

Application of the Non-Orthogonal Laguerre- L^2 Basis to the Calculation of Electron-Helium Scattering at Intermediate Energy

(Penggunaan Asas Tak Ortogon Laguerre- L^2 untuk Pengiraan Serakan Elektron-Helium pada Tenaga Pertengahan)

AGUS KARTONO & MUSTAFA MAMAT

ABSTRACT

Differential cross sections for excitation to the $n=2$ states of atomic helium by electrons were computed for incident energies in the range from 30 to 50 eV. The $n=2$ states excitation cross sections are calculated with the use of close-coupling expansion with a non-orthogonal Laguerre- L^2 basis function. The present status of agreement between theory and experiment for excitation of the ground-state was quite satisfactory.

Keywords: Atomic helium; close-coupling; differential cross sections; excitation

ABSTRAK

Pembezaan keratan rentas untuk pengujaan keadaan atom helium $n=2$ oleh elektron untuk tenaga insiden dikira dalam julat daripada 30 kepada 50 eV. Keadaan keratan rentas $n=2$ dikira dengan menggunakan pengembangan gabungan-tertutup bersama suatu fungsi asas tak-ortogon Laguerre- L^2 . Persetujuan antara teori dan eksperimen untuk pengujaan ke keadaan asas adalah agak memuaskan.

Kata kunci: Atom helium; gabungan-tertutup; mengangkat; pembezaan keratan rentas

INTRODUCTION

Electron-helium scattering is the second most simple electron-atom scattering system only being surpassed by the electron-hydrogen (e-H) problem. The former has substantial advantages from the experimental point of view and has been used as a standard against which other scattering system may be compared, normalized and calibrated. For theorists the e-H system is preferable primarily because a three-body system is easier to work with than a four-body system. For these reasons, over the years there has been a disproportional concentration of theoretical and experimental activity: a great deal of e-H theory with relatively little experimental support and vice versa for e-He system.

The study of intermediate-energy electron scattering from the helium atom is of interest from both an experimental and theoretical point of view. Helium is an important component of several different types of plasma media, such as the He-Ne laser, the Jovian atmosphere and a variety of gas discharges. Electrons of energies less than 50 eV are present in the media and it is desirable to know accurate differential cross sections for inelastic e-He scattering in order to understand these often complex plasma environments (Chutjian & Thomas 1975).

It is convenient to divide the energy region for the incident into low, intermediate and high energy regions. In the low energy region the velocity of the incident electron is of the same order or less than the velocity of the electrons

in the target which are taking an active part in the collision. In this region only a few target states can be energetically excited. The intermediate energy region extends up to energy where the velocity of the active target electrons. This is the most difficult region to treat theoretically since an infinite number of target states can be excited and also ionizing collisions are possible. Finally, high energy region is characterized by the kinetic energy of the incident electron and the net Coulomb attraction potential so the first Born or Coulomb-Born approximation will usually be applicable. Calculations in Born or Coulomb-Born approximations are legion. Invaluable as these calculations are, they are not sufficiently accurate for most applications as the temperature of plasma is high, this serves mainly to increase the ionization state of plasma and the important energy region remains below about four times the threshold excitation energy.

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. Here, we primarily concentrate on three energies 30 to 50 eV in the intermediate region. This is in the most difficult intermediate energy range, being only 5.42 to 25.42 eV above the ionization threshold. The intermediate energy region extends up to incident electron energy where the velocity of the incident electron is typically about four

times the velocity of the active target electrons. This is the most difficult region to treat theoretically since an infinite number of target states can be excited and also ionizing collisions are possible. In intermediate energies, there should be 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 average in some sense over the complete set of target eigenstates.

