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Elastic scattering of electrons by helium atoms in high energy higher order Born approximation

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Abstract. The differential cross-sections for $\bar{e}$-helium elastic scattering are calculated by using Yates *high-energy higher order Born approximations,* through $0\,(K_i^{-2})$ of the incident electron momentum, and comparisons have been made with the recent theoretical and experimental results.

Keywords. Elastic scattering; electrons; helium atoms.

1. Introduction

The development of theoretical methods for intermediate energy collisions is gaining importance. Glauber's method, the modified Glauber's method, the eikonal Born series method, the fixed-scatterer approximation, the higher order Born approximation, are some of the methods which have been applied successfully (Glauber 1959; Yates 1974; Byron and Joachain 1977; Ghosh 1977). Motivated to describe an alternative approach for the high energy expansion of the differential scattering cross-section (DCS) in terms of reciprocal powers of K_i, Yates (1979) has proposed the theoretical method of high energy higher order Born (HHOB) approximation. This method has an advantage in that the computation of the higher-order Born approximation terms is simpler. Further expressions for higher orders can be obtained in the closed form. The divergent integrals in the Glauber eikonal series (GES) method given by Yates (1974) are not present in this new treatment of HHOB. This method is very much like the modified Glauber approximation and thus has many of the attractive features of the Glauber approximation.

In this paper we examine the elastic scattering of electrons from the helium atom by the HHOB approximation method and compare the results with other recent theoretical and experimental data. In § 2 the amplitude factors for the two terms in the HHOB approximation are calculated using the Hartree-Fock wavefunction for the ground state of the helium atom. The results for the Hylleraas wavefunction are obtained as a particular case from the general results. In § 3 we discuss the results of the present calculations with the other and the experimental data.

2. Theory

In the HHOB approximation the scattering amplitudes are given by (throughout this paper atomic units are used).

$$f^{(1)}_{i\to f} = -\frac{1}{2\pi}\int dv_0 \exp(i\mathbf{q}\cdot\mathbf{r}_0)\, V_{fi}(r_0), \tag{1}$$

$$\operatorname{Im} f^{(2)}_{\mathrm{HEA}} = \frac{4\pi^3}{K_i}\int d\mathbf{p}\, U^{(2)}_{fi}(\mathbf{q}-\mathbf{p}-B_i\,\hat{\zeta};\ \mathbf{p}+B_i\,\hat{\zeta}), \tag{2}$$

$$\operatorname{Re} f^{(2)}_{\mathrm{HEA}} = -\frac{4\pi^2}{K_i}\,\mathcal{P}\int d\mathbf{p}\int_{-\infty}^{\infty}\frac{dp_z}{(p_z-B_i)}\,U^{(2)}_{fi}(\mathbf{q}-\mathbf{p}-p_z\,\hat{\zeta};\ \mathbf{p}+p_z\,\hat{\zeta})$$
$$-\frac{2\pi^2}{K_i^2}\frac{\partial}{\partial B_i}\,\mathcal{P}\int d\mathbf{p}\int_{-\infty}^{\infty}\frac{dp_z\,(p^2+p_z^2)}{(p_z-B_i)}\,U^{(2)}_{fi}(\mathbf{q}-\mathbf{p}-p_z\hat{\zeta};\ \mathbf{p}+p_z\hat{\zeta}), \tag{3}$$

where $\mathbf{q}=\mathbf{K}_i-\mathbf{K}_f$ is the momentum transfer to the target atom, K_i is the momentum of the incident electron, $B_i = \Delta E/K_i$, is the average excitation energy of the target and the symbol $\mathcal{P}$ is for the principal value of the integration.

$$V_{fi}(\mathbf{r}_0) = \langle \Psi_f(\mathbf{r}_1,\mathbf{r}_2)\,|\,V\,|\,\Psi_i(\mathbf{r}_1,\mathbf{r}_2)\rangle, \tag{4}$$

where V is the interaction between the incident electron and the target atom and is given by

$$V(\mathbf{r}_0,\mathbf{r}_1,\mathbf{r}_2) = -\frac{2}{\mathbf{r}_0}+\frac{1}{|\mathbf{r}_0-\mathbf{r}_1|}+\frac{1}{|\mathbf{r}_0-\mathbf{r}_2|}, \tag{5}$$

where $\mathbf{r}_0$, $\mathbf{r}_1$ and $\mathbf{r}_2$ are the position vectors of the incident electron and the target electrons with respect to the target nuclei. $\hat{\zeta}$ is a unit vector in the z-direction. The general form of $U^{(2)}_{fi}$ is given in the appendix. Meanings of other symbols are same as in Yates (1979). We use the Hartree-Fock wavefunction for the ground state of the helium atom as given by Byron and Joachain (1973).

$$\Psi(\mathbf{r}_1,\mathbf{r}_2) = \phi_{1s}(\mathbf{r}_1)\,\phi_{1s}(\mathbf{r}_2), \tag{6}$$

with $\quad \phi_{1s}(\mathbf{r}) = \dfrac{1}{\sqrt{4\pi}}\,[A\exp(-y_1' r)+B\exp(-y_2' r)],$

$A = 2{\cdot}60505,\quad B = 2{\cdot}08144,\quad y_1' = 1{\cdot}41,\ y_2' = 2{\cdot}61.$

The scattering amplitudes can be written as

$$f^{(1)}_{i\to f} = \sum_{k=1}^{4} C_k\left[\frac{8\,y_k^2+q^2}{(4\,y_k^2+q^2)^2}\right], \tag{7}$$

$$\operatorname{Im} f^{(2)}_{\mathrm{HEA}} = \frac{1}{\pi K_i} \sum_{\substack{k=1,2,3,4 \\ j=2,3,1,0}} \left[- A_k \left(\frac{\partial}{\partial y_k} \frac{1}{y_k^2} \right) \times \right.$$

$$\left\{ 2\, I_1 (B_i^2; y_k^2) - \frac{q^2}{q^2 + y_k^2} I_1 (B_i^2; 0) \right\} +$$

$$+ B_{kk} \int d\mathbf{p} \left\{ \frac{y_k^2}{A_1^2 B_1^2} + \frac{2}{A_1^2 B_1} + \frac{1}{y_k^2 A_1 B_1} \right\} +$$

$$\left. + B_{kj} \int d\mathbf{p} \left\{ \frac{y_k y_j}{A_2^2 B_2^2} + \frac{y_k}{y_j A_2^2 B_2} + \frac{y_j}{y_k A_2 B_2^2} + \frac{1}{y_k y_j A_2 B_2} \right\} \right], \tag{8}$$

$$\operatorname{Re}_1 f^{(2)}_{\mathrm{HEA}} = \frac{1}{\pi^2 K_i} \sum_{\substack{k=1,2,3,4 \\ j=2,3,1,0}} \left[A_k \left(\frac{\partial}{\partial y_k} \frac{1}{y_k^2} \right) \times \right.$$

$$\left\{ 2\, I_2 (B_i^2; y_k^2) - \frac{q^2}{q^2 + y_k^2} I_2 (B_i^2; 0) \right\}$$

$$- B_{kk} \left(\frac{\partial^2}{\partial y_k\, \partial y_k} \frac{1}{y_k^2 y_k^2} \right) I_4 (B_i^2; y_k^2; y_k^2)$$

$$\left. - B_{kj} \left(\frac{\partial^2}{\partial y_k\, \partial y_j} \frac{1}{y_k^2 y_j^2} \right) I_4 (B_i^2; y_k^2; y_j^2) \right], \tag{9}$$

$$\operatorname{Re}_2 f^{(2)}_{\mathrm{HEA}} = \frac{1}{2\pi^2 K_i^2} \sum_{\substack{k=1,2,3,4 \\ j=2,3,1,0}} \frac{\partial}{\partial B_i} \left[A_k \left(\frac{\partial}{\partial y_k} \right) \right.$$

$$\left\{ \frac{I_3 (B_i; 0)}{q^2 + y_k^2} + \frac{I_3 (B_i; y_k^2)}{y_k^2} - I_2 (B_i^2; y_k^2) \right\}$$

$$- \frac{B_{kk}}{2} \left(\frac{\partial^2}{\partial y_k\, \partial y_k} \frac{1}{y_k^2 y_k^2} \right) I_5 (B_i^2; y_k^2; y_k^2)$$

$$\left. - \frac{B_{kj}}{2} \left(\frac{\partial^2}{\partial y_k\, \partial y_j} \frac{1}{y_k^2 y_j^2} \right) I_5 (B_i^2; y_k^2; y_j^2) \right], \tag{10}$$

where $A_1 = |\mathbf{q} - \mathbf{p}|^2 + B_i^2 + y_k^2$; $B_1 = p^2 + B_i^2 + y_k^2$;

(C_k's, A_k's, B_{kk}'s, and B_{kj}'s are constants).

