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SOME MODIFICATIONS IN THE GLAUBER THEORY FOR ELECTRON-ATOM AND ELECTRON-MOLECULE SCATTERING

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Abstract. For the application of Glauber theory to electron-complex atom and electron-molecule scattering, the system of core electrons in an atom is replaced by the appropriate central charge density. Cosequently, the $(3z + 2)$-dimensional integral in the scattering of electrons by Z-electron atoms is reduced to one-dimensional integral. The Glauber model in this simplified form is applied to the elastic scattering of electrons by He atom. Total cross-sections for the elastic and inelastic e-Li scattering have also been calculated by the simplified Glauber Model. In the light of the above-mentioned approximations, the angular distribution of electrons distribution of electrons elastically scattered from H_2 molecule at different energies have also been computed.

1. Introduction

The Glauber approximation [1] has been successfully applied to study the scattering of charged particles by simple atoms [2-5, 22-24]. But the straightforward application of the theory to the scattering of electrons from complex atoms makes the evaluation of a cross-section rather complicated as the multiplicity of quadrature increases with the increase in number of the target electrons.

To keep the calculations manageable, several modifications in the original treatment of calculating scattering amplitudes in the case of complex atoms have been made [6, 7].

A number of works [2-5] have given procedures for reducing the Glauber amplitude to one- dimensional integral for the case of complex atoms. Also some authors [6, 7] have made calculations by using frozen core Glauber approximation.

The Glauber theory in the frozen core approximation [6] has been applied to e-Li, e-Na and e-K collisions. In these calculations the integrals have been evaluated following a procedure similar to that of Franco [2] and Walters [6]. This simplifies the problem to one quite similar to the scattering of electrons by hydrogen atoms.

Here we are presenting a method which is based upon the assumptions of Glauber [1] in which the system of core electrons has been replaced by appropriate central charge density which remains passive throughout the scattering processes. By doing so, the problem of the scattering of electrons by complex atoms has been considerably simplified without neglecting any significant features in the scattering phenomena. The $(3z+2)$-dimensional integral for the scattering amplitude for z-electron atoms has been simplified to one-dimensional integral. The validity of this method has been tested by its application to electron-helium atom elastic scattering.

A more accurate treatment with the Glauber theory may be obtained by considering the effect of all the target electrons [1, 7]. In this paper, we have also discussed the e-Li elastic and inelastic scattering where the effects of the core electrons have also been taken into account. Based upon this theory, a procedure has been developed to compute intensities of e-H_2 scattering in terms of e-H scattering amplitude.

2. e-He Elastic Scattering

In order to determine the scattering amplitude for complex atoms, the single-particle wave function is replaced by the many-particle wave function for a z-electron atom and the single-particle phase shift function by the phase shift suffered by the incident particle in passing through a configuration of target particles, i. e.

$$\psi(\mathbf{r}) \to \psi(\mathbf{r}_1, \ldots, \mathbf{r}_z) \tag{1}$$

$$\chi(\mathbf{b}-\mathbf{s}) \to \sum_{l=1}^{A} \chi_l(\mathbf{b}-\mathbf{s}_l) \tag{2}$$

where A is the number of particles. Let b denotes the impact-parameter vector relative to the origin. If r denotes the position vector of the target electron, s is the projection of r onto the plane containing b. And the incident particle imparts a momentum hq to the target. The symbols in the following text have their usual meaning [1-6].

