Elastic scattering of electrons from lithium atoms in the Glauber approximation

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The elastic scattering of electrons by lithium atoms is considered in the Glauber approximation using Franco's method for reducing the $(3Z + 2)$-dimensional integral occurring in the amplitude for the scattering of charged particles by a Z-electron atom. It is found that the involvement of the inner electrons (those in the $1s$ state) causes very little change over the frozen-core Glauber calculations.

I. INTRODUCTION

The Glauber approximation[1] has been used extensively to study scattering by hydrogen atoms.[2-8] These calculations involve the numerical evaluation of a relatively simple one-dimensional integral. Closed-form expressions have also been obtained in this case.[9,10] For the helium-target, Glauber calculations of elastic and inelastic scattering of electrons have been performed using three- and two-dimensional integral representations obtained by reducing the initial eight-dimensional (8D) integral.[11,12] In the case of electron–alkali-atom collisions, Glauber calculations have been done only in the frozen-core approximation which reduces the target to an effective one-electron system.[13-15] Thus all the applications of the Glauber approximation in atomic scattering have been restricted to the scattering by atoms having one or two "effective" electrons. The reason is that the scattering amplitude in the Glauber approximation for the scattering from a target of atomic number Z involves a $(3Z+2)$-dimensional integral which must first be reduced sufficiently before attempting any numerical calculation.

Franco[16] has proposed a method for reducing this $(3Z+2)$-dimensional integral to a 1D integral for the elastic and inelastic scattering of charged particles by arbitrary neutral atoms. His method is based (i) on the assumption that the product of the initial Φ_i and the final Φ_f wave functions of the target can be written in the form

$$\Phi_f^*\Phi_i = \sum_{k=1}^{N}\left(c_k \prod_{j=1}^{Z}[r_j^{n_{k,j}} e^{-\alpha_{k,j} r_j} \times Y_{l_j m_j}(\theta_j, \varphi_j) Y^*_{l'_j m'_j}(\theta_j, \varphi_j)]\right), \tag{1}$$

where r_j, θ_j, and φ_j are the spherical coordinates of the jth electron, and the Y_{lm} are the normalized spherical harmonics; and (ii) on carrying out the integrations over the coordinates of the target electrons without involving the impact parameter $\vec{b}$. This procedure differs from the one followed in Refs. 11 and 12 for e-He scattering. There, the impact parameter is mixed with the coordinates $\vec{r}_1(\vec{s}_1, z_1)$ and $\vec{r}_2(\vec{s}_2, z_2)$ of the target electrons to generate a new set of variables R, ξ, and ζ in place of b, s_1, and s_2. This mixing is not feasible for more than two electrons in the target. The assumption regarding the form, Eq. (1), of $\Phi_f^*\Phi_i$ is really no restriction since the wave functions usually employed in describing the atoms can always be put in that form. The result is that the final expression involves just a 1D integral over b. The only problems with this method are the evaluation of the integrand which involves the calculation of the differences between strongly divergent functions and the numerical calculation of the δ functions whenever elastic scattering is considered.[17] Thomas and Chan[17] have recently modified this procedure to eliminate these difficulties by using the properties of the modified Lommel functions, and have reported calculations for the elastic and inelastic e-He scattering.[17-19] Franco,[20] on the other hand, has used his original prescription[16] without any modifications to obtain $1S$-$2\,^1S$ excitation cross section in e-He scattering.

In the present work we have avoided the encounter with the divergent functions appearing in Franco's final expression[16] by stopping a step earlier (Sec. II). The concealed δ function in the momentum transfer q presents no numerical problem. The price to be paid for this simplification is that our final expression is a 2D integral, irrespective of the atomic number of the target, against Franco's 1D integral. Thomas and Chan[17] have also pointed out this possibility but did not pursue it. To illustrate this procedure, we consider the elastic scattering of electrons by lithium atoms.

In Sec. II we outline Franco's method. Section III contains the details of the calculation. The results are presented in Sec. IV.