$A_2 = |\mathbf{q} - \mathbf{p}|^2 + B_i^2 + y_j^2$; $B_2 = p^2 + B_i^2 + y_j^2$.

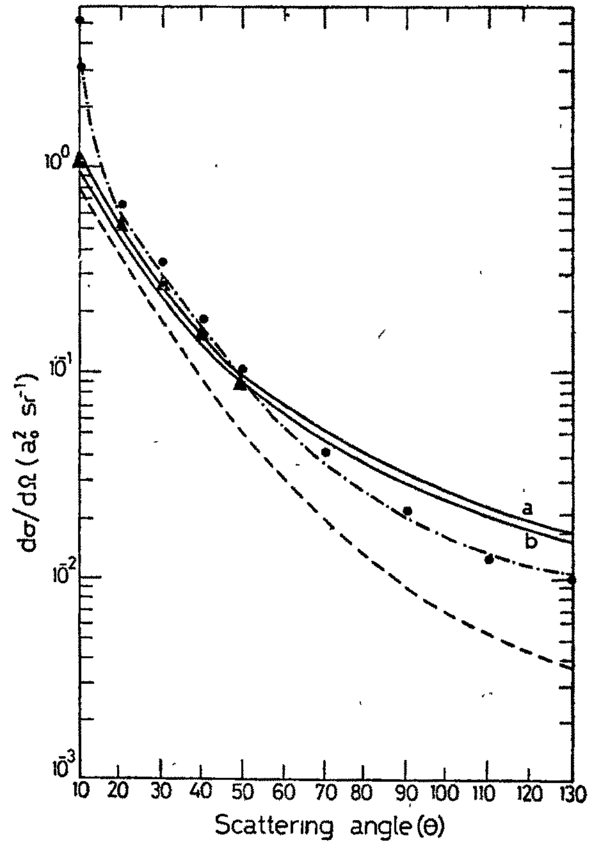

Figure 1. Differential cross-section for the elastic scattering of 200 eV electrons from the ground state of helium atom. Full curves; a and b present calculations using Hartree-Fock and Hylleraas wavefunctions respectively, chain curve; Byron and Joachain (1973, 1977), broken curve; Singh and Tripathi (1980), experimental data: ▲ Jansen *et al* (1976), ● Register *et al* (1980).

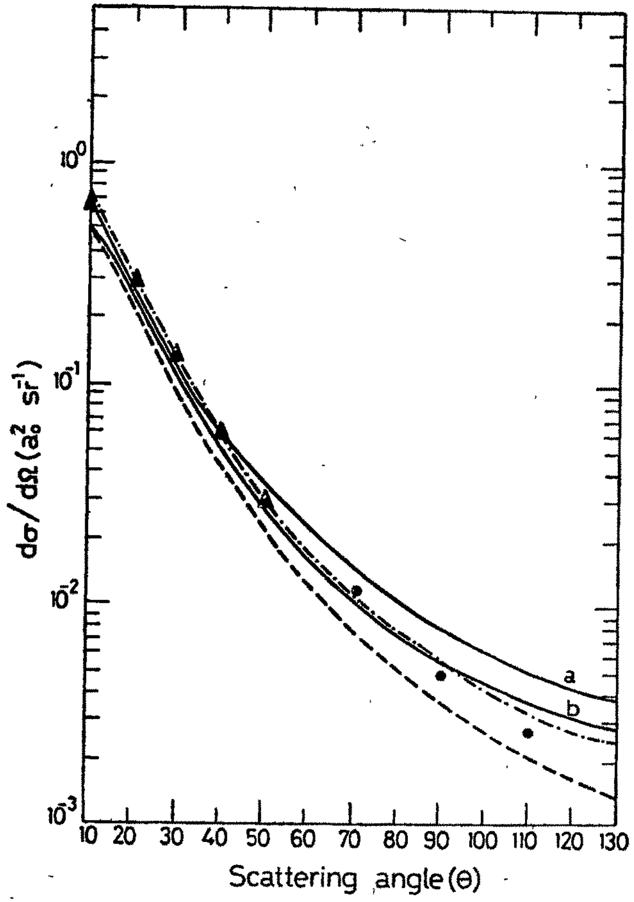

Figure 2. Differential cross-sections for the elastic scattering of 400 eV electrons from the ground state of helium atom. O, experimental data Bromberg (1974). The remaining references are same as in figure 1.

The typical integrals $I_1\,(B_i^2;\,y_1^2)$, $I_2\,(B_i^2;\,y_1^2)$, and $I_3(B_i;\,y_1^2)$ are analogous to Yates (1979). The results for the typical integrals $I_4(B_i^2;\,y_1^2;\,y_2^2)$, and $I_5(B_i^2;\,y_1^2;\,y_2^2)$ are given in the appendix. In (7), (8), (9) and (10), if $k=4, j=0$, we will get the amplitude factors corresponding to the Hylleraas wavefunction. We can write (9) and (10) as

$$\mathrm{Re}\ f^{(2)}_{\mathrm{HEA}} = \mathrm{Re}_1 + \mathrm{Re}_2, \tag{11}$$

where Re_1 and Re_2 are of the order K_i^{-1} and K_i^{-2} respectively, in (9) and (10). The differential cross-section through order K_i^{-2} for a fixed q can be approximated by

$$\frac{d\sigma}{d\Omega} = |f^{(1)}_{i\to f}|^2 + |\mathrm{Im}\,f^{(2)}_{\mathrm{HEA}}|^2 + |\mathrm{Re}_1|^2 + 2f^{(1)}_{i\to f}(\mathrm{Re}\ f^{(2)}_{\mathrm{HEA}} + fG3), \tag{12}$$

where $fG3$ is the third Glauber eikonal term of Singh and Tripathi (1980).

3. Results and discussion

We have evaluated the integrals in (8) by reducing the two-dimensional integral to one-dimensional integral. Final results for the integrations were obtained by using the Gaussian quadrature method.

In figures 1 and 2 we exhibit our results for the DCS for 200 eV and 400 eV incident energies. The wavefunctions used for these calculations are Hylleraas and the Hartree-Fock. A comparison with the recent theoretical calculations on the DCS and the experimental data is also made in these plots. It is observed that for small angles our results agree well with the experimental data, and the results of the theoretical calculations by other workers. This type of behaviour was observed by Joshipura (1981) for $\bar{e}$–H_2 DLS calculations. The results of the present calculations agree with the results of Byron and Joachain (1973). The use of the Hartree-Fock wavefunction improves the results for small angles. The improvement of the present approximation is significant at higher energies. Further it is observed that as $B_i \to 0$ the expression in (8) tends to the corresponding term given by Singh and Tripathi (1980).

In conclusion we expect that the HHOB approximation give good results at large values of K_i.