If we consider a neutral atom with z-electrons and z-protons, the profile function for this case is given by

$$T(\mathbf{b}_1, \mathbf{s}_1, \ldots, \mathbf{s}_A) = 1 - \prod_{j=1}^{z} e^{2in \ln\left(\frac{|\mathbf{b}-\mathbf{s}_j|}{\mathbf{b}}\right)}. \tag{3}$$

The Glauber scattering amplitude $F_{fi}(q)$ for collision of an electron with a many-electron atom [2, 6] can be expressed as

$$F_{fi}(q) = \frac{ik}{2\pi} \int e^{iqb} db^2 \Bigg[\partial_{fi} - \int \psi_f^*(\mathbf{r}_1, \ldots, \mathbf{r}_z) \prod_{j=1}^{z} e^{2in \ln\left(\frac{|\mathbf{b}-\mathbf{s}_j|}{\mathbf{b}}\right)} \psi_i(\mathbf{r}_1, \ldots, \mathbf{r}_z) d\mathbf{r}_1 \cdots d\mathbf{r}_z \Bigg] . \quad (4)$$

The above expression for the scattering amplitude contains multi-dimensional integrals whose evaluation is difficult.

To apply the above expression to the case of multi-electron atoms, certain simplifying assumptions regarding the structure of the target atom would have to be made.

As a first approximation, we assume that the atomic ground state wave function product may be written as

$$\psi_i^*(\mathbf{r}_1, \ldots, \mathbf{r}_z)\psi_i(\mathbf{r}_1, \ldots, \mathbf{r}_z) = \rho_1(\mathbf{r}_1) \cdots \rho_z(\mathbf{r}_z) = \prod_{j=1}^{z} \rho_j(\mathbf{r}_j) \quad (5)$$

where $\rho_j(\mathbf{r}_j)$ is the normalized density for the j-th particle. Therefore, average particle density is given by

$$\rho(\mathbf{r}) = \frac{1}{z} \sum_{j=1}^{z} \rho_j(\mathbf{r}_j) . \quad (6)$$

Since

$$e^{2in \ln\left(\frac{|\mathbf{b}-\mathbf{s}_j|}{\mathbf{b}}\right)} = 1 - T(|\mathbf{b} - \mathbf{s}_j|) ,$$

we obtain

$$\prod_{j=1}^{z} \int e^{2in \ln\left(\frac{|\mathbf{b}-\mathbf{s}_j|}{\mathbf{b}}\right)} \rho_j(\mathbf{r}_j) d\mathbf{r}_j = \prod_{j=1}^{z} \left[1 - \int \rho_j(\mathbf{r}_j) T(|\mathbf{b} - \mathbf{s}_j|) d\mathbf{r}_j \right] . \quad (7)$$

Therefore, taking logarithm on both sides of Eq. (7) and neglecting the square and higher-order terms on the right hand side (on the assumption that the phase shifts are small in this approximation), we get from Eqs (4) and (6) the elastic scattering amplitude as

$$F_{ii}(\mathbf{q}) = \frac{ik}{2\pi} \int e^{i\mathbf{q}\mathbf{b}} \left[1 - e^{-z \int \rho(\mathbf{r}) T(\mathbf{b}, \mathbf{r}) d\mathbf{r}} \right] d^2 b = ik \int J_0(q\mathbf{b}) \left[1 - e^{-z \int \rho(\mathbf{r}) T(\mathbf{b}, \mathbf{r}) d\mathbf{r}} \right] b db . \quad (8)$$

The differential cross-section for the elastic scattering is then obtained by means of the relation

$$\frac{d\sigma(q)}{d\Omega} = |F_{ii}(q)|^2 . \quad (9)$$

In the calculations we use the helium ground state wave functions given by Hylleraas [8] and Hartree-Fock [9].

3. e-Li Elastic Scattering

The treatment of a many-body target is an extension of a single-bound particle. In the formulation, we have only to replace the single-particle wave function by the many particle wave function. To be more precise, in the case of lithium atom (which is a 3-electron system), the wave function may be written as

$$\psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = U_1(\mathbf{r}_1)U_2(\mathbf{r}_2)U_3(\mathbf{r}_3) . \qquad (10)$$

This corresponds to a situation in which the interaction between the particles is neglected and the particles are distinguished by means of their positions. Therefore, the density for a three-particle system can be written as

$$\rho(\mathbf{r}) = |U_1(\mathbf{r}_1)|^2 + |U_2(\mathbf{r}_2)|^2 + |U_3(\mathbf{r}_3)|^2 . \qquad (11)$$

