gaussian quadrature based Pollaczek polynomials and the configuration interaction coefficients of the helium wave functions are determined by the roots of the three-term recurrence relation of the Pollaczek polynomials. Besides these roots, recurrence relation formula provides a powerful algorithm for performing numerical calculations. When a recurrence process of increasing index n is unstable, mention must be made of a refinement due to Miller method (see for example in Abramowitz and Stegun [16]) which enables a recurrence process of decreasing n (which will be called backward recurrence). For the Pollaczek polynomial, if the modulus of root variable is greater than 1, one will have the unstable process for the large n due to round off errors of the computer. Using Miller (backward recurrence) method, one can perform the numerical calculation without any knowledge of starting values for a large n. The most convenient way is to choose the value of the polynomial at large n as zero and $n-1$ as 1 and to perform a decreasing $-n$ process until one reaches the $n = 2$. The next step is to divide the backward recurrence value $n = 2$ by that the forward recurrence to get the constant multiplier. To ensure that the starting value of the index n is large enough, the latter step is repeated for $n = 3$. If both constant multipliers are same, the index n was chosen larger enough, otherwise one the index n is large enough and the correct values of the polynomial can be recovered simply by multiplying the backward recurrence values by constant multiplier.

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

$$\int_0^\infty dk \frac{k^2 F(x)}{E - \varepsilon_n^N - \frac{1}{2}k^2} \approx \sum_{j=1}^{N} W_j^n k_j^n F\left(k_j^n\right), \qquad (33)$$

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

$$\int_0^\infty dk \left\langle \Phi_n^N \mid k \right\rangle \left\langle k \mid \Phi_n^N \right\rangle \approx 1, \qquad (34)$$

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.

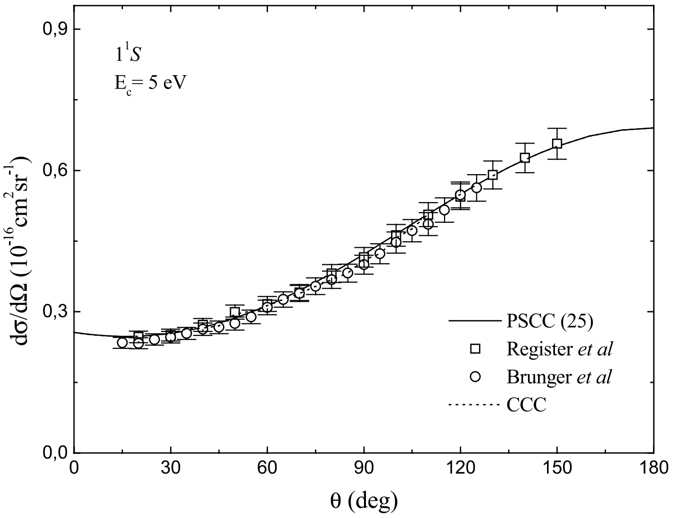

Fig. 1. Elastic differential cross-sections for electron-helium scattering at a projectile energy of 5 eV. The present calculation is denoted by PSCC, and is obtained using 25 states in the CC formalism. The calculations denoted by CCC are due to Fursa and Bray [10]. The measurements are due to Brunger et al. [17] and Register et al. [18].

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.

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. [17] at an impact energy range of 5 to 200 eV are good agreement with the more recent study by Brunger et al. [18] (1.5 to 50 eV). Therefore, the results of the experiments of Register et al. [17] (± 5 to 7% error bars) and Brunger et al. [18] (± 3.5 to 5% error bars) are presented for comparison in this work. For theory, the calculation results of Fursa and Bray [10] and Nesbet [19] 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 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