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Appendix

In this appendix several results pertinent to § 2 are tabulated. All integrations are done by standard techniques.

$$I_4(B_i^2; y_k^2; y_j^2) = -\pi^3 \Big[\operatorname{sgn}(y+q^2) \Big\{ \frac{1}{2\xi_1} - \frac{\sin^{-1} A'}{\pi\xi_1} \Big\}$$

$$- \operatorname{sgn}(y-q^2) \Big\{ \frac{1}{2\xi_2} - \frac{\sin^{-1} A''}{\pi\xi_2} \Big\} \Big]$$

$$\xi_1^2 = (y+q^2)^2 + 4q^2(B_i^2 + y_j^2)$$

$$\xi_2^2 = (y-q^2)^2 + 4q^2(B_i^2 + y_k^2)$$

$$A' = 1 - \frac{2B_i^2 (y+q^2)^2}{[(y+q^2)^2 + 4q^2 y_j^2]\,(B_i^2 + y_j^2)}$$

$$A'' = 1 - \frac{2B_i^2 (y-q^2)^2}{[(y-q^2)^2 + 4q^2 y_k^2]\,(B_i^2 + y_k^2)}$$

$$y = y_k^2 - y_j^2$$

$$I_5(B_i^2; y_k^2; y_j^2) = [I_3(B_i; y_k^2) - I_4(B_i^2; y_k^2; y_j^2)(y_j^2 + y_k^2) + I_3(B_i; y_j^2)]$$

$$I_3(B_i; y_k^2) = -\pi^3 \Big[1 - \frac{2}{\pi} \tan^{-1} \frac{y_k}{B_i} \Big]$$

We define $\overset{(2)}{U_{fi}}(q-p-x\hat{y};\, p+x\hat{y})$ as $\overset{(2)}{U_{fi}} = \langle \psi_f \,|\, \overline{V}(q-p-x\hat{y};\, r_1.r_2)$

$$\overline{V}(p+x\hat{y};\, r_1.r_2) \,|\, \psi_i \rangle$$

where $\psi_i = \psi_f$ are the state functions as defined in (6), and $\overline{V}$ is the Fourier transform of the interaction potential.

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The HHOB approximation to the elastic scattering of electrons by H(2s)

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Abstract. The high-energy higher-order Born (HHOB) approximation is applied to the elastic scattering of electrons from the excited 2s state of atomic hydrogen. Results of calculations at intermediate energies are reported along with the recent data.

The elastic scattering of electrons from the excited states of atoms plays an important role in plasma and astrophysics. The data for such processes are very scarce. An attempt is made in this present paper to apply the HHOB approximation for the calculations of the differential scattering cross section (DCS) by the intermediate-energy electrons from the excited state of hydrogen atom.

The HHOB approximation (Yates 1979), though a high-energy and small-angle approximation, has several attractive features. Firstly it is a computationally simple approximation. Secondly, in the HHOB approximation, the expressions for higher orders are obtained in closed form. Thirdly, the problem of divergent integrals in the Glauber eikonal series (Yates 1974) is avoided here. In the first part of this paper we developed the formula for DCS for the 2s state of the hydrogen atom. In the later part of this paper we discuss the results of the present paper and compare them with those of other workers.

The scattering amplitudes for the first and second Born approximations for the electron–atom scattering problem were given earlier (Rao and Desai 1981). The matrix element $V_{fi}(\boldsymbol{r}_0)$ is given by

$$V_{fi}(\boldsymbol{r}_0)=\langle\Psi_f(\boldsymbol{r}_1)|V|\Psi_i(\boldsymbol{r}_1)\rangle \tag{1}$$

where V is the interaction between the incident electron and the target atom and is given by

$$V(\boldsymbol{r}_0,\boldsymbol{r}_1)=-\frac{1}{r_0}+\frac{1}{|\boldsymbol{r}_0-\boldsymbol{r}_1|} \tag{2}$$

where $\boldsymbol{r}_0$ and $\boldsymbol{r}_1$ are the position vectors of the incident and the target electrons respectively. The wavefunction for the excited state of H(2s) can be written as

$$\Psi_{2s}(r)=\frac{1}{4(2\pi)^{1/2}}(2-r)\exp(-r/2). \tag{3}$$

The scattering amplitudes for an electron in the HHOB approximation are given in closed form as

$$f^{(1)}=\sum_{n=0}^{2}A_nD_n\left(\frac{(q^2+2y^2)}{2^2(q^2+y^2)^2}\right) \tag{4}$$

$$\operatorname{Im}f^{(2)}=-\frac{1}{k_i}\sum_{n=1}^{3}B_nD_n\frac{1}{y^2}\left(2I_1(B^2,y^2)-\frac{q^2I_1(B^2,0)}{(q^2+y^2)}\right) \tag{5}$$

$$\operatorname{Re}_1 f^{(2)}=\frac{1}{\pi k_i}\sum_{n=1}^{3}B_nD_n\frac{1}{y^2}\left(2I_2(B^2,y^2)-\frac{q^2I_2(B^2,0)}{(q^2+y^2)}\right) \tag{6}$$

$$\operatorname{Re}_2 f^{(2)}=\frac{1}{2\pi k_i^2}\sum_{n=1}^{3}B_nD_nD'\left(\frac{I_3(B^2,0)}{(q^2+y^2)}-\frac{I_3(B^2,y^2)}{y^2}-I_2(B^2,y^2)\right) \tag{7}$$

$$F^{(3)}_{\mathrm{GES}}=-\frac{\pi}{16k_i^2}\sum_{n=1}^{3}C_nD_n\frac{1}{(q^2+y^2)}\left[4\left(\log\frac{q^2+y^2}{qy}\right)^2+\tfrac{1}{3}\pi^2-2A(q,y^2)\right] \tag{8}$$

where

$$A(q,y^2)=2[\log(q/y)]^2+\tfrac{1}{6}\pi^2+\sum_{n=1}^{\infty}\left(-\frac{q^2}{y^2}\right)^n\frac{1}{n^2} \qquad \text{when } q/y\leqslant 1$$

$$=-\sum_{n=1}^{\infty}\left(-\frac{y^2}{q^2}\right)^n\frac{1}{n^2} \qquad \text{when } q/y>1$$

$D_n=\partial^n/\partial^n y$, $D'=\partial/\partial B$, and the A_n, B_n and C_n are the constants given below

$A_0=1.999$, $A_1=1.999$, $A_2=0.500$, $B_1=0.159$, $B_2=0.159$,

$B_3=0.0398$, $C_1=0.0398$, $C_2=0.0398$, $C_3=0.00995$ and $y=1$.

$B=\Delta E/k_i$ where ΔE is the average excitation energy obtained from Joachain *et al* (1977b), and $f^{(1)}$ is the first Born approximation, $\operatorname{Im}f^{(2)}$, $\operatorname{Re}_1 f^{(2)}$ and $\operatorname{Re}_2 f^{(2)}$ are the imaginary, real parts of order $(1/k_i)$ and order $(1/k_i^2)$, amplitudes in the second Born approximation respectively, and $F^{(3)}_{\mathrm{GES}}$ is the third Glauber eikonal series term derived using Yates (1974). The typical integrals $I_1(B^2,y^2)$, $I_2(B^2,y^2)$ and $I_3(B^2,y^2)$ in these amplitudes are similar to Yates (1979). The direct scattering amplitude in the present approximation is given as

$$F_d=f^{(1)}+\operatorname{Re}_1 f^{(2)}+\operatorname{Re}_2 f^{(2)}+F^{(3)}_{\mathrm{GES}}+\mathrm{i}\operatorname{Im}f^{(2)}. \tag{9}$$

The leading term (Ochkur 1963) of the first-order exchange amplitude is also included in the present DCS calculations. The exchange amplitude is given as

$$g_{\mathrm{ex}}=\sum_{n=0}^{2}-\frac{F_nD_n}{k_i^2}\left(\frac{y}{(q^2+y^2)^2}\right) \tag{10}$$

where the F_n are the constants given below

$F_0=2$, $F_1=2$ and $F_2=0.5$.