A new expansion of the three-body Coulomb wave functions in a non-orthogonal Laguerre-type function basis and the frozen-core model is used to calculate the three-body Coulomb Hamiltonian. It is shown that discretization of the radial kinetic energy and the Coulomb problem in the attractive case for the helium ground state ($1s$) give the modified Pollaczek polynomials, whereas the other discretization of the radial kinetic energy and the Coulomb problem in the attractive and electron-electron potential case for the helium excitation states give a new modified Pollaczek polynomial. The resulting three-term recurrence relation is shown to be a special case of the Pollaczek polynomials which is a set of orthogonal polynomials having a nonempty continuous spectrum in addition to an infinite discrete spectrum. The completeness relation of the three-body Coulomb wave functions is calculated in term of the configuration interaction coefficient via the Gaussian quadrature. It is shown that the weights and configuration interaction coefficients converge to the certain number for different basis size (Kartono & Mamat 2010a).

For intermediate energies, there should be 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 average in some sense over the complete set of target eigenstates (Kartono & Mamat 2011).

The close-coupling 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 the ways to approximate the continuum states is positive-energy pseudostates formed from the non-orthogonal Laguerre- L^2 basis function (Kartono & Mamat 2010b). 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 close-coupling equations by numerical quadrature. The convergence of such a method can be determined by increasing the order of the quadrature until scattering amplitudes are stable to a specified accuracy, for example 1% (Bray & Stelbovics 1992).

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 from the electron-helium atom scattering to complex atoms calculations.

The primary purpose of this paper was 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 used a detailed description of the helium target which was presented by Winata and Kartono (2004). 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.

EXPANSION OF THE HELIUM TARGET WAVE FUNCTIONS

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 basis function:

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

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:

$$H = H_1 + H_2 + V_{12}, \quad (2)$$

where:

$$H_i = K_i + V_i = -\frac{1}{2}\nabla_i^2 - \frac{Z}{r_i}, \quad (3)$$

for $i = 1, 2$, is the one-electron Hamiltonian of the He^+ ion ($Z = 2$), and:

$$V_{12} = \frac{1}{r_{12}}, \quad (4)$$

is the electron-electron potential. Atomic units (a.u.) are assumed throughout.

Although 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

$$\langle \Phi_m \left| -\frac{1}{2}\nabla_1^2 - \frac{Z}{r_1} - \varepsilon_{n_1} \right| \Phi_n \rangle = 0, \quad (5)$$

in order to get a good description of the He^+ ion state, where ε_{n_1} 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:

$$\langle \Phi_m \left| -\frac{1}{2}\nabla_2^2 - \frac{Z}{r_2} + \frac{1}{r_{12}} - \varepsilon_{n_2} \right| \Phi_n \rangle = 0, \quad (6)$$

where ε_{n_2} is the energy associated with the excitation states of the helium atom.

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 able to obtain 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). For examples, the all of roots and resulting eigenvalues for nS excited states are presented in Table 1.

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

$$\left(C_{Ni}^{W(\alpha\beta)} \right)^2 = \frac{2^{2l}}{\pi} \frac{\lambda_l}{(1 - X_{Ni}^{(\alpha\beta)})} W_{Ni}^{(\alpha\beta)}, \quad (7)$$

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:

$$W_{Ni}^{(\alpha\beta)} = \frac{\pi \Gamma(N + 2l + 1)}{2^{2l} \Gamma(N + 1)} \frac{1}{P_{N-1}^{(\alpha\beta)}(X_{Ni}^{(\alpha\beta)}) \frac{d}{dx} P_N^{(\alpha\beta)}(X_{Ni}^{(\alpha\beta)})}. \quad (8)$$

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:

$$\lim_{r_0 \rightarrow \infty} \Psi(x_0, x_1, x_2) = \chi(\sigma) \exp(i\vec{k}_i \cdot \vec{r}_0) \Phi_i(x_1, x_2), \quad (9)$$

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

$$\begin{aligned} \langle \vec{k}_f^{(-)} \Phi_f | T | \Phi_i \vec{k}_i^{(+)} \rangle &= \langle \vec{k}_f^{(-)} \Phi_f | V | \Phi_i \vec{k}_i^{(+)} \rangle + \\ &\sum_n \int_n \int_k d^3k \frac{\langle \vec{k}_f^{(-)} \Phi_f | V | \Phi_n \vec{k} \rangle \langle \vec{k} \Phi_n | T | \Phi_i \vec{k}_i^{(+)} \rangle}{E^{(+)} - \varepsilon_n - k^2}, \end{aligned} \quad (10)$$

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

$$\left(\varepsilon_k^{(\pm)} - K_0 \right) |k^{(\pm)}\rangle = 0. \quad (11)$$

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

$$E - \varepsilon_n - k_n^2/2 = 0. \quad (12)$$

and exist only for open channels n such that $E = \varepsilon_i - k_n^2/2 > \varepsilon_n$.