The elastic amplitude $F_{ii}(q)$ for e-Li scattering may be calculated from the equation

$$F_{ii}(\mathbf{q}) = ik \int J_0(qb) \left[1 - e^{-z\int \rho(\mathbf{r})T(\mathbf{b},\mathbf{r})d\mathbf{r}}\right] bdb . \qquad (12)$$

4. e-Li Inelastic Scattering

As long as the energy difference between the initial state i and the final state f is small compared to the incident energy, the scattering amplitude is given by

$$F_{fi}(\mathbf{k} - \mathbf{k}') = \frac{ik}{2\pi} \int e^{i\mathbf{q}\mathbf{b}} d^2\mathbf{b} \langle f|T(\mathbf{b}, \mathbf{s}_1, \ldots, \mathbf{s}_A)|i\rangle \qquad (13)$$

where the profile function

$$T(\mathbf{b}, \mathbf{s}_1, \ldots, \mathbf{s}_A) = 1 - e^{i\chi(\mathbf{b},\mathbf{s}_1,\ldots,\mathbf{s}_A)}$$

$$e^{i\chi(\mathbf{b},\mathbf{s}_1,\ldots,\mathbf{s}_A)} = \prod_{j=1}^{z} e^{2in_g \ln\left(\frac{|\mathbf{b}-\mathbf{s}_j|}{\mathbf{b}}\right)}$$

and

$$\langle f|e^{i\chi}|i\rangle = \int \psi_f^*(\mathbf{r}_1, \ldots, \mathbf{r}_z) \prod_{j=1}^{z} e^{2in_g \ln\left(\frac{|\mathbf{b}-\mathbf{s}_j|}{\mathbf{b}}\right)} \psi_i(\mathbf{r}_1, \ldots, \mathbf{r}_z) d\mathbf{r}_1 \cdots d\mathbf{r}_z . \qquad (14)$$

In this model, a single-electron (i. e. the outermost electron) is assumed to participate in a transition. We separate its wave function from that of the remaining electrons by writing

$$\psi_i(\mathbf{r}_1, \ldots, \mathbf{r}_z) = U_i(\mathbf{r}_1)\phi_0(\mathbf{r}_2, \ldots, \mathbf{r}_z)$$

and

$$\psi_f(\mathbf{r}_1,\ldots,\mathbf{r}_z) = U_f(\mathbf{r}_1)\phi_0(\mathbf{r}_2,\ldots,\mathbf{r}_z)\,. \tag{15}$$

The remaining electrons, e g. those in closed shells, play no active role in the transition. Therefore,

$$\begin{aligned}\langle f|e^{i\chi}|i\rangle = &\int U_f^*(\mathbf{r}_1)e^{2in_g \ln\left(\frac{|\mathbf{b}-\mathbf{s}_j|}{b}\right)}U_i(\mathbf{r}_1)d\mathbf{r}_1 \\ &\times \int \phi_0^*(\mathbf{r}_2,\ldots,\mathbf{r}_z)\prod_{j=2}^{z} e^{2in_g \ln\left(\frac{|\mathbf{b}-\mathbf{s}_j|}{b}\right)}\phi_0(\mathbf{r}_2,\ldots,\mathbf{r}_z)d\mathbf{r}_2\cdots d\mathbf{r}_z\,.\end{aligned} \tag{16}$$

The final expression for inelastic scattering is

$$\begin{aligned}F_{fi}(\mathbf{q}) = &\frac{ik}{2\pi}\int e^{i\mathbf{q}\mathbf{b}}\Big[\partial_{fi} - \int U_f^*(\mathbf{r}_1)e^{2in_g \ln\left(\frac{|\mathbf{b}-\mathbf{s}_j|}{b}\right)}U_i(\mathbf{r}_1)d\mathbf{r}_1 \\ &\times e^{-(z-1)\int \rho(\mathbf{r})T(\mathbf{b},\mathbf{r})dr}\Big]d^2b\end{aligned} \tag{17}$$

where $U_i(\mathbf{r}_1)$ and $U_f^*(\mathbf{r}_1)$ are the ground state and the excited state wave functions of the valence electrons.