From the equations (9) and (10) the DCS through order $(1/k_i^2)$ can be approximated using the following equation:

$$\mathrm{d}\sigma/\mathrm{d}\Omega=\tfrac{1}{4}|F_d+g_{\mathrm{ex}}|^2+\tfrac{3}{4}|F_d-g_{\mathrm{ex}}|^2. \tag{11}$$

We present, in figure 1, our results for the differential scattering cross sections, with and without the exchange term, for 200 eV. The results are compared with the results of Joachain *et al* (1977b). As expected it is observed that at small angles the HHOB approximation results are in good agreement with the results of other workers. Our results are slightly higher than the results of Joachain *et al* (1977b). This type of behaviour for e^-–He-atom elastic scattering was also observed earlier by Rao and Desai (1981).

The results for the higher impact energy 400 eV are shown in figure 2. The agreement of the results with those of other workers is very good. We observed from the figures that the behaviour of the HHOB approximation remains the same as for the ground state H(1s), and the exchange contribution to the direct scattering amplitude is small.

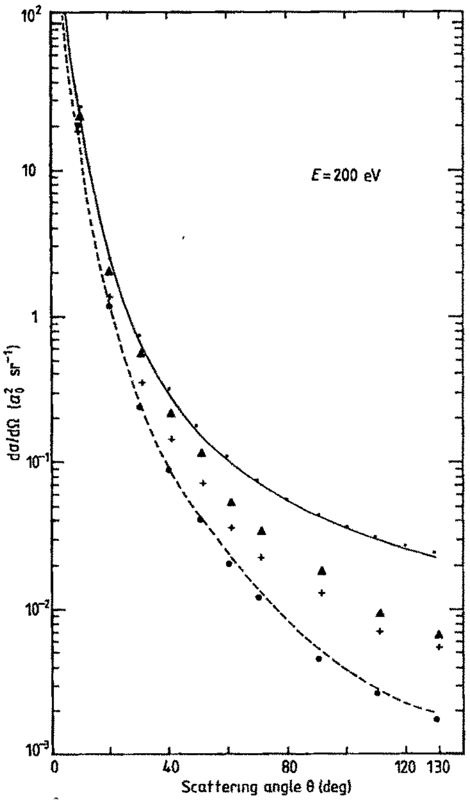

Figure 1. Differential scattering cross section for the elastic scattering of 200 eV electrons from H(2s). Small dots and full curve, present HHOB approximation with and without exchange term; ▲, simplified second Born approximation of Joachain *et al* (1977a); broken curve, static approximation of Joachain *et al* (1977b); +, EBS approximation of Joachain *et al* (1977b), ●, optical model of Joachain and Winters (1980).

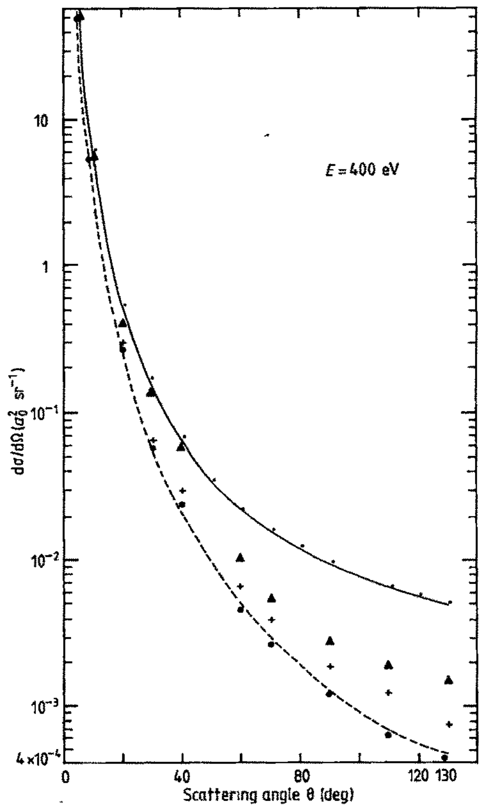

Figure 2. Differential scattering cross section for the elastic scattering of 400 eV electrons from H(2s). The rest of the caption is the same as for figure 1.

We conclude that the disagreement at large angles with other workers (Joachain *et al* 1977b, Joachain and Winters 1980) is due to the fact that the Born series is slowly convergent at large angles. Our results will be improved by taking higher-order Born terms in the HHOB approximation of Yates (1979).

Acknowledgments

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Application of HHOB Approximation to e$^-$-Li Elastic Scattering

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High energy higher-order Born (HHOB) approximation as proposed by AC Yates [*Phys Rev A* (*USA*), 19 (1979) 1550] is applied to calculate the elastic differential cross-sections and total collisional cross-sections for e$^-$-Li elastic scattering at intermediate energies. Results of the calculations are compared with recent theoretical results of F W Byron and C J Joachain [*Phys Rev A* (*USA*), 4 (1981) 1817] and the experimental data of Williams *et al.* [*J Phys B* (*GB*), 9 (1976) 1529, 1576].

1 Introduction

The HHOB approximation proposed by Yates[1] is one of the successfully applied high energy, small angle approximation. This HHOB approximation yields reliable results for elastic scattering processes[2-4]. In the case of e$^-$-He atom scattering, results[2] obtained using this approximation are very encouraging.

In the present paper, we have calculated the elastic differential scattering cross-section (DCS) and total collisional cross-section (TCS) for e$^-$-Li elastic scattering. The first and second terms in the Born approximation are calculated within the framework of HHOB approximation[1], the third term is calculated using the Glauber eikonal series (GES) of Yates[5]. We have used the one-electron wavefunction for Li atom as suggested by Walters[6]. It was investigated by Mathur *et al.*[7] that at both intermediate and high energies, the differences between the scattering parameters obtained by using one- or three-electron wavefunctions of Li atom were not very appreciable. Keeping this in mind, we have used the one-electron wavefunction for the Li atom.

2 Theory

Atomic units are used in this study. $\mathbf{K}_i$, $\mathbf{K}_f$ and $\mathbf{q}=\mathbf{K}_i-\mathbf{K}_f$, represent the incident, final momenta of scattered electron, and the momentum transfered to the target atom, respectively, during the collision process. The DCS for fixed q through $O(1/k_i^2)$ can be approximated as:

$$\frac{d\sigma}{d\Omega}=|F^{(1)}|^2+|\mathrm{Im}\,F^{(2)}|^2+|\mathrm{Re}_1\,F^{(2)}|^2+2F^{(1)}[\mathrm{Re}_1\,F^{(2)}+\mathrm{Re}_2\,F^{(2)}+F^{(3)}_{GES}] \quad \ldots(1)$$

where $F^{(1)}$ is the first Born approximation, $\mathrm{Im}\,F^{(2)}$, $\mathrm{Re}_1\,F^{(2)}$ and $\mathrm{Re}_2\,F^{(2)}$ are the imaginary and real parts of order $(1/k_i)$ and order $(1/k_i^2)$ amplitudes in the second Born approximation respectively, and $F^{(3)}_{GES}$, the third GES term is derived using Yates[5]. The matrix element $V_{fi}(\mathbf{r}_0)$ is given as:

$$V_{fi}(\mathbf{r}_0)=\langle\Psi_f(\mathbf{r}_1)|V|\Psi_i(\mathbf{r}_1)\rangle \quad \ldots(2)$$

where V is the interaction between the incident electron and the Li atom and is given as:

$$V_0(\mathbf{r}_0,\mathbf{r}_1)=-\frac{1}{r_0}+\frac{1}{|\mathbf{r}_0-\mathbf{r}_1|}+V_c \quad \ldots(3)$$

