A Distorted Wave Method Applied to Study the $2^3P$ Excitation of Helium Atom by Electron Impact

James Mugambi Linturi*, J Okumu** and C S Singh**
*Department of Physical Sciences South Eastern University College
(A Constituent College of University of Nairobi), Kitui, Kenya
**Physics Department, Kenyatta University, Nairobi, Kenya
e-mail: j_l_mug@yahoo.com

Received 7 October 2010, Revised 10 January 2011, Accepted 29 January 2011

Abstract

The distorted wave method has been applied to calculate the differential and integral cross sections for $1^1S-2^3P$ excitations of helium atom by electron impact in the energy range of 40-200 eV. The initial distortion potential is taken as the static potential of the helium (target) atom in the initial state ($1^1S$) while the final distortion potential is taken as the average of the initial- and final-state static potentials of helium atom. The distorted waves are determined by partial wave expansion method by expanding it in terms of spherical harmonics and the radial equation corresponding to distorted waves is solved by use of Numerov method. A computer program DWBA1 written for e-H scattering by Madison and Bartschat is modified to perform the numerical calculations for e-He scattering and the results obtained are compared with experimental and theoretical results. The present results for $1^1S-2^3P$ transition are in a good agreement with experimental and theoretical results.

Keywords: Distorted wave method, Helium, Electron impact, DWBA1, Numerov method

1. Introduction

Electron-impact excitation of helium has been an important testing ground for many experimental as well as theoretical methods in atomic physics. Specifically electron collision processes involving helium are important in a large variety of systems and environment (various discharge and laser systems, fusion plasmas, planetary and astrophysical environment). If the differential cross section for particular scattering process for helium is known accurately, then this may be used to normalize data pertaining to other collision processes involving complex atoms. It is because of this potential application that considerable importance is attached to the determination of accurate cross section for electron-helium scattering.

In this paper both differential and total cross sections are calculated since it is misleading to judge the success of a theoretical method purely on the agreement of the total cross section with the experimental measurement. Differential cross section (DCS) is known to provide better insight into a collisional process than the total cross section and should be calculated for the reliable assessment of a theoretical method. The present work reassesses the available data for the collision processes involving helium atom from its ground state ($1^1S$) to the excited states $2^3P$, using the distorted wave method proposed by Singh. This method has already been applied to study the magnetic-sublevel differential cross section for electron impact excitation of $2^3P$ state of helium and to study the electron impact excitation of $2^3S$ state of helium atom, but it has never been applied to study the excitation to triplet states which occurs through exchange process. So it would be interesting to see how it works for $1^1S-2^3P$ excitation of helium atom by electron impact and see how the results obtained compares with other theoretical and experimental results available.

The results obtained are compared with first order many body theory (FOMBT) results of Trajmar, R-matrix Results of Fon et al, distorted wave methods results of Srivastava, convergent close coupling results of Fursa and Bray and experimental results among others. The present results are in qualitative agreement with the experimental results. For all our calculations we have used the computer program DWBA1 developed by Madison and Bartschat that was written for electron-hydrogen scattering. The code was modified to fit electron-helium scattering.

2. Theory

The total Hamiltonian of the electron-helium system can be written as,

$$H = H_A + T + V$$

where $H_A$ is the Hamiltonian of the helium atom, $T$ is the kinetic energy of projectile electron and $V$ is the interaction potential between the incident electron and atom. They are given by

$$T = -\nabla^2_o$$

$$V = \frac{2}{r_{01}} + \frac{2}{r_{02}} + \frac{2Z_N}{r_0}$$

Both $T$ and $V$ are in Rydberg units.

The subscript 0 refers to the projectile electron and subscript 1 and 2 refers to the bound atomic electrons, $r_{01}$ and $r_{02}$ are the distances between
the projectile electron and the atomic electrons 1 and 2 respectively and \( Z_n \) is the nuclear charge that is equal to 2 for helium.

