Elastic Scattering of Electrons by Helium Atoms in Born Approximation

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Abstract: Elastic scattering phenomena arising in electron-helium scattering are dominant processes. The determination of accurate elastic differential cross sections for electron-helium scattering has a considerable importance. An accurate calculation of the plane-wave first Born exchange amplitude of electrons elastic scattering by helium atoms is reported. The direct and exchange amplitudes are calculated analytically from the Hartree-Fock orbital wave functions by using a variational method. The forms of these wave functions are very suitable for analytical calculations and powerful to generalize to more complex atomic systems. The interaction potential is modelled by the static Coulomb interaction between the incident electron and the atomic system. The differential cross sections are calculated at intermediate energies taking into account the exchange effects. We have established in the high energies region, by neglecting the exchange effects, the analytical expressions of the total and momentum transport cross sections suitable for the calculation of the plasma transport properties. A very compact form of the Born amplitude has been proposed as a finite series of Gaussian functions, which represents a major tool in the calculations of differential cross sections of two-electron atomic systems. Numerical results are used to analyze the contribution of the exchange amplitude to the differential cross sections at intermediate and high energies. The differential cross sections are calculated for the energy range 30-400 eV. We find good agreement in high energy domain scattering with experimental results and other sophisticated calculations without using any adjustable parameter.

Keywords: Differential Cross Section, Elastic Scattering, Exchange Amplitude, Electron Transport, Helium

1. Introduction

Many research has been done in the recent past to study the elastic diffusion of electrons by atoms, ions, molecules or solids both theoretically and experimentally [1-9]. The differential cross section for elastic scattering of electrons by neutral atoms has been investigated by many authors [10-13]. Many theoretical models are employed to deal with the interaction potential during the diffusion process [14]. Y. Kucut et al. have presented a new potential set by deriving a formula for the depth of the real and imaginary parts of the optical potential for ⁶He elastic scattering at low energies [15].

In this paper, we present a theoretical approach to such processes based on a detailed study of the first Born approximation. We proceed to the accurate calculation of both the direct and exchange amplitudes. Our method applies essentially to the regions of intermediate and high energy. In the low energy domain, the first Born approximation will be inappropriate because many processes can occur as wave distortion, polarization of the target... The introduction of the exchange term in the evaluation of the differential cross section contributes to a significant improvement of the first Born approximation results. The choice of the shape of the radial wave functions is crucial for determining the exchange term. To describe the quantum process of the scattering of an incident particle given by a potential, we must first study the behavior over time of the wave packet which represents the quantum state of this particle. The characteristics of this wave packet are assumed to be known for the long and post-collision times when the particle has not yet been affected by the interaction potential. We know that the future evolution of the wave packet is obtained immediately if we apply the fundamental theorem of the superposition of stationary states. This is the reason why we are going to study the eigenvalue...
equation of the Hamiltonian of relative motion. We investigate directly on these stationary states and not on the wave packet. The eigenstates of the Hamiltonian of relative motion must verify the Schrodinger equation which the exact analytical resolution is only possible so far for simple atomic systems. For complex systems, several approximation methods exist, either numerical or analytical [16-18]. In this work, the radial functions of the Slater type with variational parameters are been used. This choice reduces drastically the difficulties linked to analytical calculations but also the time of numerical calculation. However, we lose precision in the results obtained with these radial functions. The polarization effects, which are energy-dependent, are not taken into account in this study. The potential due to the polarization can be neglected in the asymptotic region for diffusion since it is proportional to $r^{-4}$ in comparison to the Coulomb static potential which is in $r^{-1}$.

In low energy scattering, the projectile polarizes the target. The polarization potential must be introduced in the determination of the differential cross section. The first Born approximation can predict the correct scattered amplitude for small target which has relatively small atomic number $Z$. On the other hand, the calculation of the phase is inaccurate in the first Born approximation [19]. At low scattering energies, and especially near the scattering center, the interaction substantially changes the state of the projectile, so the approach by the plane wave function becomes inaccurate. It appears the phenomena of distortion of the wave functions. It is necessary in calculations, to take account these effects.