In practice, no numerical method for solving the coupled T -matrix equations in the form (10) 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 both i, f and n are in 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:

$$\langle \Phi_m^N | H_T | \Phi_n^N \rangle = \varepsilon_n^N \delta_{mn}, \quad (13)$$

and have the property:

TABLE 1. The roots and pseudostates energies ($\varepsilon_{i\alpha} + \varepsilon_{i\beta}$) (a.u.) which were produced from non-orthogonal Laguerre- L^2 expansions are shown for the ground states, $\lambda_{i\alpha} = 4.0$ for $N_\alpha = 1, {}^1, {}^3S$ excited states, $\lambda_{i\beta} = 0.93$ for $N_\beta = 5, 10, 15, 20$. Powers of ten are denoted by the number in brackets

N_β	i	$x_{i\beta}$	1S	$x_{i\beta}$	3S
5	1	0.66808090(+1)	-2.145	0.13282618(+1)	-2.175
	2	-0.35185507(+1)	-2.060	0.41686718(+1)	-2.068
	3	-0.16628586(+1)	-2.027	-0.50627876(+1)	-2.024
	4	-0.35362914	-1.949	-0.15819399(+1)	-2.022
	5	0.68283608	-1.430	0.38607842	-1.757
10	1	0.66808089(+1)	-2.145	0.13250302(+1)	-2.175
	2	-0.35195686(+1)	-2.060	0.41686005(+1)	-2.068
	3	-0.18855244(+1)	-2.033	-0.50659650(+1)	-2.036
	4	-0.14455480(+1)	-2.020	-0.21120690(+1)	-2.022
	5	-0.10519270(+1)	-2.003	-0.15184051(+1)	-2.001
	6	-0.57415939	-1.971	-0.10145974(+1)	-1.956
	7	-0.77645763(-1)	-1.908	-0.42011142	-1.851
	8	0.37253183	-1.765	0.16170720	-1.521
	9	0.72269176	-1.333	0.63352830	-1.150
	10	0.93569806	1.234	0.92129230	0.622
15	1	0.66808089(+1)	-2.145	0.13250260(+1)	-2.175
	2	-0.35195686(+1)	-2.060	0.41686005(+1)	-2.068
	3	-0.18857648(+1)	-2.033	-0.50659650(+1)	-2.036
	4	-0.14816654(+1)	-2.021	-0.21123202(+1)	-2.024
	5	-0.12887558(+1)	-2.014	-0.15654176(+1)	-2.015
	6	-0.10902887(+1)	-2.005	-0.13298493(+1)	-2.005
	7	-0.84176699	-1.991	-0.10998427(+1)	-1.989
	8	-0.56057641	-1.970	-0.81221773	-1.963
	9	-0.26506416	-1.938	-0.48953736	-1.922
	10	0.27839887(-1)	-1.886	-0.15626455	-1.850
	11	0.30247889	-1.799	0.16520870	-1.714
	12	0.54481143	-1.635	0.45456512	-1.405
	13	0.74294921	-1.272	0.69410085	-0.462
	14	0.88776305	-0.193	0.86942456	5.279
	15	0.97358844	6.027	0.97091398	7.258
20	1	0.66808089(+1)	-2.145	0.13250260(+1)	-2.175
	2	-0.35195686(+1)	-2.060	0.41686005(+1)	-2.068
	3	-0.18857648(+1)	-2.033	-0.50659650(+1)	-2.036
	4	-0.14819681(+1)	-2.021	-0.21123202(+1)	-2.024
	5	-0.13084548(+1)	-2.014	-0.15656459(+1)	-2.016
	6	-0.11979999(+1)	-2.010	-0.13501023(+1)	-2.011
	7	-0.10705412(+1)	-2.004	-0.12233178(+1)	-2.004
	8	-0.91232049	-1.995	-0.10829059(+1)	-1.995
	9	-0.73101700	-1.983	-0.90766420	-1.982
	10	-0.53401026	-1.967	-0.70670226	-1.963
	11	-0.32808692	-1.946	-0.48919027	-1.937
	12	-0.11972151	-1.916	-0.26355659	-1.900
	13	0.84878801(-1)	-1.873	-0.37805456(-1)	-1.845
	14	0.27982937	-1.809	0.18045213	-1.759
	15	0.45966677	-1.710	0.38408549	-1.612
	16	0.61946674	-1.543	0.56657397	-1.334
	17	0.75496825	-1.231	0.72214597	-0.713
	18	0.86269873	-0.543	0.84592530	1.156
	19	0.94010779	1.480	0.93416906	12.146
	20	0.98575646	12.975	0.98492723	13.250