The general T-matrix in two potential approach for an electron colliding with an N-electron atom is given by (Madison and Bartschat):

\[
T_{fi} = (N+1) 
\left\{ \chi_f^0(1,...,N) | H - U_f | A \Psi^+_i(0,...,N) \right\} + \left\{ \chi_f^0(1,...,N) | U_f | \Psi_i(1,...,N) \beta_i \right\} \tag{4}
\]

where \( \beta_i \) is the initial plane wave (eigenfunction for an isolated projectile) and \( \Psi_i^+ \) is the total wave function of the electron-atom system satisfying the Schrödinger equation

\[
H \Psi_i^+ = E \Psi_i^+ \tag{5}
\]

with outgoing wave boundary conditions.

\( \Psi_i \) and \( \Psi_f \) are the properly antisymmetrized initial and final atomic wave functions for the isolated target atom, \( A \) is the antisymmetrization operator which is generally expressed as

\[
A = \frac{1}{N+1} (1 - \sum_{i=1}^{N} P_{ia}) \tag{6}
\]

where \( P_{ia} \) is the operator that exchanges \( i \)-th atomic electron and the projectile electron. For electron-helium system the T-Matrix will take the form

\[
T_{fi} = 3 \left\{ \chi_f^0(1,2) | H - U_f | A \Psi^+_i(0,1,2) \right\} + \left\{ \chi_f^0(1,2) | U_f | \Psi_i(1,2) \exp(i k, r_o) \right\} \tag{7}
\]

and

\[
A = \frac{1}{3} (1 - P_{10} - P_{20}) \tag{8}
\]

The potential \( U_f \) in equation (4) is an arbitrary distortion potential for the projectile electron, which is used to calculate \( \chi_f^0 \) by solving the equation

\[
\left( \nabla_0^2 - U_f + k_f^2 \right) \chi_f^0 = 0 \tag{9}
\]

where the \( - \) superscript denotes the incoming wave boundary conditions. \( k_f \) is the final state wave vector of the projectile electron and \( k_f^2 \) gives the kinetic energy (in Rydberg) of the projectile electron in the final state. Since we will be choosing \( U_f \) as some combination of static potentials of the target states, for inelastic collision (as we have considered) the second term on the right hand side of equation (7) will vanish due to the orthogonality of the atomic wave functions since \( U_f \) depends only on the single coordinate of the projectile. Therefore, equation (7) reduces to:

\[
T_{fi} = 3 \left\{ \chi_f^0(1,2) | H - U_f | A \Psi^+_i(0,1,2) \right\} \tag{10}
\]

To evaluate equation (10) we will make some approximation due to the fact that \( \Psi_i \) cannot be evaluated without making some approximation. In distorted-wave approach, \( \psi_f \) is expressed in terms of a product of an initial-state distorted wave \( \chi_f^+ \chi_i^+ \) and an initial state atomic wave function \( \psi_i \). Thus in the first order distorted wave Born approximation, \( \psi_i \) will be replaced by \( \psi_i(1,2) \psi_i(0) \), where \( \chi_i^+ \) is a solution to the wave equation

\[
\left( \nabla_0^2 - U_f + k_f^2 \right) \chi_i^+ = 0 \tag{11}
\]

where \( U_f \) is an arbitrary potential chosen for the distortion of the initial state projectile electron wave function, \( k_f \) is the initial wave vector of the projectile electron and \( k_f^2 \) gives the kinetic energy (in Rydberg units) of the projectile electron in the initial state. \( \chi_i^+ \) Satisfies the outgoing wave boundary conditions. 

Now the T-Matrix to be used will be given by

\[
T_{fi} = \left\{ \chi_f^0(0) \psi_f(1,2) | H - U_f | \psi_i(1,2) \chi_i^+(0) \right\} \tag{12}
\]

Expanding equation (12) it gives

\[
T_{fi} = T_{fi}^d - T_{fi}^{ex} \tag{13}
\]

where

\[
T_{fi}^d = \left\{ \chi_f^0(0) \psi_f(1,2) | H - U_f | \psi_i(1,2) \chi_i^+(0) \right\} - \left\{ \chi_f^0(0) \psi_f(1,2) | U_f | \psi_i(1,2) \chi_i^+(0) \right\} \tag{14}
\]

and

\[
T_{fi}^{ex} = \left\{ \chi_f^0(0) \psi_f(1,2) | H - U_f | \psi_i(1,2) \chi_i^+(0) \right\} + \left\{ \chi_f^0(0) \psi_f(1,2) | U_f | \psi_i(1,2) \chi_i^+(0) \right\} \tag{15}
\]