Since the interaction between the incident electron and the target atom has been assumed to be spin-independent and the exchange effect has not been taken into account, the spin functions of the initial and final atomic states remain the same. This fact has been assumed beforehand in writing down the expression (17) which is given in detail by Walters [6]. For the excitation from state i to state f the differential cross-section is

$$\frac{d\sigma_{fi}}{d\Omega} = \frac{k_f}{k_i}|F_{fi}(q)|^2 \tag{18}$$

and the total cross-section is

$$\sigma_{fi} = \int \frac{k_f}{k_i}|F_{fi}(q)|^2 \sin\theta d\theta d\phi \tag{19}$$

where θ, ϕ are the angles in spherical co-ordinates specifying the direction of k_f relative to k_i.

For testing the validity of this theory we have calculated the total inelastic cross-section of e-Li, 2s→2p resonance transition. In the case of e-Li inelastic scattering the core part of expression (17) is similar to the helium atom. The cross-section for the direct excitation of the 2s→2p transition of lithium can be calculated from the knowledge of the scattering amplitude for all the three transitions 2s→2p, 2s→2p+1 and 2s→2p−1. For excitation to the 2p state, the scattering amplitude vanishes identically. This is the consequence of the Glauber theory where q is perpendicular to k_i; the direction of k_i being the axis of quantization for atomic wave functions. The 2s→2p+1 amplitudes are identical but differ by a phasefactor $e^{i\phi}$.

5. e-H_2 Scattering

Molecular hydrogen H_2 is one of the most abundant trace gases in the atmosphere. In view of the importance of such gases, we present in this paper a theoretical model in the light of Glauber multiple scattering theory [1] for e-H_2 molecule scattering. The electron diffraction is one of the most powerful methods for investigating molecular structure and fortunately, the Glauber multiple scattering theory is also a diffraction approximation. Based upon this fact, a procedure has been developed for calculating the intensities of e-H_2 scattering in terms of e-H scattering within the framework of Glauber multiple scattering [2].

In the Glauber multiple scattering theory the collision of an electron with a hydrogen molecule is similar to the case of collisions between a single particle and deutron [1]. Franco [2] has studied the e-H elastic scattering in which the interactions of the incident particle with both the target electron and the target proton are treated explicitly. Moreover, the target proton has been considered to be infinitely heavy and the exchange scattering is neglected which is generally very small at high energies above $\approx$100 eV for e-H scattering.

Let the origin of co-ordinates be placed at the proton, and let b denote the impact parameter vector relative to the origin and r denote the position vector of the target electron.

The complete scattering amplitude [2, 6] is given by

$$F_{fi}(\mathbf{q}) = \frac{ik}{2\pi}\int \psi_f^*(\mathbf{r})T(\mathbf{b},\mathbf{r})\psi_i(\mathbf{r})e^{i\mathbf{q}\mathbf{b}}d^2\mathbf{b}d\mathbf{r}\,. \tag{20}$$

Here $T(\mathbf{b},\mathbf{r})$ is the profile function, ψ_i is the initial state wave function and ψ_f is the final state wave function and the incident particle imparts a momentum hq to the target. The two-dimensional integration over the impact parameter vector is over a plane perpendicular to the direction of the incident beam, the vector q is perpendicular to k, and

$$T(\mathbf{b},\mathbf{r}) = 1 - e^{i\chi(\mathbf{b},\mathbf{s})}$$

where $\chi(\mathbf{b},\mathbf{s})$ is the phase shift corresponding to the impact parameter $\mathbf{b}$.