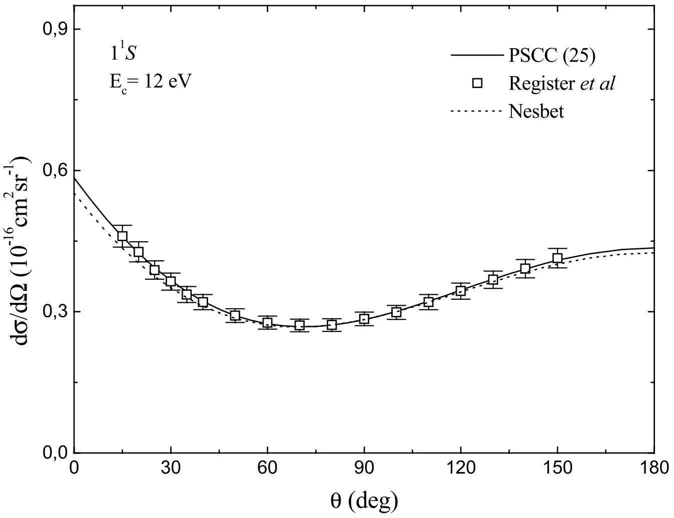

Fig. 2. Elastic differential cross-sections for electron-helium scattering at a projectile energy of 12 eV. The present calculation is denoted by PSCC, and is obtained using 25 states in the CC formalism. The calculations denoted by variational method are due to Nesbet [19]. The measurements are due to Register et al. [18].

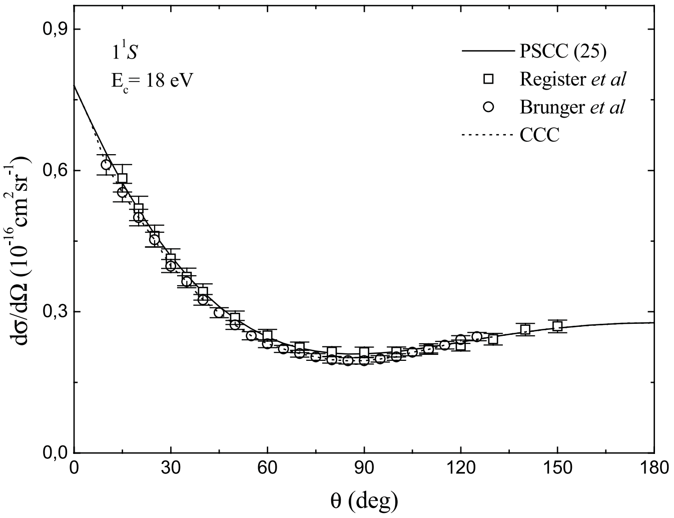

Fig. 3. Elastic differential cross-sections for electron-helium scattering at a projectile energy of 18 eV. The present calculation is denoted by PSCC, and is obtained using 25 states in the CC formalism. The calculations denoted by CCC are due to Fursa and Bray [10]. The measurements are due to Brunger et al. [17] and Register et al. [18].

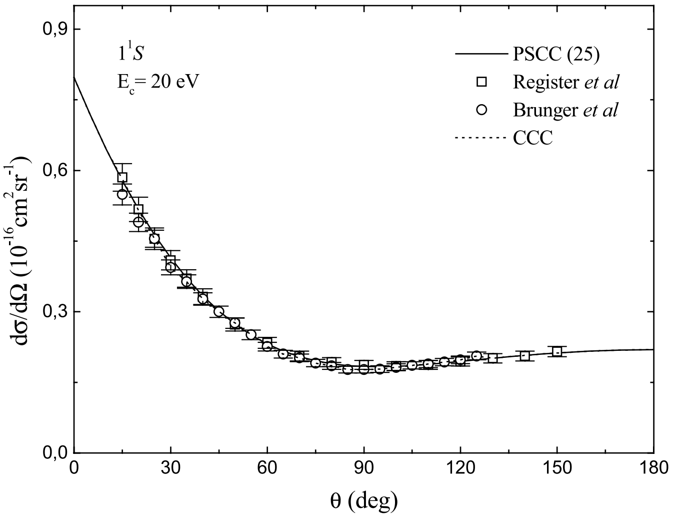

Fig. 4. Elastic differential cross-sections for electron-helium scattering at a projectile energy of 20 eV. The present calculation is denoted by PSCC, and is obtained using 25 states in the CC formalism. The calculations denoted by CCC are due to Fursa and Bray [10]. The measurements are due to Brunger et al. [17] and Register et al. [18].