Since it is only the triplet states that are being considered the direct part \( (T_{fi}^d) \) of the T-matrix in equation (13) is zero since we are not considering the spin dependent interaction. In the exchange T-matrix \( (T_{fi}^{ex}) \) the last two terms are neglected because the overlap integral of the continuum and the bound electron wave functions will be negligible. This is due to the oscillatory nature of the distorted wave which causes this integral to vanish, particularly when the distorted wave oscillates significantly more rapidly than the bound-state wave functions, which is the case for intermediate to high projectile energies. Thus equation (15) reduces to

\[
T_{fi}^{ex} = \left\{ \chi_f^0(0) \psi_f(1,2) | H - U_f | \psi_i(0,2) \chi_i^+(1) \right\} + \left\{ \chi_f^0(0) \psi_f(1,2) | U_f | \psi_i(0,2) \chi_i^+(1) \right\} \tag{16}
\]

Substituting the interaction potential in equation (16) we get
\[ T^\text{ex}_{ji} = 2 \left\langle \chi_j(0) \psi_j(1,2) \right| \frac{Z}{r_0} \left| \psi_j(0,2) \chi_j^*(1) \right\rangle - 2 \left\langle \chi_j(0) \psi_j(1,2) \right| \frac{Z}{r_0} \left| \psi_j(0,2) \chi_j(1) \right\rangle + 2 \left\langle \chi_j(0) \psi_j(1,2) \right| \frac{Z}{r_0} \left| \psi_j(1,0) \chi_j^*(2) \right\rangle + 2 \left\langle \chi_j(0) \psi_j(1,2) \right| \frac{Z}{r_0} \left| \psi_j(1,0) \chi_j(2) \right\rangle \]

(17)

On the same ground of the overlap integral of the bound state and the continuum wave functions we neglect the second, third, fourth and sixth terms in the above equation. So, we finally get the exchange matrix as

\[ T^\text{ex}_{ji} = 2 \left\langle \chi_j(0) \psi_j(1,2) \right| \frac{Z}{r_0} \left| \psi_j(0,2) \chi_j^*(1) \right\rangle + 2 \left\langle \chi_j(0) \psi_j(1,2) \right| \frac{Z}{r_0} \left| \psi_j(1,0) \chi_j^*(2) \right\rangle \]

(18)

Before evaluating the T-matrix element, it is important to mention the atomic wave functions to be used and choice and evaluation of the static potentials

3. Atomic Wave Functions

For ground state (1S) of the helium atom, we will use the Hartee-Fock wave function i.e.9

\[ \psi_j(r_1, r_2) = \phi_j(r_1) \phi_j(r_2) \]

(19)

where

\[ \phi_j(r) = \frac{N_1}{\sqrt{4\pi}} (\exp(-pr) + c \exp(-qr)) \]

with \( N_1=2.60505 \), \( p=1.41 \), \( q=2.61 \), and \( c=0.799 \).

For the excited state (2P) we will use the wave function given as

\[ \psi_{2P}(r_1, r_2) = \frac{1}{\sqrt{2}} \left[ \phi_{j_1}(Z, r_1) \phi_{j_2}(Z', r_2) - \phi_{j_1}(Z, r_2) \phi_{j_2}(Z', r_1) \right] \]

(21)

where \( \phi_{j_1,m}(\xi, r) \) are the hydrogenic orbitals with nuclear charge \( \xi \), which are given by

\[ \phi_{j_1}(r) = \left( \frac{Z}{a_0} \right)^{\frac{3}{2}} \frac{2}{a_0} \exp\left( -\frac{Zr}{a_0} \right) J_{2m}(r) \]

and

\[ \phi_{j_2}(r) = \left( \frac{Z'}{a_0} \right)^{\frac{3}{2}} \frac{2r}{a_0^3} \exp\left( -\frac{Z'z}{a_0} \right) J_{2m}(r) \]

With \( Z=1.99, Z'=1.1 \) and \( a_0=1 \) and \( \chi_{i,m}(r) \) are the spherical harmonics.