$$\sum_n \int \Phi_n(x_1, x_2) f_n(x_0) = \lim_{N \rightarrow \infty} \sum_{n=1}^N \Phi_n^N(x_1, x_2) f_n^N(x_0), \quad (14)$$

With these definitions, the sum and integral in the Lippmann-Schwinger equation (13) become a single sum over N , with the target states and energies being replaced by $|\Phi_n^N\rangle$ and ε_n^N , respectively. We define:

$$\begin{aligned} \langle \vec{k}_f^{(-)} \Phi_f^N | T | \Phi_i^N \vec{k}_i^{(+)} \rangle &= \langle \vec{k}_f^{(-)} \Phi_f^N | V | \Phi_i^N \vec{k}_i^{(+)} \rangle + \\ &\sum_{n=1}^N \int d^3k \frac{\langle \vec{k}_f^{(-)} \Phi_f^N | V | \Phi_n^N \vec{k} \rangle \langle \vec{k} \Phi_n^N | T | \Phi_i^N \vec{k}_i^{(+)} \rangle}{E^{(+)} - \varepsilon_n^N - k^2}, \end{aligned} \quad (15)$$

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:

$$\langle \vec{k} \Phi_f | T | \vec{k}_i \Phi_i \rangle = \lim_{N \rightarrow \infty} \langle \vec{k} \Phi_f^N | T | \vec{k}_i^{(+)} \Phi_i^N \rangle, \quad (16)$$

for the physical T -matrix elements.

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 (17) in the limit of large N and that $\lim_{N \rightarrow \infty} \Phi_n^N = \Phi_n$ and $\lim_{N \rightarrow \infty} \Phi_n^N = \Phi_n$. This ensures that the limiting procedure (18) gives the correct T -matrix amplitudes (13) for the transitions to $2S$ level.

The partial wave Lippmann-Schwinger equation corresponding to (18) for the reduced T -matrix elements are:

$$\begin{aligned} &\langle L_f k_f^{(-)}, f \pi_f l_f s_f \| T_{\text{NS}}^{JN} \| L_i k_i^{(+)}, i \pi_i l_i s_i \rangle \\ &= \langle L_f k_f^{(-)}, f \pi_f l_f s_f \| V_{\text{NS}}^{JN} \| L_i k_i^{(+)}, i \pi_i l_i s_i \rangle \end{aligned}$$

$$+ \sum_{n=1}^N \sum_{l, L} \sum_k \int \frac{\langle L_f k_f^{(-)}, f \pi_f l_f s_f \| V_{\text{NS}}^{JN} \| L k^{(-)}, n \pi l s \| T_{\text{NS}}^{JN} \| L_i k_i^{(+)}, i \pi_i l_i s_i \rangle}{E^{(+)} - \varepsilon_n^N - \varepsilon_k}. \quad (17)$$

The differential cross sections for scattering from channel i to channel f at an angle θ is

$$\begin{aligned} \frac{d\sigma_{fi}}{d\Omega} &= (2\pi)^4 \frac{k_f \hat{S}^2}{k_i \hat{I}^2} \\ &\sum_m \sum_{L_i, L_f} \left| \langle L_f k_f^{(-)}, n_f \pi_f l_f s_f \| T_{\text{NS}}^{JN} \| L_i k_i^{(+)}, n_i \pi_i l_i s_i \rangle \right|^2. \end{aligned} \quad (18)$$

The solution of equations (17) and (18) is calculated by Gaussian-type quadrature method.