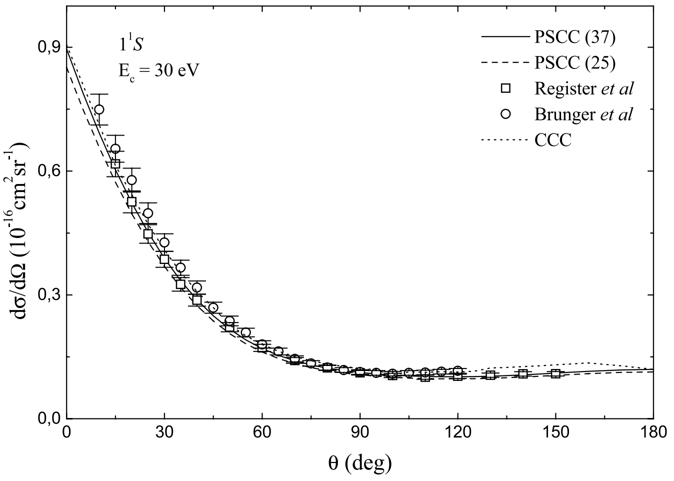

Fig. 5. Elastic differential cross-sections for electron-helium scattering at a projectile energy of 30 eV. The present calculation is denoted by PSCC, and is obtained using 25 and 37 states in the CC formalism. The calculations denoted by CCC are due to Fursa and Bray [10]. The measurements are due to Brunger et al. [17] and Register et al. [18].

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. [18] at an impact energy range of 30 to 50 eV, particularly at the forward angles.

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 et al. [20] and Truhlar et al. [21] (±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

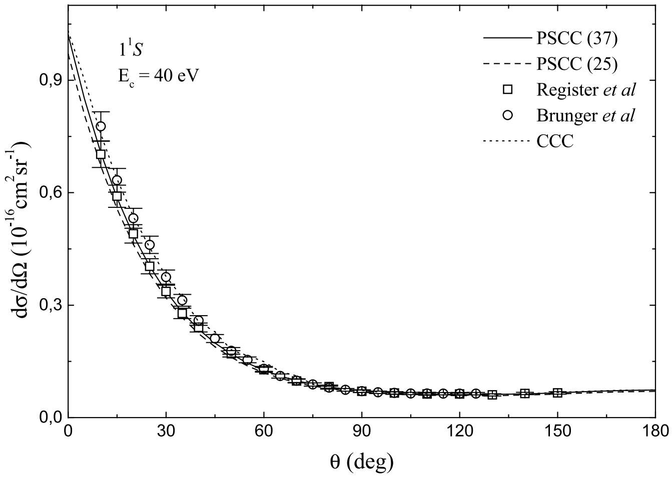

Fig. 6. Elastic differential cross-sections for electron-helium scattering at a projectile energy of 40 eV. The present calculation is denoted by PSCC, and is obtained using 25 and 37 states in the CC formalism. The calculations denoted by CCC are due to Fursa and Bray [10]. The measurements are due to Brunger et al. [17] and Register et al. [18].

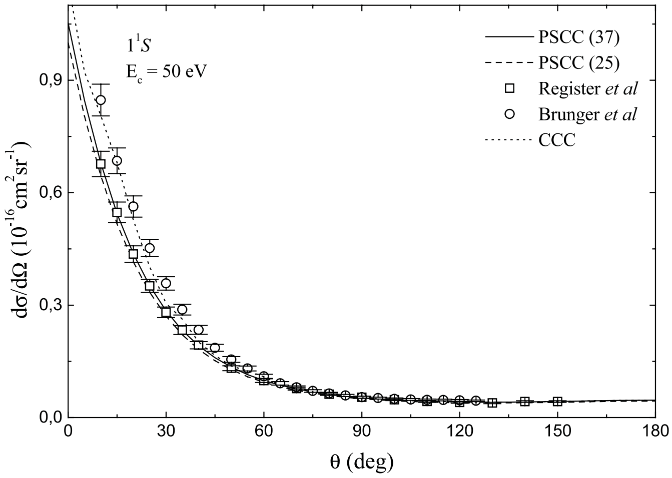

Fig. 7. Elastic differential cross-sections for electron-helium scattering at a projectile energy of 50 eV. The present calculation is denoted by PSCC, and is obtained using 25 and 37 states in the CC formalism. The calculations denoted by CCC are due to Fursa and Bray [10]. The measurements are due to Brunger et al. [17] and Register et al. [18].

considerably below the measurements of Trajmar et al. [20] and Truhlar et al. [21]. 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 basis functions. For example, we show the spectrum for case of $\lambda_l = 0.93$ and varying N (see Refs. [12,15]). The negative-energy levels converge, with increasing N, to the true bound states. The positive-energy states do not converge but provide a dense covering of the continuous spectrum in the limit $N \to \infty$. The expanding nature of the spectrum for positive energies is due to the fact that the roots of the Pollaczek polynomials are determined in the variable X rather than energy and in that variable they are regularly spaced in the interval $X \in [-1, 1]$.