4. Distortion Potential

Though the choice of the distortion potential is arbitrary, the common choice is either the potential of the target atom in its initial or final state, or any linear combination of the two. In this study the distorted waves are generated as suggested by Singh. Here the initial state distorted wave is due to static potential of helium atom in the initial state (1S) and the final state distorted wave will be generated by the average of the initial state static potential \((U_i)\) and final state \((U_f)\) static potential of helium atom as given below

\[ U_i = \{ \psi_j \} \]

and

\[ U_f = \frac{1}{2} \{ \psi_j \} \{ \psi_j \} + \{ \psi_j \} \{ \psi_j \} \]

The reason for this choice is that when the electron is in the initial state, for all the time it is in the field of the initial state of the target. Hence the distortion potential for the projectile electron in the initial state should be taken as the static potential of the target atom in the initial state. When the energy from the projectile electron is transferred to the target atom, the atom takes time (relaxation time) to go to the final state. Because of this time lag between the time of energy transfer and the instant when the atom reaches its final state, the projectile electron in its final state ‘sees’ a potential that is intermediate between the initial-state and final-state static potentials. Hence the final state distortion potential is taken as the average of the initial- and final-state static potentials of helium atom.

5. Evaluation of the T-Matrix

Because of the symmetrical nature of both the initial \( \psi_j(r_1, r_2) \) and final \( \psi_j(r_1, r_2) \) wave functions of helium atom, as given by equations (19) and (21), with respect to \( r_1 \) and \( r_2 \), the two terms in the T-matrix \( T_{ji}^{\text{ex}} \) (given by equation (18)) will be equal. Thus, we evaluate the first term of equation (18) by substituting the atomic wave functions given in equations (19) and (21) as follows

\[ 2 \left\langle \chi_j(0) \psi_j(1,2) \right| \frac{Z}{r_0} \left| \psi_j(0,2) \chi_j^*(1) \right\rangle = 2 \left\langle \chi_j(0) \psi_j(1,2) \right| \frac{Z}{r_0} \left| \psi_j(1,0) \chi_j^*(2) \right\rangle \]

Expanding the right hand side of (22) we get it as

\[ 2 \left\langle \chi_j(0) \psi_j(1,2) \right| \frac{Z}{r_0} \left| \psi_j(0,2) \chi_j^*(1) \right\rangle = 2 \left\langle \chi_j(0) \psi_j(1,2) \right| \frac{Z}{r_0} \left| \psi_j(1,0) \chi_j^*(2) \right\rangle \]

(22)
The radial distorted wave equation (28) for initial and final states is solved using Numerov method and the differential cross-section for the triplet state for helium atom are obtained using the relation

$$\frac{d\sigma}{d\Omega} = 4\pi^4 \frac{k_f}{k_i} \left| T_{fi}^{\text{ex}} \right|^2$$

where \( k_i \) and \( k_f \) are initial and final wave vectors respectively and \( T_{fi}^{\text{ex}} \) is as given in equation (23) for \( 2^3\text{P} \) transitions. The total cross section is calculated using the formulae

$$\sigma = \int_{0}^{\pi} d\theta \int_{0}^{2\pi} d\phi \sin \theta d\theta d\phi$$

6. Results and Discussions

Distorted wave method (present model) have been applied to calculated the total and differential cross sections for the spin forbidden transitions

\( \text{e} + \text{He} (1^1S) \rightarrow \text{e} + \text{He} (2^3\text{P}) \)

at impact energies ranging from 40 to 200 eV. In presenting our results we will discuss the differential and integral cross sections separately

6.1 1^1S-2^3P transition

At 40 eV (figure 1) the present DWM calculations are compared with the experimental results of\(^{12}\) and theoretical calculations for CCC75\(^{50}\). Present calculations are in qualitative agreement in shape with both experimental measurements and theoretical calculations, but not in quantitative agreement. This discrepancy may be attributed to the fact that first order distorted wave methods do not give good results at lower incident energies. The present result has a peak at around 60° while other results have a peak at 40°.