The independent model is adopted here by neglecting the correlation effects between the two atomic electrons. The model is expected to be less applicable for diffusion. The Hartree-Fock slater wave functions are widely used in various atomic processes due to their applicability in different calculations. Natalie M. Cann et al. have evaluated the differential cross sections by using the explicit correlated wave functions with $N=100$ number of terms [20]. In their work, they did not take into account the exchange amplitude for the elastic scattering from the helium ground state. Jorge L. S. Lino proposed a development of the Schwinger multichannel method for the elastic scattering of positrons by helium atom. The method is based on the first Born approximation with the inclusion of the polarization potential [21].

The present work is structured as followed. In section 2 of this paper, the Born direct and exchange amplitude are derived. The analytical expression of the total and momentum transport cross sections are established. Section 3 presents our results in different energy region for differential cross sections. We compare our results with some theoretical and experimental data for electron-helium scattering.

$$\phi(r) = 0.76838 \chi_1 + 0.22346 \chi_2 + 0.04082 \chi_3 - 0.0994 \chi_4 + 0.00230 \chi_5$$  

where $\chi_i$ are in the following form:

$$\chi_i = 2 \zeta^{3/2} \exp(-\zeta r)$$  

From index 1 to 5 the values of $\zeta$ are respectively: 1.41714, 2.37682, 4.39628, 6.52699, 7.94252. The radial function of equation (5) must be normalized by division by $\sqrt{N}$.

2. Born Amplitudes

The initial channel wave function which consists of the incident electron and the bound electrons, will be described as the product of two wave functions, one describing the incident electron and the other reflecting the dynamics of the bound electrons. The incident electron state will be given by the plane wave according to the first Born approximation. Bound states wave function of the ground state of the target is solution to two-system Schrödinger equation. The interaction potential between the electron and the atomic system is the static Coulomb potential averaged over the target state $\psi_0(r_1, r_2)$

$$V(r) = \left[\psi_0(r_1, r_2) \left(-\frac{Z}{r_0} + \frac{1}{r_{01}} + \frac{1}{r_{02}}\right)\psi_0(r_1, r_2)\right]  

$$

where $r_{ij} = |r_i - r_j|$. The vector positions of the free and the two bound electrons are respectively $r_0$, $r_1$ and $r_2$. Due to the normalization of the atomic wave functions and the indistinguishable of the atomic electrons, the integration with respect to $r_1, r_2$ gives [6]

$$V(r) = -\frac{Z}{r} + \int \frac{\rho(r')}{|r - r'|} \, dr'$$  

The total electron density of the two-electron system is:

$$\rho(r_2) = 2 \int [\psi_0(r_1, r_2)]^2 \, dr_2$$

For helium and the two-electron systems, the density $\rho$ is exactly evaluated by using both Hartree-Fock and Hylleraas types wave functions from reference [22]. $V(r)$ can be seen as the potential of an electron in the static field of a helium atom in ist’s state $\psi_0$. It can be really evaluated by using the explicit form of Hartree wave function $\psi_0(r_1, r_2) = \phi(r_1)\phi(r_2)$. In the Hartree Approximation, one assumes that the eigen-states of the total Hamiltonian can be written as a product of single particle states. The variational approximation is then used to derive an equation for these single-particle states. The atomic orbital function $\phi(r)$ in the following form:

$$\phi(r) = A \exp(-ar) + B \exp(-br)$$  

For the helium atom [23], the constants are $A = 2.60505, B = 2.08144, \alpha = 1.41, \beta = 2.61$. The analytical function of helium and some atoms wave functions are established by Carla Roetti and Enrico Clementi [24]. The helium radial function from this reference is given by:

$$N = 8 \sum_{k=1}^{5} \sum_{l=1}^{5} C_l C_j \frac{(\zeta_i \zeta_j)^{3/2}}{(r_i r_j)^{3/2}}$$

$C_k$ are coefficients of $\chi_k$ in equation (5). We have written python code to deal with the variational method, generalized to atoms and ions with two electrons. The results obtained are recorded in table 1. We rewrite this function in a compact way
for convenient usage as:

\[ \phi(r) = \sum_{i=1}^{N} C_i \exp(-c_i r) \]  

(8)