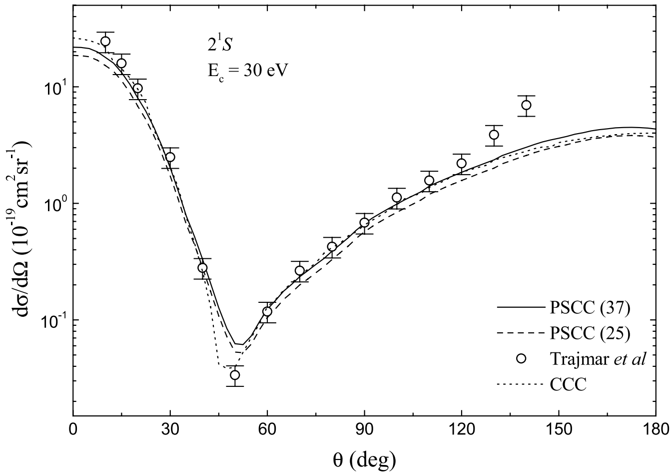

Fig. 8. The 2^1S differential cross-sections for electron-helium scattering at a projectile energy of 30 eV. The present calculation is denoted by PSCC, and is obtained using 25 and 37 states in the CC formalism. The measurements are due to Trajmar et al. [20]. The calculations denoted by CCC are due to Fursa and Bray [10].

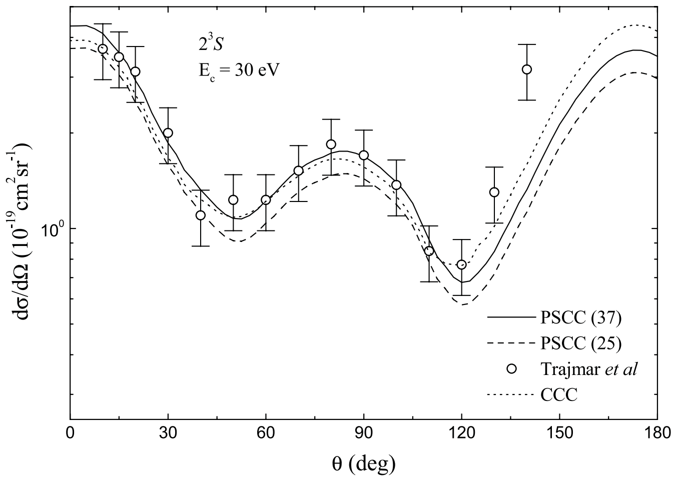

Fig. 9. The 2^3S differential cross-sections for electron-helium scattering at a projectile energy of 30 eV. The present calculation is denoted by PSCC, and is obtained using 25 and 37 states in the CC formalism. The measurements are due to Trajmar et al. [20]. The calculations denoted by CCC are due to Fursa and Bray [10].

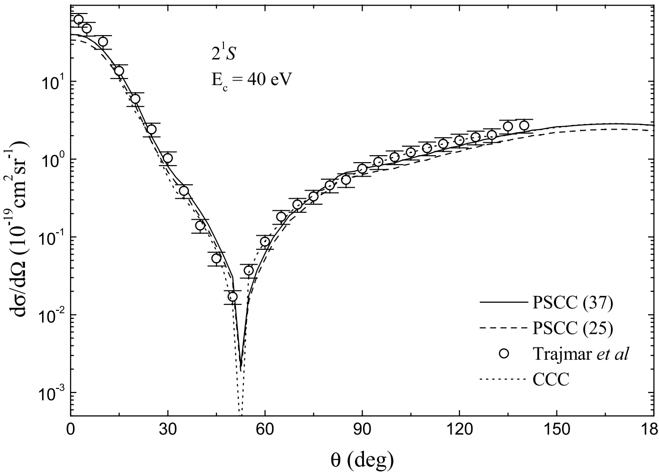

Fig. 10. The 2^1S differential cross-sections for electron-helium scattering at a projectile energy of 40 eV. The present calculation is denoted by PSCC, and is obtained using 25 and 37 states in the CC formalism. The measurements are due to Trajmar et al. [20]. The calculations denoted by CCC are due to Fursa and Bray [10].