where

$$V_c=-2\left[\frac{1}{\mathbf{r}_0}+2.7\right]\exp(-5.4\,r_0)$$

V_c is the core potential and $\mathbf{r}_0$, $\mathbf{r}_1$, are the position vectors of the incident and target electrons, with respect to the target nuclei. The wavefunction used for the ground state of lithium atom is

$$\Psi_{2s}(r)=A\,r\exp(-y_1'r)+B\exp(-y_2'r) \quad \ldots(4)$$

where $A=0.11252$; $B=-0.42204$; $y_1'=0.65$; $y_2'=2.7$. In the calculation of higher order terms, we have neglected the core potential V_c contribution. It was shown by Guha and Ghosh[8] that V_c will not affect the cross-section appreciably. The closed form of the amplitude factors in the HHOB approximation are given as:

$$F^{(1)}=\sum_{n=0}^{2}D_nA_n\left[\frac{2}{y_n^3(q^2+y_4^2)}+\frac{1}{y_n^3(q^2+y_n^2)}+\frac{5.4\,y_4}{y_n^3(q^2+y_4^2)^2}+\frac{1}{y_n(q^2+y_n^2)^2}\right] \quad \ldots(5)$$

$$\mathrm{Im}\,F^{(2)}=-\sum_{n=1}^{3}\left[\frac{B_n}{k_i}D_n\frac{1}{y_n^2}\left\{2I_1-\frac{q^2}{(q^2+y_n^2)}I_1^0\right\}\right] \quad \ldots(6)$$

$$\mathrm{Re}_1\,F^{(2)}=\sum_{n=1}^{3}\left[\frac{B_n}{\pi k_i}D_n\frac{1}{y_n^2}\left\{2I_2-\frac{q^2}{(q^2+y_n^2)}I_2^0\right\}\right] \quad \ldots(7)$$

$$\mathrm{Re}_2\,F^{(2)}=\sum_{n=1}^{3}\left[\frac{B_n}{2\pi k_i^2}D_n\frac{\partial}{\partial B_i}\left\{\frac{I_3^0}{(q^2+y_n^2)}+\frac{I_3}{y_n^2}-I_2\right\}\right] \quad \ldots(8)$$

$$F^{(3)}_{GES}=-\sum_{n=1}^{3}\left[\frac{C_n}{k_i^2}D_n\frac{1}{(q^2+y_n^2)}\left\{4\left\{\log\left(\frac{q^2+y_n^2}{y_nq}\right)\right\}^2+\frac{\pi^2}{3}-2A(q,y_n^2)\right\}\right] \quad \ldots(9)$$

where

$$A(q, y_n^2) = 2\left(\log\frac{q}{y_n}\right)^2 + \frac{\pi^2}{6} + \sum_{m=1}^{\infty}\left(-\frac{q^2}{y_n^2}\right)^m \Big/ m^2 \qquad \text{when } \frac{q}{y_n} \leq 1$$

$$= -\sum_{m=1}^{\infty}\left(\frac{y_n^2}{q^2}\right)^m \Big/ m^2 \qquad \text{when } \frac{q}{y_n} > 1$$

where

$$D_n = \frac{\partial^n}{\partial^n y_n}, \quad B_i = \frac{\Delta E}{k_i} = \frac{0.0745}{k_i}.$$

where ΔE is average excitation energy obtained from Vanderpoorten[9].

A_n's, B_n's, C_n's and y_n's are constants with following values:

$A_0 = 8.95318 \quad A_1 = 4.7740 \quad A_2 = 0.63640$

$B_1 = 0.71247 \quad B_2 = 0.37990 \quad B_3 = 0.05064$

$C_1 = 29.73803 \quad C_2 = 2.49206 \quad C_3 = 0.00710$

$y_0 = 5.4 \quad y_1 = 3.4 \quad y_2 = 1.3$

$y_1 = 5.4 \quad y_2 = 3.4 \quad y_3 = 1.3 \quad y_4 = 5.4$

The typical integrals I_1, I_1^0 and I_2, I_2^0, I_3, I_3^0 are analogous to Yates[1]. The total cross-section can be calculated using the optical theorem:

$$\sigma_{\text{tot}} = \frac{4\pi}{k_i}\,\text{Im}\,F^{(2)} \quad (q=0) \qquad \ldots(10)$$

Using this optical theorem, we have also calculated the total collisional cross-sections for elastic scattering of electrons by helium atoms. The results are presented in Table 1.

3 Results and Discussion

Differential scattering cross-sections (DCS)—Using Eq. (1) we have calculated the DCS at incident energies 20, 60, 100 and 200 eV. In the Figs 1-4, the curves (a) and (b) represent the present DCS with and without $\text{Re}_2 F^{(2)}$ contribution respectively. Figs 1 and 2 show the present results along with the measured values of Williams *et al.*[12] Results of the present study made at 20 eV are compared with the close coupling results of Issa[13] and eikonal Born series results[14] in Fig. 1. Results of present study made at 60 eV are compared with the two potential eikonal approximation results of Tayal *et al.*[15] and optical potential approximation results of Vanderpoorten[16] in Fig. 2. Figs 3 and 4 show the present results along with the corrected static approximation results of Tayal *et al.*[17] and the eikonal-Born series results[14]. It is observed from the figures that at small angles, the present DCS results agree closely with the other results at 200 eV than at lower incident energies. The difference between the curves (a) and (b) exhibits the importance of the term $\text{Re}_2 F^{(2)}$.

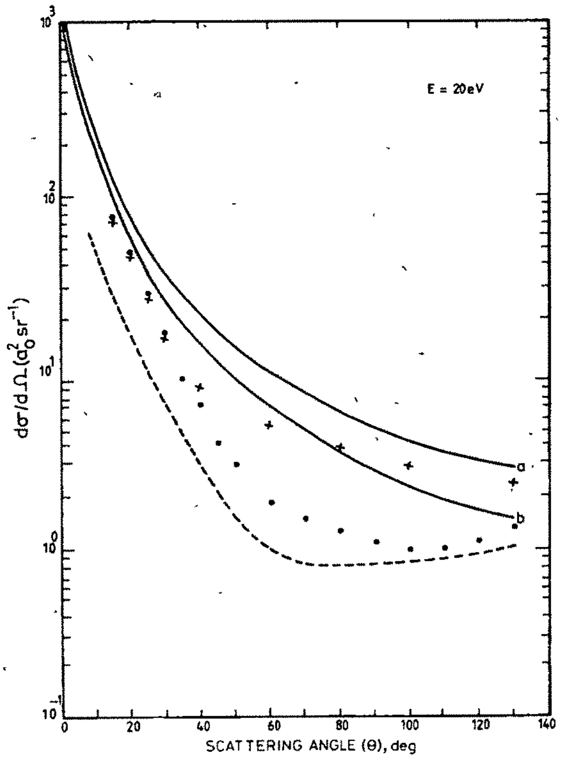

Fig. 1—DCS for e⁻-Li elastic scattering at 20 eV [solid curves (a) and (b) present calculations in HHOB approximation with and without Re $F^{(2)}$ contribution respectively; broken curve represents close-coupling results of Issa[13], ●, data points of Williams *et al.*[12], and +, eikonal Born series results[14]]

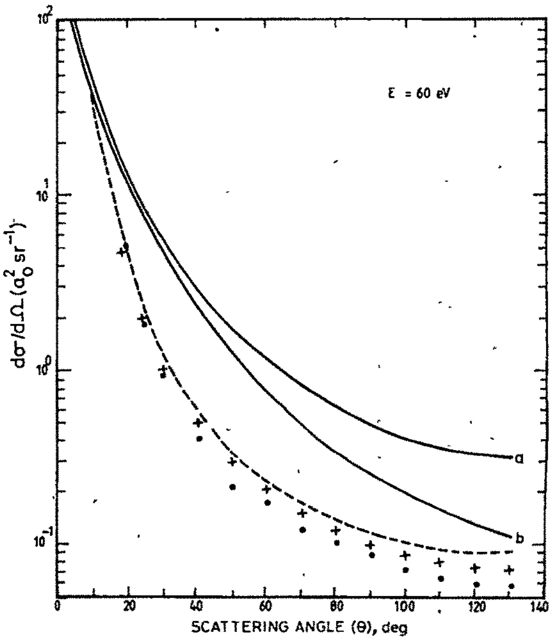

Fig. 2—DCS for e⁻-Li elastic scattering at 60 eV [solid curves (a) and (b) present calculation in HHOB approximation with and without Re $F^{(2)}$ contribution respectively; broken curve represents results of Tayal *et al.*[15], +, results of Vanderpoorten[16], and ●, data points of Williams *et al.*[12]