With this notation, we calculate the function \( V(r) \) as:

\[ V(r) = -2 \sum_{i=1}^{N} \frac{a_i}{a_i^2} (2 + a_i r) e^{-a_i r} \]  

(9)

\( V(r) \) represents the average electrostatic interaction of the incident electron with the set of atomic electrons. Consider the more ready question; we find the sum of the mean values of the quantity \([r - r_i]^{-1}\). It can be seen as a screening potential. Hence, to the first Born approximation the elastic scattering amplitude is defined as:

\[ f_B = -\frac{1}{2\pi} \int e^{i q \cdot r} V(r) \, dr \]  

(10)

where \( q = k_1 - k_2 \). Momentum vectors of incident and scattered electron are respectively \( k_1 \) and \( k_2 \). Let us remember that we assume the momentum conservation \( k_1 = k_2 = k \). Equation (10) is nothing but the Fourier transform of the potential \( V(r) \). If \( \theta \) is the angle between the two momentum vectors it follows

\[ q = 2 k \sin \frac{\theta}{2} \]  

(11)

We have implicitly chosen the polar axis in the direction of the incident electron momentum vector \( k_1 \). Using the Bethe integral

\[ \int e^{i q \cdot r} r^{-a} \, dr = \frac{4\pi}{q^2 + a^2} \]  

(12)

we perform calculation of the integral in equation (10) as

\[ f_B = \frac{1}{2\pi} \sum_{i=1}^{N} \frac{a_i}{a_i^2} \int \frac{1}{q^2 + a_i^2 + (q + a_i)^2} \]  

(13)

In general, it can be shown that the limit of the first Born amplitude is

\[ f_B = f_0 = 16 \sum_{i=1}^{N} \frac{a_i}{a_i^2} \neq 0 \]  

(14)

The first Born amplitude is a monotonically decreasing function of the transfer momentum as \( q \to +\infty \). The form of the amplitude \( f_B \) of equation (13) may well be replaced by the Gaussian type function as

\[ f_B = \sum_{i=0}^{N} B_i \exp(-b_i q^2) \]  

(15)

with \( b_0 = 0 \) and \( B_0 = f_0 \) given by equation (14). The other parameters are obtained by making a fit of the function \( f_B(q) \) of the equation (13) using programming languages such as Python, Matlab, Gnuplot etc. This form is more suitable for evaluating the differential cross section and the total and transport sections. If we want to make corrections to the first approximation of Born, we must add in the Born development the higher order terms in our calculations. The calculations of these higher order terms will be very cumbersome. Instead, we will just take into account only the exchange term. The first Born exchange amplitude is given in the case of electron-helium elastic scattering by \( g_B = -Z g_1 + g_2 + g_3 \). The different terms of the exchange amplitude are in the following form

\[ g_1 = -\frac{1}{2\pi} \langle \phi(r) e^{i k_2 r_1} \rangle \frac{1}{r_1} \langle e^{i k_1 r} \phi(r_1) \rangle \]  

(16)

\[ g_2 = -\frac{1}{2\pi} \langle \phi(r) e^{i k_2 r_1} \rangle \frac{1}{r_1} \langle e^{i k_1 r} \phi(r_1) \rangle \]  

(17)

\[ g_3 = -\frac{1}{2\pi} \langle \phi(r_2) \phi(r) e^{i k_2 r_1} \rangle \frac{1}{r_1} \langle e^{i k_1 r} \phi(r_1) \rangle \]  

(18)

The evaluation of these three terms of the exchange amplitude is more complicated. After straightforward calculations we find

\[ g_1 = -4 \sum_{i=1}^{N} \frac{a_i b_i c_i}{[k^2 + a_i^2] [k^2 + b_i^2]} \]  

(19)

\[ g_2 = -\sum_{i=1}^{N} b_i^2 a_i c_i \langle 0 | k, a_i, b_i \rangle \]  

(20)

\( c_i, a_i \) and \( b_i \) are respectively elements of

\[ cc = [A^2, B^2, A B, A B] \]  

(21)

\[ aa = [\alpha, \beta, \alpha, \beta] \]  

(22)

\[ bb = [\alpha, \beta, \beta, \alpha] \]  