For elastic scattering of electrons by the hydrogen in its ground state [2]

$$\psi_i = \psi_f = (\pi a_0^3)^{-\frac{1}{2}}e^{-\frac{r}{a_0}}$$

where a_0 is the first Bohr radius. The scattering amplitude for e-H_2 scattering in terms of Glauber e-H scattering can be written as

$$\begin{aligned} f_{\text{e-H}_2}(\mathbf{q}) =& f_{\text{eH}}(q^2)S\left(\frac{\mathbf{q}}{2}\right) + f_{\text{e-H}}(q^2)S\left(\frac{\mathbf{q}}{2}\right) \\ &+ \left(\frac{i}{2\pi k}\right)\int d^2q'\, f_{\text{eH}}\left(\left|\mathbf{q}' - \frac{\mathbf{q}}{2}\right|\right) f_{\text{eH}}\left(\left|\mathbf{q}' - \frac{\mathbf{q}'}{2}\right|\right) S(\mathbf{q}) \end{aligned} \tag{21}$$

with

$$S(\mathbf{q}) = \int d^3r\, e^{i\mathbf{q}\mathbf{r}}|\phi_0(\mathbf{r})|^2\,.$$

In Eq. (21), the effects of single and double scattering are explicitly separated. The first two terms are the amplitudes for single scattering by each of the two target particles. The third term contributes only for molecular configurations in which the incident particle can pass through the two regions of interaction surrounding the two electrons.

Hence the differential cross-section for e-H scattering can be computed in terms of Eq. (21).

6. Results and Discussion

6.1. e-He Scattering

The present formulations have been applied to e-He elastic scattering for incident electron energies 100 and 500 eV. The results are presented in Figs 1 and 2 and are compared with that obtained from the Born approximation. The present calculations using Hartree-Fock wave functions are in fair accord with calculations of Franco and Thomas [3] and Thomas and Chan [5] and also with the available experimental data [13, 14, 16]. This is much better at low momentum transfers and at higher energies and it is evolving from the Glauber theory also which is particularly applicable for small angle scattering at high impact energies. Further, we find that the results obtained by using the Hartree-Fock wave function are superior to those obtained by using the Hylleraas wave function, especially at small scattering angles. It appears that the difference between the cross-sections at high energies using the Hartree-Fock and Hylleraas wave functions shows a decreasing trend as we go to larger scattering angles. It is probably due to the fact that the wide angle scattering is dominated by the interaction with the nucleus of the helium atom and is independent of the detailed shape of the electron cloud.

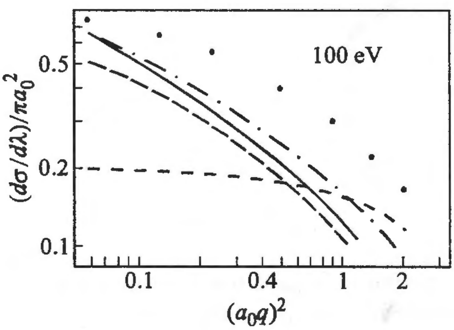

Fig. 1.

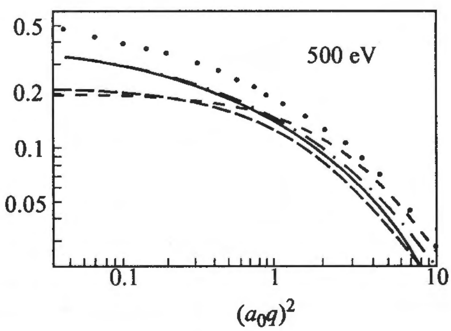

Fig. 2.