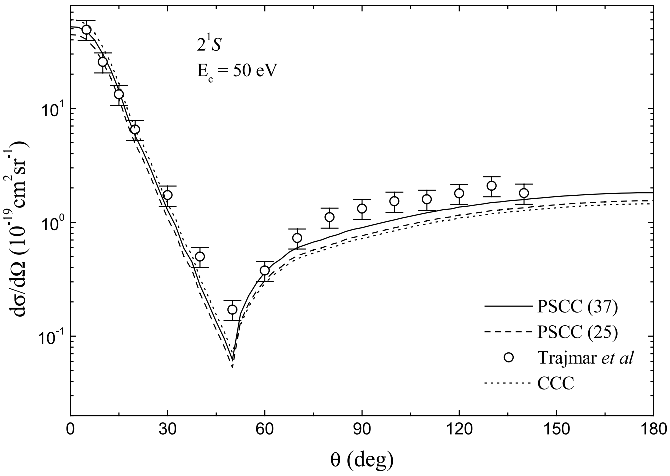

Fig. 12. The 2^1S differential cross-sections for electron-helium scattering at a projectile energy of 50 eV. The present calculation is denoted by PSCC, and is obtained using 25 and 37 states in the CC formalism. The measurements are due to Trajmar et al. [20]. The calculations denoted by CCC are due to Fursa and Bray [10].

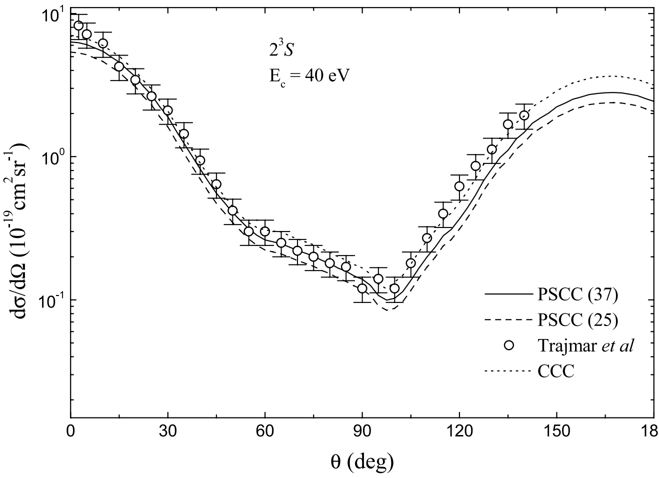

Fig. 11. The 2^3S differential cross-sections for electron-helium scattering at a projectile energy of 40 eV. The present calculation is denoted by PSCC, and is obtained using 25 and 37 states in the CC formalism. The measurements are due to Trajmar et al. [20]. The calculations denoted by CCC are due to Fursa and Bray [10].

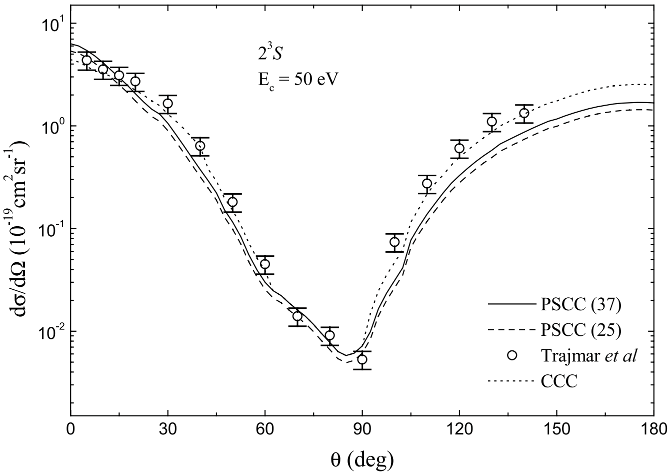

Fig. 13. The 2^3S differential cross-sections for electron-helium scattering at a projectile energy of 50 eV. The present calculation is denoted by PSCC, and is obtained using 25 and 37 states in the CC formalism. The measurements are due to Trajmar et al. [20]. The calculations denoted by CCC are due to Fursa and Bray [10].

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.