(23)

The function \( I_{00}(k, a_i, b_i) \) is a three-denominator Lewis integrals

\[ I_{00}(k, a_i, b) = \int \frac{d\rho}{\rho^2 ([p - k_i]^2 + a^2) ([p - k_j]^2 + b^2)} \]  

(24)

The third term \( g_3 \) is split into two factors as \( g_3 = g_{31} \cdot g_{32} \)

\[ g_{31} = \frac{\alpha A}{(k^2 + a^2)^2} + \frac{\beta B}{(k^2 + b^2)^2} \]  

(25)

\[ g_{32} = -8 \sum_{i=1}^{N} c_i a_i \langle 0 | U(\alpha) + B U(\beta) \rangle \]  

(26)

The auxiliary function \( U(x) \) has the following form

\[ U(x) = \frac{1}{k^2 + a^2} - \frac{1}{(k^2 + a^2)^2} - \frac{a_i (a_i + x)}{[k^2 + (a_i + x)^2]^2} \]  

(27)

Here the coefficients are

\[ cc = [A^2, B^2, 2 A B] \]  

(28)

\[ aa = [2, \alpha, \beta, \alpha + \beta] \]  

(29)

The auxiliary function \( I_{00}(X, Y) \) is analytically evaluated by R. R. Lewis, Jr [25]

\[ I_{00}(X, Y) = \frac{1}{\sqrt{X - Y^2}} \log \frac{Y + j \sqrt{X - Y^2}}{Y - j \sqrt{X - Y^2}} \]  

(30)

where \( X = X(a_i, a_2) \), \( Y = Y(a_i, a_2) \). The quantity \( X - Y^2 \) is always positive definite for real values of the parameters and variables.

\[ X = [a^2 + (a_1 + a_2)^2] (a_1^2 + k^2) (a_2^2 + k^2) \]  

(31)

\[ Y = a_1 (a_1^2 + k^2) + a_2 (a_2^2 + k^2) \]  

(32)
The second derivative of $I_{00}(X,Y)$ in equation (17) can be written as

$$\sigma = \frac{d^2I_{00}(k, a_1, a_2)}{d\theta d\phi} = X_{11} I_{10} + Y_{11} I_{01} + X_{10} \left[ X_{01} I_{20} + Y_{01} I_{11} \right] + Y_{10} \left[ X_{01} I_{11} + Y_{01} I_{02} \right]$$

The $I_{mn}$ are the partial derivatives with respect to $(X_0 \equiv X, Y_0 \equiv Y)$, and $X_{mn}, Y_{mn}$ are the partial derivatives with respect to $(a_1, a_2)$ as [26]:

$$I_{mn} = \frac{\partial^{m+n} I_{00}(X,Y)}{\partial X^m \partial Y^n}$$

$$X_{mn} = \frac{\partial^{m+n} X_{00}}{\partial a_1^m \partial a_2^n}$$

The n-th derivatives of $I_{00}(X,Y)$ has a lower limit when $T$ tends to zero. This lower limit is equal to $2Y$. The condition of zero momentum transfer corresponds to the zero scattering angle ($T = 0$) or to a zero energy ($E = 0$) scattering.

The elastic differential cross section $\sigma(\theta)$ in atomic units $\alpha_0^2/\pi r$ is given by [27]

$$\sigma(\theta) = \sum_{i=1}^{2} \sum_{j=1}^{3} A_{ij} \left[ \frac{a_i^2}{(s + a_i^2)(s + a_j^2)} \right]^2 + \frac{a_i^2 a_j^2}{(s + a_i^2)(s + a_j^2)} + \frac{a_i^2 a_j^2}{(s + a_i^2)(s + a_j^2)}$$

with $A_{ij} = 64 A_i A_j/(\alpha_0 a_i)^3$. With this last form of the differential cross section expressed according to the square of the modulus of the transfer moment, one can give the analytical expressions of the two quantities $\sigma_T$ and $\sigma_M$ as:

$$\sigma_T(k) = \frac{\pi}{k^2} \sum_{i=1}^{2} \sum_{j=1}^{3} A_{ij} \left[ \alpha_{ij}(2k^2) - \alpha_{ij}(0) \right]$$

$$\sigma_M(k) = \frac{\pi}{2k^2} \sum_{i=1}^{2} \sum_{j=1}^{3} A_{ij} \left[ \beta_{ij}(2k^2) - \beta_{ij}(0) \right]$$