II. METHOD

In the Glauber approximation, the amplitude $F_{fi}(\vec{q})$ of a particle with momentum $\hbar\vec{k}_i$ by a Z-electron atom, which undergoes a transition from an initial state i with wave function Φ_i to a final state f with wave function Φ_f, is given by[1,2]

$$F_{fi}(\vec{q}) = \frac{ik_i}{2\pi}\int \Phi_f^*(\vec{r}_1, \ldots, \vec{r}_Z)\Gamma(\vec{b}, \vec{r}_1, \ldots, \vec{r}_Z) \times \Phi_i(\vec{r}_1, \ldots, \vec{r}_Z)e^{i\vec{q}\cdot\vec{b}}\, d^2b\, d^3r_1 \cdots d^3r_Z , \tag{2}$$

where $\hbar\vec{q} = \hbar(\vec{k}_i - \vec{k}_f)$ is the momentum transfer which the incident particle imparts to the target, and $\vec{r}_1, \ldots, \vec{r}_Z$ are the coordinates of target electrons relative to the nucleus. The momentum transfer $\vec{q}$ is assumed to lie in the plane of the impact parameter $\vec{b}$. The profile function Γ is given by

$$\begin{aligned}\Gamma(\vec{b}, \vec{r}_1, \ldots, \vec{r}_Z) &= 1 - \exp[i\chi_{\text{tot}}(\vec{b}, \vec{r}_1, \vec{r}_2, \ldots, \vec{r}_Z)] \\ &= 1 - \prod_{j=1}^{Z} e^{i\chi(\vec{b}, \vec{s}_j)} \\ &= 1 - \prod_{j=1}^{Z}\left(\frac{|\vec{b} - \vec{s}_j|}{b}\right)^{2i\eta} ,\end{aligned} \tag{3}$$

where $\eta = e^2/\hbar v = 1/k_i$ (using Rydberg atomic units), v is the initial speed of the incident electron in the lab system (same as the center-of-mass system in our case), and $\vec{s}_j$ is the projection of $\vec{r}_j$ onto the plane of $\vec{b}$. Combining Eqs. (2) and (3), the expression for the scattering amplitude $F_{fi}(\vec{q})$ takes the form

$$F_{fi}(\vec{q}) = \frac{ik_i}{2\pi}\int d^2b\, e^{i\vec{q}\cdot\vec{b}}\left\{1 - \int \Phi_f^*\Phi_i\left[\prod_{j=1}^{Z}\left(\frac{|\vec{b} - \vec{s}_j|}{b}\right)^{2i\eta}\right] d^3r_1 \cdots d^3r_Z\right\} . \tag{4}$$

The contribution of the first term in curly brackets in Eq. (4), though proportional to the 2D δ function $\delta^2(\vec{q})$, cannot be ignored, for otherwise the integrand over b would not tend to zero, as it should, for large values of the impact parameter b, and would create numerical difficulties.

For the product $\Phi_f^*\Phi_i$, we prefer the form

$$\Phi_f^*\Phi_i = \prod_{j=1}^{Z}\left(\sum_{k=1}^{N_j} c_{k,j} r_j^{n_{k,j}} e^{-\alpha_{k,j} r_j}\right) \times Y_{l_j m_j}(\theta_j, \varphi_j) Y^*_{l'_j m'_j}(\theta_j, \varphi_j) , \tag{5}$$

which can be obtained by regrouping the terms in Eq. (1). For elastic scattering by lithium atoms only s states are involved, i.e., $l_j = l'_j = m_j = m'_j = 0$ for all j. Thus

$$\Phi_f^*\Phi_i = (4\pi)^{-3}\prod_{j=1}^{3}\left(\sum_{k=1}^{N_j} c_{k,j} r^{n_{k,j}} e^{-\alpha_{k,j} r_j}\right) \tag{6a}$$

$$= (4\pi)^{-3}\prod_{j=1}^{3}\sum_{k=1}^{N_j} c_{k,j}(-1)^{1+n_{k,j}} \times \left(\frac{\partial}{\partial\alpha_{k,j}}\right)^{1+n_{k,j}} \frac{e^{-\alpha_{k,j} r_j}}{r_j} . \tag{6b}$$