6.2. e-Li Scattering

The formalism for the inelastic scattering Glauber model has been applied to the case of e-Li scattering. The results of calculations for the total cross-sections for electron-lithium elastic scattering are compared with those of Born approximation and also with the experimental data of Perel et al [10] in Fig. 3. At the low energies, our results are distinctly different from those of the Born approximation, but are close to the experimental data. Though we have ignored the exchange effects, even then our calculations are in better agreement with the experimental data in the low-energy range. It might be mentioned that the measurements are available only up to energies ≈ 10 eV. The present results are also consistent with that of Walters [6] who used the frozen core approximation for such calculations. The results of the calculation for the total cross-section of lithium 2s→2p resonance transition is shown in Fig. 4 and is compared with a number of available theoretical calculations and the experimental data of Hughes and Hendrickson [11]. The present results are in good agreement with the experiment and also with the available calculated data. The resonance peak based on our curve and the experimental curve tend to merge with each other.

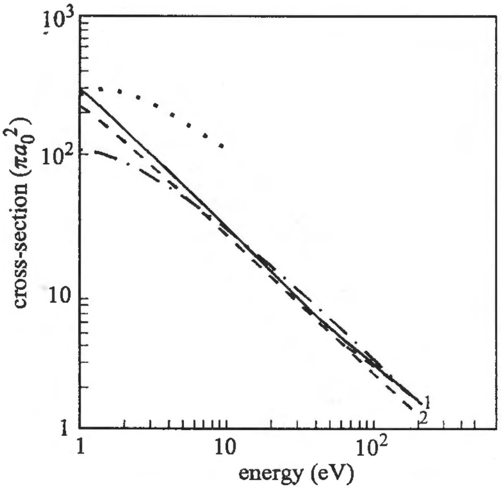

Fig. 3.

Also shown in the figure are the cross-sections obtained by the frozen core Glauber approximation [6], the close coupling approximation [15], and the Vainshitein model [9]. In the Walters calculations, the total cross-section peak lies at a higher energy than that obtained by us. The two curves are almost identical at high energies. The slight difference which we note in these two calculations may be due to the different choices of atomic wave functions. We also find that the Born calculation gives a much higher cross-section as compared to the Glauber theory and the experimental data at low energies; but at high energies the Born calculations merge with the results of the Glauber theory. The inability of a weak coupling approximation to take into account strong coupling between the initial and final states of the resonance transition is obvious from the same figure. The Glauber approximation (without exchange) is strictly justified only at "high energies". At very low energies (Fig. 4), the cross-sections from Glauber theory tend to fall rapidly. We find that by taking into consideration the core electrons, the Glauber theory excitation gives fairly good results.

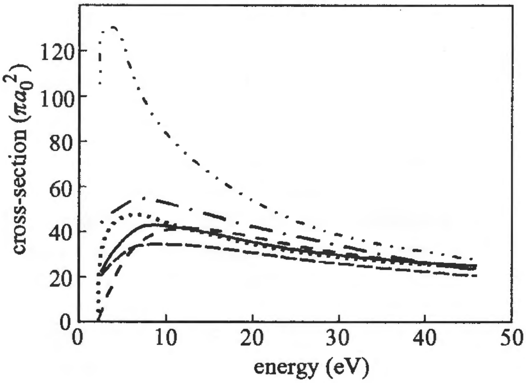

Fig. 4.

6.3. e-H_2 Scattering

Figs 5*a*, *b* and *c* present theoretical results of the angular distribution of electrons elastically scattered from H_2 molecule at the energies 100 eV, 200 eV and 912 eV respectively and are compared with the experimental data of Webb [18] and William [19]. From these figures we notice that the agreement between the theory and the experiment is satisfactory for the whole angular range.

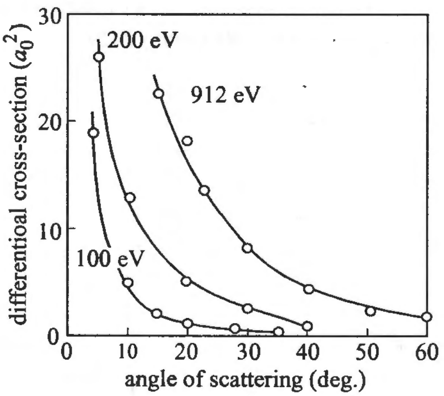

Fig. 5.

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