In the previous double summation, we will pay attention to the case where the index $i = j$, which gives a different result for $i \neq j$.

$$[\alpha_{ij}(s)] = M \begin{bmatrix} 1 \\ a_i^2 \\ a_j^2 \end{bmatrix}$$

$$[\beta_{ij}(s)] = M \begin{bmatrix} 1 \\ a_i^2 \\ a_j^2 \end{bmatrix}$$

The matrix elements $M_{nk}$ are defined as:

$$M_{11} = \frac{1}{a_i^2 - a_j^2} \log\left(\frac{s + a_i^2}{s + a_j^2}\right)$$

$$M_{12} = \frac{1}{a_i^2 - a_j^2} \log\left(\frac{s + a_i^2}{s + a_j^2}\right)$$

$$M_{13} = \frac{1}{a_i^2 - a_j^2} \log\left(\frac{s + a_i^2}{s + a_j^2}\right)$$

$$M_{14} = \frac{2 \log\left(\frac{s + a_i^2}{s + a_j^2}\right)}{(a_i^2 - a_j^2)^3} \left( \frac{a_i^2 a_j^2}{(a_i^2 - a_j^2)} \right)$$

In the case of $i \neq j$ we have

$$M_{21} = \frac{1}{a_i^2 - a_j^2} \left[ a_i^2 \log(s + a_j^2) - a_j^2 \log(s + a_i^2) \right]$$

$$M_{22} = \frac{a_i^2}{a_i^2 - a_j^2} \log\left(\frac{s + a_i^2}{s + a_j^2}\right)$$

$$M_{23} = \frac{a_i^2}{a_i^2 - a_j^2} \log\left(\frac{s + a_i^2}{s + a_j^2}\right) - \frac{a_i^2}{a_i^2 - a_j^2} \log\left(\frac{s + a_i^2}{s + a_j^2}\right)$$
The total momentum transport cross section is necessary for the calculation of energy averaged momentum transport cross section. Plasma transport properties depend strongly on these cross sections determination.

3. Results

In table 1, we have given the variational parameters and the corresponding energy for some systems with two electrons. These parameters fully determine the normalized radial wave function. Besides the normalization condition, the radial wave function also satisfies the finitude condition. We can see that these high energy orbitals are further from the nucleus than for low atomic number ions. The variational parameters increase with the atomic number, so that it will be easier to tear off an electron for high Z ions than for low atomic number ions. The 1s orbital is further from the nucleus than for low Z ions. Hence their relatively weak bond to the nucleus.

Table 1. Variational atomic wave functions parameters of two-electrons systems and their corresponding ground state energies.

| $\theta$ | Direct | Exchange | Ref. [28] | Shyn [29] |
|----------|--------|----------|-----------|-----------|
| 6        | 0.157287 | 0.182852 | 0.1381989 | 0.275 |
| 12       | 0.118649 | 0.137041 | 0.1373959 | 0.173 |
| 24       | 0.050271 | 0.056707 | 0.0575412 | 0.101 |
| 25       | 0.046481 | 0.052302 | 0.0531684 | 0.061 |
| 30       | 0.031429 | 0.034888 | 0.0358690 | 0.035 |
| 36       | 0.019931 | 0.021722 | 0.0227400 | 0.021 |
| 48       | 0.008729 | 0.009120 | 0.0100289 | 0.0092 |
| 60       | 0.004343 | 0.004324 | 0.0050576 | 0.0047 |
| 72       | 0.002428 | 0.002293 | 0.0028712 | 0.0024 |
| 84       | 0.001499 | 0.001339 | 0.0017979 | 0.0015 |
| 96       | 0.001006 | 0.000850 | 0.0012215 | 0.0010 |
| 108      | 0.000726 | 0.000580 | 0.0008894 | 0.00070 |
| 120      | 0.000557 | 0.000422 | 0.0006878 | 0.00055 |
| 132      | 0.000452 | 0.000327 | 0.0005614 | 0.00054 |
| 144      | 0.000387 | 0.000268 | 0.0004813 | 0.00047 |
| 156      | 0.000346 | 0.000233 | 0.0004322 | 0.00047 |