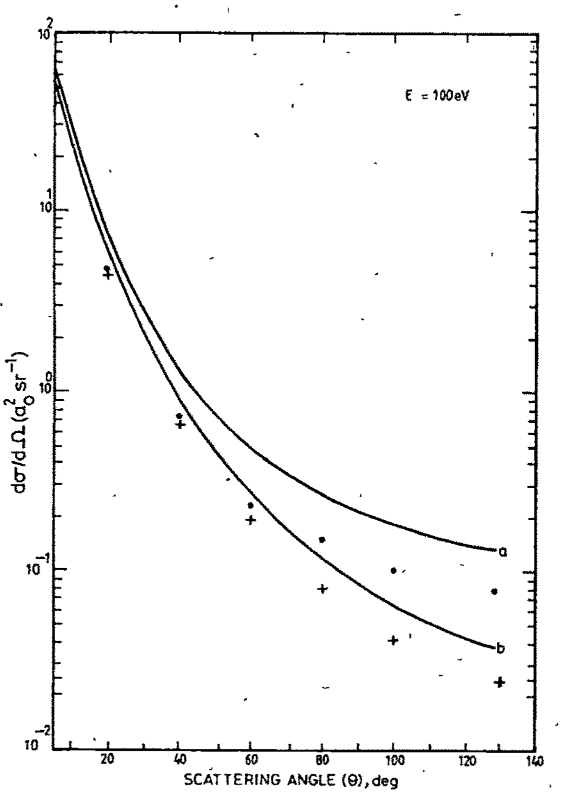

Fig. 3—DCS for e⁻-Li elastic scattering at 100 eV [solid curves (a) and (b) present calculations in HHOB approximation with and without Re $F^{(2)}$ contribution respectively, ● and + are corrected static approximation and eikonal Born series results taken from Ref 17]

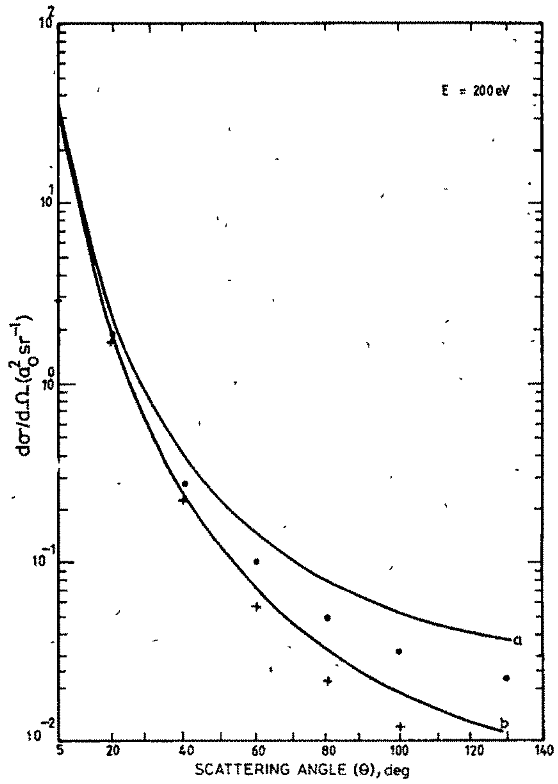

Fig. 4—DCS for e⁻-Li elastic scattering at 200 eV [The legend is same as for Fig. 3]

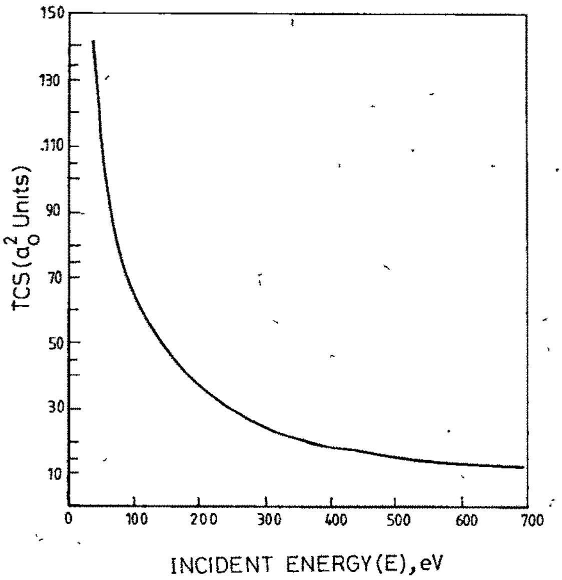

Fig. 5—TCS for e⁻-Li elastic scattering at incident energies ranging from 40 to 700 eV [solid curve present calculation in HHOB approximation]

Table 1—Total Collisional Cross-sections (in units of a_0^2) for Electron-Helium Scattering

Energy (eV)	Present results	Byron & Joachain[10]	de Heer & Jansen[11]
100	4.94	4 57	4 05
200	2.93	2.90	2.68
300	2 14	2 14	2 03
400	1 69	1.72	1 66
500	1 42	1 45	1 39
700	1.08	1 10	1.06

Total collisional cross-sections (TCS)—Using Eq. (10) we have calculated the total cross-sections for e⁻-Li scattering, at the incident energies from 40 eV to 700 eV. The results of the calculations are exhibited in Fig. 5. The TCS results for He-atom are given in Table 1 and these results are also found to be in good agreement with the other results[10,11] at large incident energies.

From an analysis of our previous results[2,3] and the present ones, we conclude that the HHOB approximation leads to very good results at large incident energies. The values of DCS will be further improved at large angles by inclusion of higher-order Born terms of Yates[1].

Acknowledgement

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ANGULAR DISTRIBUTION OF ELECTRONS SCATTERED INELASTICALLY BY HYDROGEN ATOMS

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YATES[1] approximation is a small angle and high energy approximation. The main advantage of this approximation is that it is computationally simple and higher order Born terms can be obtained in the closed form. Here there is no problem of divergent integrals. This approximation is further simplified and has been applied to various atoms for the elastic processes[2-4]. In all these problems, first two Born terms were derived according to Yates[1] and the third Born term was approximated by the third Glauber elkonal series (GES) term of Yates[5]. At small angles very good results were obtained for elastic process by Rao and Desai[2-4]. In the present paper an attempt is made to calculate differential cross-section (DCS) for H(1S–2S) inelastic scattering.