NUMERICAL RESULTS

In this paper it was our aim to demonstrate that the PSCC method was able to provide a relatively accurate description of electron-helium scattering at projectile energy of intermediate region. We introduced the approximation of treating the helium target by the frozen-core model, where we restricted one of the electrons to be the $1s$ He^+ orbital. The frozen-core model approximation reduced convergence studies to treating only one-electron excitation.

Our tests of this approximation for intermediate energy excitation scattering require many expansion states. The former has 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 . For large bases used, calculations are close to the limit of our desktop workstation computational resources.

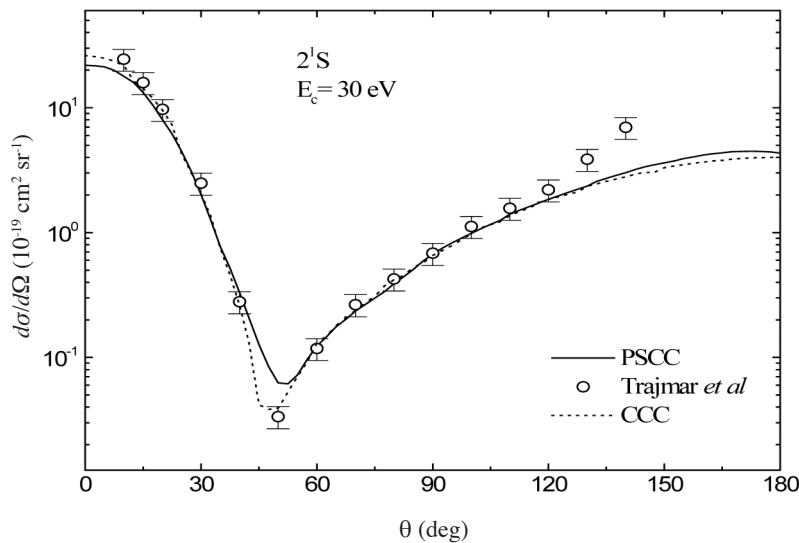


FIGURE 1. The 2^1S differential cross sections for electron-helium scattering at a projectile energy of 30 eV. The present calculation is denoted by PSCC and is obtained using 37 states in the CC formalism. The measurements are due to Trajmar et al. (1992). The calculations denoted by CCC are due to Fursa and Bray (1995)