At low scattering angles, the correction due to the exchange effect provides an improvement in the determination of the differential cross section. According to the data in table 1, from angles greater than 84 degrees, the exchange term brings no improvement to the first Born approximation. Our calculations are in good agreement with the relativistic results of the reference [28]. Nevertheless, the two theories had difficulty in correctly estimating the differential cross-section at low angles diffusion. In this area, many physical phenomena can occur alongside diffusion such as absorption, excitation followed by de-excitation.

We represent in the figure 1, the variation of the radial distribution of the helium atom in the ground state. Our calculations give the same results as those of reference [23]. The probability of finding an electron in the 1s orbital for this configuration is approximately $r = 0.564103$, with an approximate value equal to 0.866448. We note a slight difference between our results and those calculated by Roetti and Clementi [24]. However, the general appearance of the different density curves are similar. In view of the orbital energy found at -0.91795 u.a by these authors, we can estimate that our results are quite correct.

Figure 2. Differential cross section for 50 eV. Star symbols are the present first Born with exchange. Full circle curve is from Shyn [29], open circle are from D. F. Register et al. [1] and full triangle are from M. J. Brunger et al. [8]. Solid line is from relativist calculations of A. Jablonski et al. [28].

Figure 3 shows our differential cross sections at 100 eV compared with the relativist calculations of Ref. [28] and experimental results of Ref. [29]. As observed, our results exhibit reasonable agreement with [28] study. In comparison with the experimental data, the two theories differential cross sections are too small for forward scattering electrons.
Nevertheless, for high impact energies as in figures 4 and 5 we observe good agreement with experimental differential cross section.

Figure 3. Differential cross section for 100 eV. Star symbols curve is the present first Born approximation with exchange, full circle curve is from Shyn [29] and solid line is from relativist calculations of A. Jablonski et al. [28].

Figure 4. Differential cross section for 200 eV. Star symbols curve is the present first Born approximation with exchange, full circle curve is from Shyn [29] and solid line is from relativist calculations of A. Jablonski et al. [28].

Figure 5. Differential cross section for 400 eV. Star symbols curve is the present first Born approximation with exchange, full circle curve is from Shyn [29] and solid line is from relativist calculations of A. Jablonski et al. [28].

Figure 6 shows the elastic electron helium scattering at energies 30, 50, 80, 100 and 200 eV. We note in this graph a progressive decrease of the maximum with the increase of the energy of the incident electron. A completely predictable result due to the dependence of the amplitude of Born in \( k^{-2} \). It is interesting to note that in the small angle region, all curves converge approximately to the same value. This convergence is due to the \((1 - \cos \theta)\) factor that multiply the energy \( k^{-2} \) in the momentum expression. We recall that all differential cross sections are multiplied by \( \sin \theta \) for better clarity to the representation. At the upper limit of the scattering angle, the differential cross section naturally converges to zero, due to the multiplication by the sine function.

4. Conclusion

Calculated differential cross sections for electron elastic scattering by helium atom are presented. We also presented the atomic variational parameters and plotted the density variation of the ground state. Differential cross section have been calculated in the first Born approximation from the variational Hartree-Fock wave functions for the helium atom. These calculations provide an extensive set of elastic differential cross sections for electron-helium collisions. Exchange amplitude is explicitly calculated and introduced to the first Born approximation. Detailed comparisons between the first Born approximation with exchange and the relativistic calculations of Jablonski et al. were presented. Numerical calculations have been performed in energy range from 30 eV to 400 eV and for all scattering angles 0° - 180°. The comparisons show that, at low energies electron impact, we note a reasonable agreement. But consideration of both distortion and polarization effects in the calculations at low energies collision should significantly improve this agreement. At high energies, the first Born approximation provide an accurate differential cross sections. It should be noted that differential cross sections and their absolute values are very important in our quantum mechanical description of electron-atom interaction. We have provided a consistent set of analytical expressions suitable to machine code implementation.

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