Yates[1] method for the elastic collision of electrons by the H-atom is extended to the inelastic collision of electrons by the H-atom for H(1S–2S). The results for the scattering amplitudes for this process are given as

$$\operatorname{Im} F^{(2)} = \left(A + B\frac{\partial}{\partial\lambda}\right) \operatorname{Im} f^{(2)}_{\text{HEA}}, \qquad (1)$$

$$\operatorname{Re} F^{(2)} = \left(A + B\frac{\partial}{\partial\lambda}\right) \operatorname{Re} f^{(2)}_{\text{HEA}}, \qquad (2)$$

where $\operatorname{Im} f^{(2)}_{\text{HEA}}$ and $\operatorname{Re} f^{(2)}_{\text{HEA}}$ are the imaginary and real parts of the second Born approximation for the elastic case[1]. These are functions of q, λ and β_i. In the present case the numerical values of these quantities are $\lambda = 1.5$, $\beta_i = \Delta E / k_i$, where ΔE is the average excitation energy[6] and $q = k_i - k_f$, k_i and k_f are the initial and final momenta of the scattered electron. In the equations (1) and (2) the constants A and B are given as

$$A = 0.3536, \quad B = 0.1768.$$

The third term of Yates[5] for the present case is given as

$$F^{(3)}_{\text{GES}} = \left(C + D\frac{\partial}{\partial\lambda}\right) F(\lambda, q) \qquad (3)$$

where $C = -0.1187$, $D = -0.0559$ and $F(\lambda, q)$ is similar to the expression given by Rao and Desai[3]. The first Born scattering amplitude is given as

$$F^{(1)} = -\frac{11.3137}{(q^2 + 2.25)^3} \qquad (4)$$

The direct scattering amplitude is given as

$$F_d = F^{(1)} + \operatorname{Re} F^{(2)} + F^{3}_{\text{GES}} + i\, \operatorname{Im} F^{(2)} \qquad (5)$$

from this equation the DCS through order $(1/k^2)$ can be approximated as

$$\frac{d\sigma}{d\Omega} = \frac{k_f}{k_i}\left| F_d \right|^2 \qquad (6)$$

Figures 1 and 2 show the present DCS results at incident energies 100 and 200 eV respectively. The present DCS curves reproduce the curves of other results[7,8]. At 100 eV our results are higher than the other results[7,8]. The results are good at 200 eV than at 100 eV. For the checking of our results, we compared our imaginary part with the imaginary part of Byron and Latour[6], and it is observed that there is very nice agreement at all angles. These results are displayed in figure 3.

We conclude that the present results will be improved at higher incident energies and the inclusion

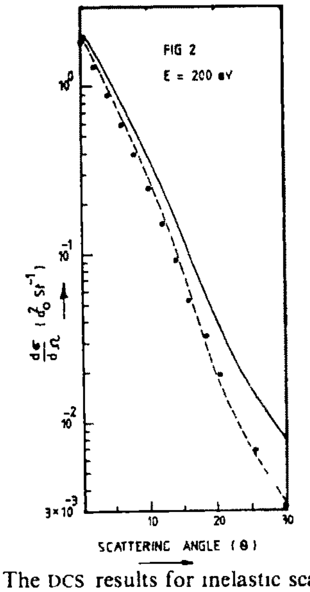

Figure 1. The DCS results for inelastic scattering of electrons by H-atom at incident energy 100 eV solid curve—present results, Broken Curve—results of Unnikrishnan and Prasad[7], solid circles—results of Glauber[8].

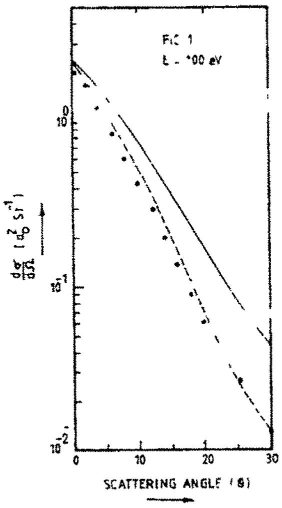

Figure 2. The DCS results at incident energy 200 eV. The references are same as in figure 1.

of third Born term[1] instead of third GES[5] will improve our results over the entire angular range.

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6 August 1982

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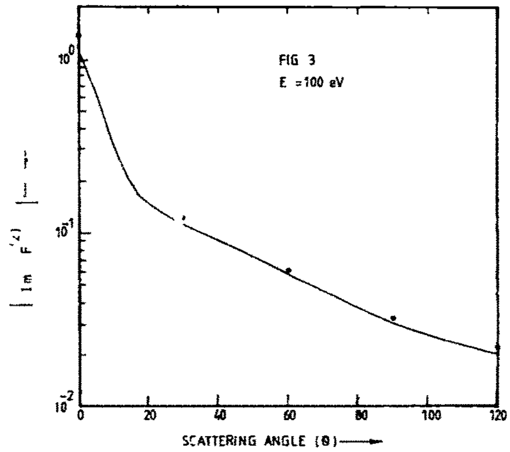

Figure 3. Comparison of present imaginary part and the imaginary part of Byron and Latour[6] at incident energy 100 eV

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Elastic and inelastic scattering of electrons by lithium atoms

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Abstract : An analytical expression for the differential scattering cross section (DCS) is obtained through order (K_i^{-2}), for the elastic and inelastic scattering of electrons by lithium atoms. Yates high energy higher order Born (HHOB) and Glauber eikonal series (GES) approximations are used for these derivations. The exchange scattering amplitudes for these processes are obtained by using Lewis integral technique. The present scattering amplitudes are compared with the recent scattering amplitudes of Rao and Desai.

1. Introduction

The scattering of electrons by lithium atom is one of the interesting and encouraging problems in the recent years. The data for this $\bar{e}-$Li collision process is very scarce. Motivated by this, we have derived an expression for the DCS through $0(K_i^{-2})$. Yates (1979) high energy higher order Born (HHOB) approximation is used to derive two terms of the Born approximation and Glauber eikonal series (GES) of Yates (1974) is used to derive the third GES term. These two approximations were used by Rao and Desai (1981-83) for hydrogen, helium and lithium atoms, at intermediate and high incident energies. The results obtained by means of these approximations were very encouraging.

The aim of the present paper is to obtain scattering amplitudes for DCS through $0(K_i^{-2})$ for elastic and inelastic collision processes of $\bar{e}-$Li interaction. The wave functions choosen for the ground and excited states of lithium atom are as used by Mathur *et al* (1972). The basic scattering amplitudes were given by Rao and Desai (1981). Here we give only the closed form of the scattering amplitudes for elastic and inelastic processes for the Li-atom. The first order exchange scattering amplitudes is calculated using the Lewis (1956) integral techniques and this exchange term is included in the DCS formula. The total interaction in this problem is divided into two parts. First part similar to the

$\bar{e}-H$ interaction and the second part is considered as core obtained by the inner target electrons. The core interaction is neglected in the higher order scattering amplitudes. The present elastic scattering amplitude expressions are compared with the recent expressions of Rao and Desai (1983).

2. Theory

Throughout this work atomic units are used. The wave function for the ground (2*s*) state of Li-atom is given as

$$\Psi_{2s}(r)=\frac{1}{\sqrt{4\pi}}\left[\sum_{i=1}^{2}A_i\ e^{-y_i r}+\sum_{j=3}^{6}A_j r\ e^{-y'_j r}\right] \tag{1}$$

and for the excited (2*p*) state of Li-atom is given as

$$\Psi_{2p}(r)\ =\ Ar\ e^{-y'r} \tag{2}$$

where $A=0.22805$, $y'=0.5227$ and A'_is and y'_is are constants given by Clementi (1965).

For the elastic scattering $(2s-2s)$ the initial and final states of the target atom are assumed to be same. The substitution of eq. (1) in the second Born approximation (Rao and Desai 1981) gives the corresponding imaginary and real contributions to the scattering amplitude. The closed form of these amplitudes are given as

$$Im\ F^{(2)}=\tfrac{1}{4}\left[\sum_{i=1}^{4}D_i F(y_i)-\sum_{j=1}^{8}E_j DF(y_j)+\sum_{k=1}^{16}F_k D^2F(y_k)\right] \tag{3}$$

$$Re\ F^{(2)}=\tfrac{1}{4}\left[\sum_{i=1}^{4}D_i G(y_i)-\sum_{j=1}^{8}E_j DF(y_j)+\sum_{k=1}^{16}F_k D^2 F(y_k)\right] \tag{4}$$

$$GES^{(3)}=\tfrac{1}{4}\left[\sum_{i=1}^{4}D_i H(y_i)-\sum_{j=1}^{8}E_j DH(y_j)+\sum_{k=1}^{16}F_k D^2F(y_k)\right] \tag{5}$$

where D is differentiation operator and the functions $F(y)$, $G(y)$ and $H(y)$ are the corresponding scattering amplitudes for $\bar{e}-H$ atom scattering [Yates (1979, 74)].