At 50 eV (figure 2) the present results are compared with same theoretical results as for 40 eV and with the experimental results\(^{12}\). The present results are in best agreement with the experimental results of Trajmar et al.\(^{51}\). The close coupling results are not in good agreement with the experimental results at intermediate scattering angles (40°-120°). The present result shows a peak at 50°, experimental results\(^{50}\) have a peak at 40° while other results have a peak at around 45°.
At 80 eV (figure 3) the present results are compared with the experimental results of Yagishita et al. and theoretical calculations: R-matrix, CCC75 and FOMBT. The present results are in a close agreement with the experimental results of Yagishita et al. All the results have peaks at around 25°.

At 100 eV (figure 4) the present results are compared with experimental results and theoretical results; R-matrix, 11-state R-matrix and CCC75. Present results are in reasonably good agreement with experimental results as well as theoretical results. The present results are in best agreement with the experimental results of Trajmar et al. for scattering angles ≥110°. Both the present and other theoretical results have a peak at around 10°.

At 200 eV (figure 5) the present results are compared with experimental results of Yagishita et al. and theoretical results: 11-state and 7-state R-matrix, R-matrix, FOMBT, and CCC75. The present results are in qualitatively good agreement with other theoretical calculations and experimental results. Both the present results, experimental results and all theoretical calculations have a peak at around 10°.

In general the present DWM results for 1S-2P transition are in good agreement with most theoretical calculations and experimental results at all electron incident energies except at 40 eV. Also, the experimental and theoretical results have a peak that shifts towards the left (lower scattering angles) with the increase of incident electron energy. If we ignore the 40 eV results for 2P excitation, the present differential cross section results for 1S-2P transition are in good agreement with the corresponding theoretical and experimental results.

Figure 1. Differential cross section for 1S-2P excitation of helium by electron impact at 40eV. Theoretical results: — Present DWM, — — — CCC75. Experimental results: ■, ◊.

Figure 2. Same as figure 1 but for 50 eV. ● Experimental results of Trajmar et al., (1992).

Figure 3: Same as figure 1 but for 80 eV. Theoretical results: —— R-Matrix (Fon et al., 1979), —— FOMBT and ▼ Experimental results of Yagishita et al.,

Figure 4: Same as figure 1 but for 100 eV. Theoretical results: —— R-Matrix (Trajmar et al., 1992), —— 11-state R-matrix (Nakazaki et al., 1991). Experimental results: ● an ▼ Yagishita et al.
6.2 Integral cross Sections (1S-2P transition)

The present integral cross sections result (figure 6) for 1S-2P transition are compared with the experimental results of de Heer and theoretical results: CCC756, FOMBT7, R-matrix5). The present results show a close agreement with the R-matrix in the energy range of 40-80 eV but for energies ≥ 100 eV, the present results are higher than the experimental and other theoretical results.

7. Conclusions

If we ignore the 40 eV results for 2P excitation, the present differential cross section results for 1S-2P transition are in good agreement with the corresponding theoretical and experimental results. Since it is the differential cross section results which give a better test of any theoretical method because DCSs reflect more clearly the characteristics of the interacting potential and are more dependent on the target wave functions and approximation method used than the integral cross-sections, we can say that the present distorted wave method worked well for 1S-2P transition.

Looking at the performance of this method 1S-2P excitation in helium by electron impact, we recommend the following: 1) Further studies to be carried out to find the effect of including the terms which were neglected while evaluating the T-matrix elements, on the ground that these terms involved the overlap integral of bound and continuum wave functions; 2) The present method to be extended to study excitation of atoms to higher l-states e.g. D-state; 3) The present method to be extended in the study of excitation from an excited state e.g. metastable state (2S or 2P) to other excited states.

References