4 Conclusions and future work

Our aim in this paper has been to develop a framework for the solution of the CC equations using the non-orthogonal Laguerre-L^2 basis expansions for the helium atom target, which can be increased to arbitrary basis size, hence enabling overall convergence of the differential and total cross-sections to be studied systematically. The methods developed are numerically stable and our calculations have been limited only by the local computing facilities available.

Generally, we have demonstrated that the PSCC method using a non-orthogonal Laguerre-L^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.

Table 1. Total cross-sections (10^{-16} cm^2) for 5 to 50 eV electrons scattering on the ground state of helium. The calculations are denoted by CCC are due to Fursa and Bray [10]. The experimental estimates are due to Register et al. [17] (3% error) and Brunger et al. [18] (1% error).

E_c (eV)	PSCC (37)	CCC [10]	Register et al. [17]	Brunger et al. [18]
5	5.385	-	5.25 ± 0.16	5.32 ± 0.04
12	4.109	-	3.96 ± 0.12	-
18	3.274	-	3.22 ± 0.10	3.34 ± 0.06
20	3.034	-	3.03 ± 0.09	2.98 ± 0.01
30	2.236	2.47	2.34 ± 0.07	2.30 ± 0.01
40	1.890	2.03	1.94 ± 0.06	1.67 ± 0.08
50	1.571	1.76	1.69 ± 0.05	1.47 ± 0.01

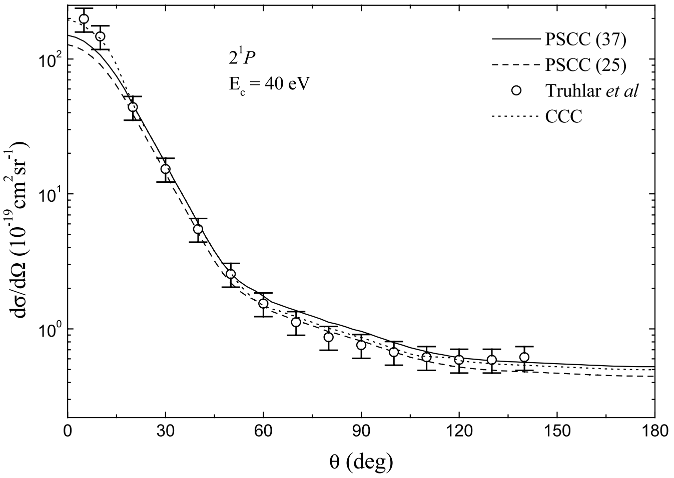

Fig. 14. The 2^1P differential cross-sections for electron-helium scattering at a projectile energy of 40 eV. The present calculation is denoted by PSCC, and is obtained using 25 and 37 states in the CC formalism. The measurements are due to Truhlar et al. [21]. The calculations denoted by CCC are due to Fursa and Bray [10].

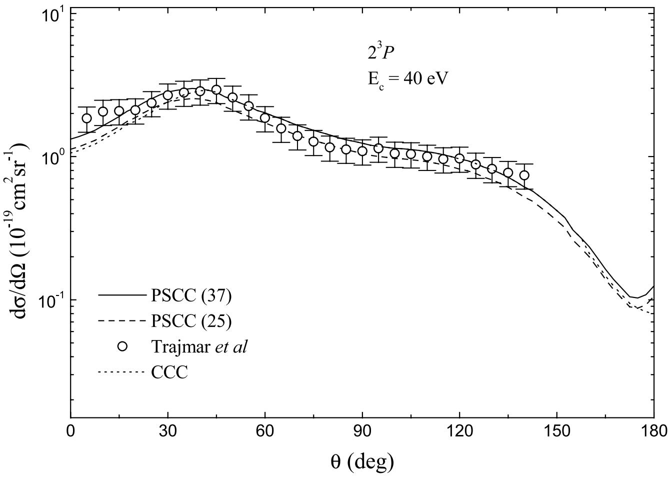

Fig. 15. The 2^3P differential cross-sections for electron-helium scattering at a projectile energy of 40 eV. The present calculation is denoted by PSCC, and is obtained using 25 and 37 states in the CC formalism. The measurements are due to Trajmar et al. [20]. The calculations denoted by CCC are due to Fursa and Bray [10].

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.

At a later stage, we will present the calculations of the differential, integrated and total cross-sections for large bases used. To examine convergences studies, in the most difficult intermediate energy region, we will also present the convergence of the PSCC method with the inclusion of G states and many continuum states.

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