For the inelastic scattering $(2s-2p)$ the final state of the target atom is assumed as $2p$ state. Following the similar procedure as discussed above, we will get the three scattering amplitudes similar to eqs. (3), (4) and (5).

The first order exchange scattering amplitude (Joachain 1975) is obtained by using the wave function (1) and the integral techniques of Lewis (1956). The exchange amplitude for this elastic process is given as

$$T_{ex} = -2\sum_{ij}^{6} A_{ij}(-1)^{m+n}\frac{1}{y_i y_j} D^m D^n \frac{\tan^{-1}}{f_1}\left(\frac{f_1}{f_2}\right) \tag{6}$$

where

$$f_1^2 = q(K_1^2+y_j^2)(K_1^2+y_i^2)+(y_i^2-y_j^2)^2 K_1^2$$
$$f_2 = y_j(K_1^2+y_i^2)+y_i(K_1^2+y_j^2)$$

m and n in the eq. (6) are the powers of the target coordinate r in the wave functions. This elastic exchange term can be easily extended to inelastic process.

Now the DCS $0(K_i^2)$ can be obtained from the following equation.

$$\frac{d\sigma}{d\Omega} = \frac{K_f}{K_i}\left| F^{(1)} + Re\,F^{(2)} + GES^{(3)} + T_{ex} + Im\,F^{(2)} \right|^2 \tag{7}$$

Here $F^{(1)}$ is the first Born amplitude. This expression is not given which is straightforward and lengthy expression.

3. Results and discussion

Present elastic scattering amplitudes are compared with the recently reported amplitudes of Rao and Desai (1983). The DCS and total cross sections can be compared with this recent results of Rao and Desai (1983).

Finally we conclude that these new scattering amplitudes will generate good results than the earlier results of Rao and Desai (1983). Inclusion of the exchange term is the reason for this conclusion. The DCS calculations are in progress.

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AN ANALYTICAL STUDY OF HIGHER ORDER BORN TERMS IN THE STATIC FIELD

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THE closed forms of the elastic scattering amplitudes in the static field are obtained by using the Yates high energy higher order Born approximation. The differential scattering cross-section through order $(1/K_i^2)$ is obtained for elastic electron-atom scattering. Total cross-sections for the elastic scattering of the electrons by lithium atom are calculated. The results show good agreement with compared data.

In this communication we report the elastic scattering amplitudes developed for a z-electron atom. The approximation given by Yates[1] is used in these derivations. We have treated e-atom interaction as the static field[2,3] due to z-electron target. Additional advantages in this case are that all the Yates[1] elastic scattering amplitudes are simplified and one can calculate DCS (differential cross-sections), TCS (total cross-sections) very easily for any atom. One can also standardise the computer programme for the calculation of DCS and TCS for any target atom. The static potential can be defined as

$$V_{st}(r_0) = \langle \psi_i | V | \psi_f \rangle \tag{1}$$

where ψ_i and ψ_f are the initial and final state wave functions of the target atom and V is the interaction between the incident electron and the target atom. The static potential $V_{st}(r_0)$ can be obtained[2,3] for different atoms. Analytical expression for the static potential can be given as

$$V_{st}(r_0) = Z \left| \sum_{i=1}^{N} \right| R_i \left| e \frac{-Y_i r_0}{r_0} \right. \tag{2}$$

where R_i's and Y_i's are obtained from[2,3] for different atoms. The fourier form of $V_{st}(r_0)$ is given as

$$V_{st}(r_0) = \int d\mathbf{p} \exp(-i\mathbf{p}\cdot\mathbf{b}_0) \int_{-\infty}^{\infty} dp_z \exp(-ip_z Z_0)\, V_{st}(p + p_z\hat{z}) \tag{3}$$

where

$$V_{st}(p+p_z\hat{z}) = \frac{Z}{2\pi^2} \sum_{i=1}^{N} \frac{R_i}{(p^2+p_z^2+y_i^2)} \tag{4}$$

The aim of the present work is to study all the Yates[1] amplitudes in the static field These amplitudes are obtained by the substitution of equation in Yates[1] approximation. The corresponding three Born terms are given as

$$f^{(1)}_{i\to f} = -2Z \sum_{i=1}^{N} \frac{R_i}{(q^2 + y_i^2)} \tag{5}$$

$$\mathrm{Im}\, f^{(2)}_{\mathrm{HEAS}} = \frac{Z^2}{\pi K_i} \sum_{i,j=1}^{N} R_i R_j\, I_1(B_i^2, y_i^2, y_j^2) \tag{6}$$

$$\mathrm{Re}\, f^{(2)}_{\mathrm{HEAS}} = \frac{Z^2}{2\pi K_i} \sum_{i,j=1}^{N} R_i R_j \Big[I_2(B_i^2, y_i^2, y_j^2) + \frac{1}{2K_i}\frac{\partial}{\partial B_i}\left\{ I_3(B_i^2, y_i^2) - y_i^2 I_2(B_i^2, y_i^2, y_j^2)\right\}\Big] \tag{7}$$

$$f^{(3)}_{\mathrm{HEAS}} = f_{1s}^{(3)} + f_{2s}^{(3)} \tag{8}$$

where

$$f_{1s}^{(3)} = \frac{Z^3}{2\pi^2 K_i^2} \sum_{i,j,K=1}^{N} R_i R_j R_K\, I_4(q^2, u, v, w,)$$

Similarly one can obtain $f_{2s}^{(3)}$ by using the present approximation and the computation procedure given by Yates[1]. The closed form of the all I_n's in the above expressions were given[1,4-6]. The elastic scattering amplitude through $(1/K_i^2)$ can be given as

$$F_{as} = f^{(1)}_{i\to f} + \mathrm{Re}\, f^{(2)}_{\mathrm{HEAS}} + f^{(3)}_{\mathrm{HEAS}} + i\,\mathrm{Im}\, f^{(2)}_{\mathrm{HEAS}} \tag{9}$$

Total cross-section can be obtained using the optical theorem[1].

$$\sigma^{\mathrm{tot}} \doteq \frac{4\pi}{K_i}\, \mathrm{Im}\, f^{(2)}_{\mathrm{HEAS}}(0) \tag{10}$$

where

$$\mathrm{Im}\, f^{(2)}_{\mathrm{HEAS}}(0) = \frac{Z^2}{K_i}\left[\left[\sum_{i\neq j} \frac{R_i R_j}{(y_i^2 - y_j^2)}\right] \log \frac{B_i^2 + y_i^2}{B_i^2 + y_j^2} + \sum_{i=j} \frac{R_i^2}{(B_i^2 + y_i^2)}\right]$$

is the imaginary part of the second Born Term in the forward direction The meaning of all the symbols are same as Yates[1].

Using σ^{tot} we have calculated TCS for lithium atom[3]. The results are given below

TABLE I

TCS in units of (πa_0^2) for lithium atom

Incident Energy E eV	Present results	Results of Guha and Gosh[8]
50	6 295	7.511
60	5 260	6 034
100	3.152	3 379
150	2 106	2.183
200	1 577	1.614

To confirm our results these terms have been compared with the corresponding Born Terms of Yates[1] and the two types of Born terms show good agreement. The most notable observation is that when $B_i \to 0$ few of the Yates[1] integrals were divergent and cancelled with the opposite types of integrals. However, in the present studies there are no divergent integrals as can be seen from equation (10). In order to see the validity of the present approach we have calculated TCS for lithium atom using the optical theorem[7]. The TCS results are found to be in good agreement at higher incedent energies with the other data[8].

The present calculations are simpler than the Yates[1] approximation and one can calculate TCS and DCS very easily for any atom Further work is in progress

2 December 1982

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