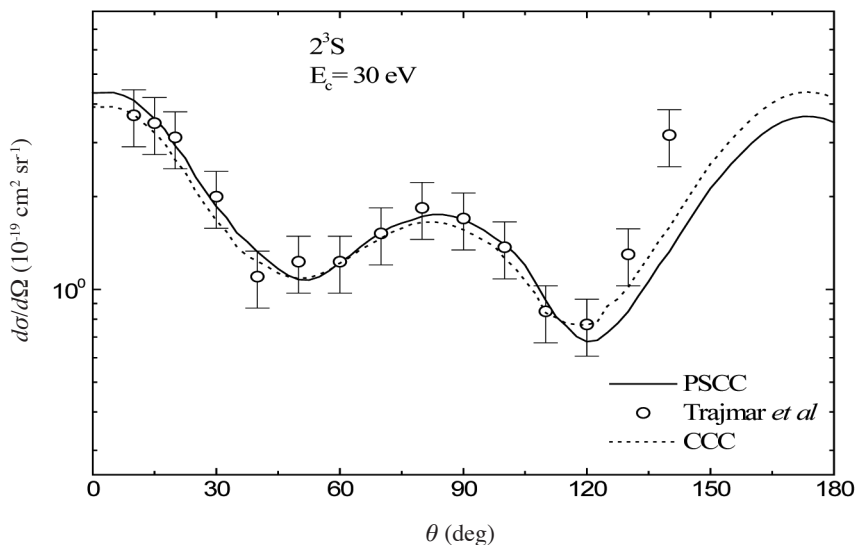


FIGURE 2. The 2^3S differential cross sections for electron-helium scattering at a projectile energy of 30 eV. The present calculation is denoted by PSCC and is obtained using 37 states in the CC formalism. The measurements are due to Trajmar et al. (1992). The calculations denoted by CCC are due to Fursa and Bray (1995)

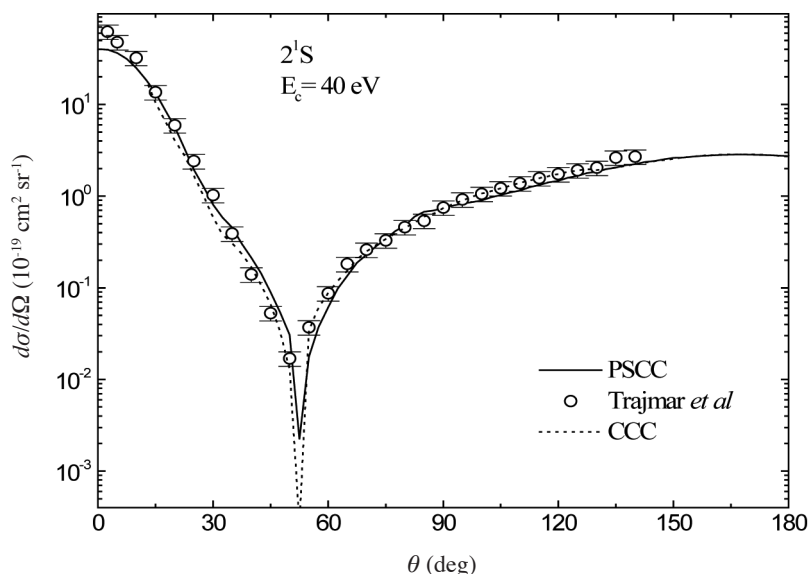


FIGURE 3. The 2^1S differential cross sections for electron-helium scattering at a projectile energy of 40 eV. The present calculation is denoted by PSCC and is obtained using 37 states in the CC formalism. The measurements are due to Trajmar et al. (1992). The calculations denoted by CCC are due to Fursa and Bray (1995)

In Figures 1 to 6, we present the excitation differential cross sections the 2^1S and 2^3S state calculated by the PSCC method for electron-helium scattering on the ground state at a range of projectile energies of 30 to 50 eV. These are compared to some of the available experiments and theories. From the figures, we see that there is essentially complete qualitative, and often quantitative, agreement between the PSCC calculation and experiment of Trajmar et al. (1992) (± 19 to 20% error bars). We noted one exception to this at the forward and backward angles for the 2^1S and 2^3S excitation, where the PSCC theory was considerably below the measurements of Trajmar et al. (1992).

The best of the other calculations was the CCC calculation of Fursa and Bray (1995). The difference between the PSCC and CCC calculations were predominantly due to the inclusion of the different basis size and the type of basis in the close-coupling formalism. Fursa and Bray (1995) use the orthogonal Laguerre basis to constructive of the helium target.

Discrepancy with experiments and other theories is still substantial at an impact energy range of 30-50 eV. The discrepancy between this work and experiments suggests that slightly large bases used calculations are necessary to get better accuracy.

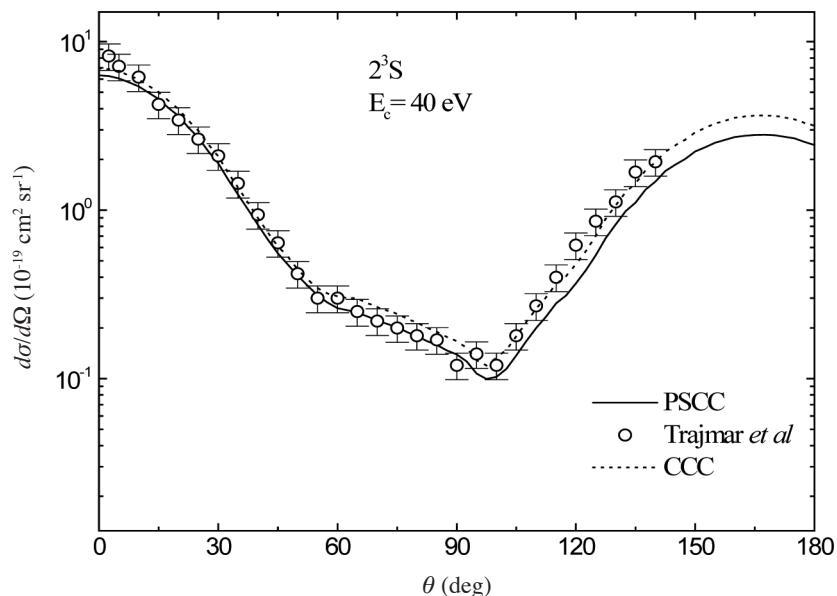


FIGURE 4. The 2^3S differential cross sections for electron-helium scattering at a projectile energy of 40 eV. The present calculation is denoted by PSCC and is obtained using 37 states in the CC formalism. The measurements are due to Trajmar *et al.* (1992). The calculations denoted by CCC are due to Fursa and Bray (1995)

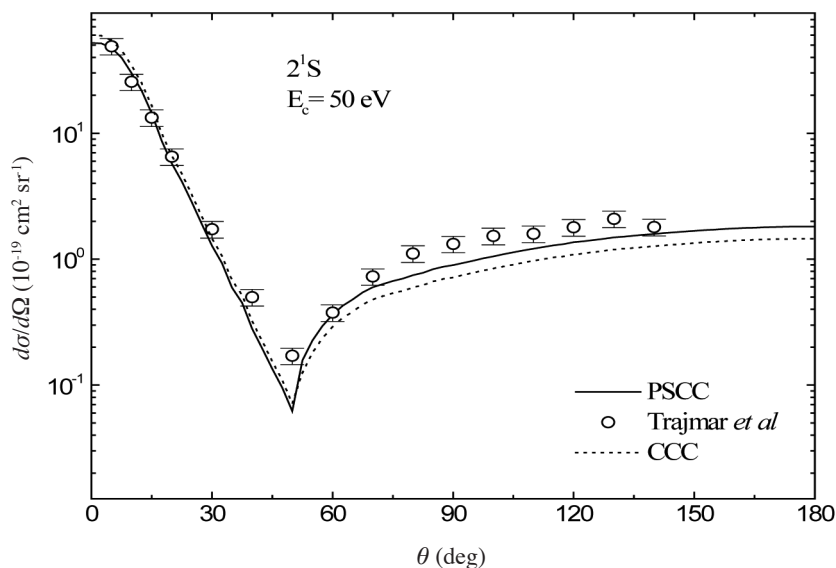


FIGURE 5. The 2^1S differential cross sections for electron-helium scattering at a projectile energy of 50 eV. The present calculation is denoted by PSCC and is obtained using 37 states in the CC formalism. The measurements are due to Trajmar *et al.* (1992). The calculations denoted by CCC are due to Fursa and Bray (1995)

CONCLUSION

We have presented some results of recent PSCC calculations applied to the electron-helium system. Specially, differential cross sections for excitation to the 2^3S and 2^1S states of atomic helium by electrons were computed for incident energies in the range from 30 to 50 eV. Generally we found satisfactory agreement between theory and experiment for excitation transitions involving the ground state. 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. At a later stage, we will present the calculations of the excitation differential cross sections for larger bases. To examine the convergences, 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.

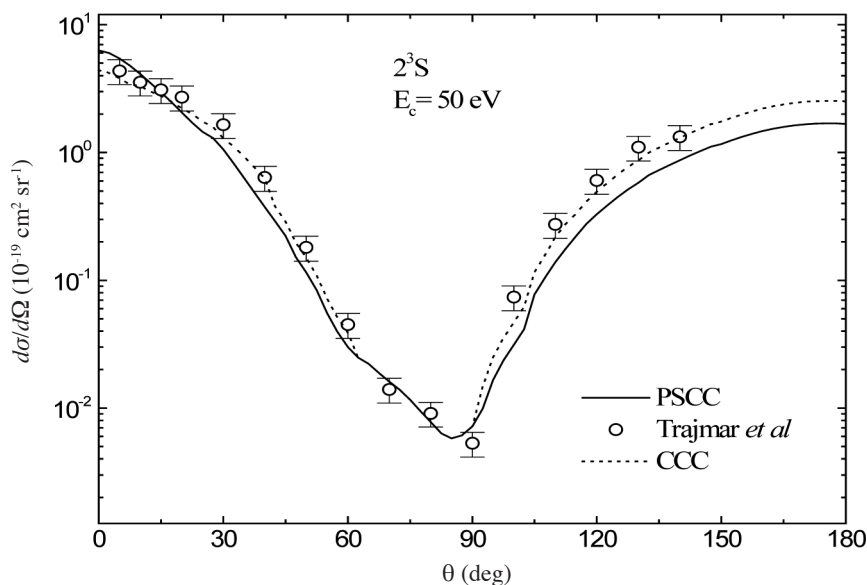


FIGURE 6. The 2^3S differential cross sections for electron-helium scattering at a projectile energy of 50 eV. The present calculation is denoted by PSCC and is obtained using 37 states in the CC formalism. The measurements are due to Trajmar et al. (1992). The calculations denoted by CCC are due to Fursa and Bray (1995)

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REFERENCES

- Bray, I. & Stelbovics, A.T. 1992. Convergent close-coupling calculations of electron-hydrogen scattering. *Phys. Rev. A* 46: 6995-7011.
- Chutjian, A. & Thomas, L.D. 1975. Experimental and (first-order many-body) theoretical differential and integral cross-sections for excitation of $n=3$ states of He by electron-impact at 29.2 and 39.7 eV. *Phys. Rev. A* 11: 1583-1595.
- Fursa, D.V. & Bray, I. 1995. Calculation of electron-helium scattering. *Phys. Rev. A* 52: 1279-1297.
- Kartono, A. & Mamat, M. 2010a. The three-body coulomb potential polynomials. *Malaysian Journal of Mathematical Sciences* 4(1): 33-54.
- Kartono, A. & Mamat, M. 2010b. The application of the pseudostate-close-coupling method using a non-orthogonal Laguerre- L^2 basis for electron-helium scattering. *Applied Mathematical Sciences* 4(27): 1309-1328.
- Kartono, A. & Mamat, M. 2011. A study of the pseudostate-close-coupling method using a non-orthogonal Laguerre- L^2 basis in the intermediate energy. *Malaysian Journal of Mathematical Sciences* 5(1): 61-83.
- Trajmar, S., Register, D.F., Cartwright, D.C. & Csanak, G.J. 1992. Differential and integral cross section for electron impact excitation of the n^3S , n^1S and n^3P ($n=2, 3$) levels in He. *J. Phys. B: At. Mol. Opt. Phys.* 25: 4889-4910.
- Winata, T. & Kartono, A. 2004. Study of non-orthogonal Laguerre- L^2 method for helium atom. *Eur. Phys. J. D: At. Mol. Opt. Phys.* 28: 307-315.

Agus Kartono & Mustafa Mamat*
 Institute of Oceanography and Environment
 Universiti Malaysia Terengganu
 Mengabang Telipot
 21030 Kuala Terengganu, Terengganu
 Malaysia

Mustafa Mamat*
 Department of Mathematics
 Faculty of Sciences and Technology
 Universiti Malaysia Terengganu
 Mengabang Telipot
 21030 Kuala Terengganu, Terengganu
 Malaysia

*Corresponding author; email: mus@umt.edu.my

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