Using Eq. (6b) in Eq. (4), and carrying out the integration over φ_b, gives

$$F_{fi}(\vec{q}) = ik_i\int_0^\infty db\, J_0(qb) b\left[1 - (4\pi)^{-3}\prod_{j=1}^{3}\sum_{k=1}^{N_j} c_{k,j}(-1)^{1+n_{k,j}}\left(\frac{\partial}{\partial\alpha_{k,j}}\right)^{1+n_{k,j}} I(\alpha_{k,j}, b)\right] , \tag{7}$$

where

$$I(\alpha_{k,j}, b) = \int \frac{e^{-\alpha_{k,j} r_j}}{r_j}\left(\frac{|\vec{b} - \vec{s}_j|}{b}\right)^{2i\eta} d^3r_j . \tag{8}$$

It is worth mentioning here that the limit as $b \to \infty$ of the second term in Eq. (7) is unity. The integral in Eq. (8) can be performed by introducing cylindrical coordinates $\vec{s}_j, z_j$ for $\vec{r}_j$ and following the methods of Franco[16] and Thomas and Gerjuoy,[9] to give

$$\begin{aligned} I(\alpha_{k,j}, b) &= 2\int_0^\infty ds_j\, s_j \int_0^\infty dz_j (s_j^2 + z_j^2)^{-1/2} \exp[-\alpha_{k,j}(s_j^2 + z_j^2)^{1/2}] \int_0^{2\pi} d\varphi \left(1 + \frac{s_j^2}{b^2} - \frac{2s_j}{b}\cos\varphi\right)^{i\eta} \\ &= 2b^2\int_0^\infty ds\, K_0(\alpha_{k,j} bs) s \int_0^{2\pi} d\varphi (1 + s^2 - 2s\cos\varphi)^{i\eta} \\ &= 2b^2\left(-\pi 2^{1+2i\eta}\frac{\Gamma(1+i\eta)}{\Gamma(1-i\eta)}\right)\int_0^\infty ds\, sK_0(\alpha_{k,j} bs)\int_0^\infty dt\, t^{-2i\eta}\frac{d}{dt}[J_0(t)J_0(st)] \\ &= 2b^2E(\eta)\int_0^\infty dt\, t^{-2i\eta}\frac{d}{dt}\left(J_0(t)\int_0^\infty ds\, sK_0(\alpha_{k,j} bs)J_0(st)\right) \\ &= 2b^2E(\eta)\int_0^\infty dt\, t^{-2i\eta}\frac{d}{dt}\left(\frac{J_0(t)}{t^2 + (\alpha_{k,j} b)^2}\right) , \end{aligned} \tag{9}$$

where

$$E(\eta) = -\pi 2^{1+2i\eta}\left(\frac{\Gamma(1+i\eta)}{\Gamma(1-i\eta)}\right) . \tag{10}$$

Franco[16] integrates Eq. (9) by parts, to get[21]

$$I(\alpha_{k,j}, b) = 4i\eta b^2 E(\eta) \int_0^\infty dt \frac{t^{-2i\eta-1} J_0(t)}{(t^2+\alpha_{k,j}^2 b^2)}$$

$$= 4i\eta b^2 E(\eta)[E_1(\eta)(\alpha_{k,j}b)^{-2-2i\eta}{}_0F_1(-;\ 1;\ \tfrac{1}{4}\alpha_{k,j}^2 b^2) + E_2(\eta)\,{}_1F_2(1;\ 2+i\eta,\ 2+i\eta;\ \tfrac{1}{4}\alpha_{k,j}^2 b^2)] , \tag{11}$$

where

$$E_1(\eta) = \tfrac{1}{2}\Gamma(-i\eta)\Gamma(1+i\eta)$$

and

$$E_2(\eta) = \frac{\Gamma(-1-i\eta)}{2^{3+2i\eta}\Gamma(2+i\eta)} .$$

The hypergeometric functions appearing in Eq. (11) are themselves divergent functions of $\alpha_{k,j}b$ although their combination as appearing in Eq. (11) is convergent. This can be clearly seen by carrying out the differentiation indicated in Eq. (9).

$$I(\alpha_{k,j}, b) = -2b^2 E(\eta)$$

$$\times \int_0^\infty dt\, t^{-2i\eta}\left[\frac{J_1(t) + 2tJ_0(t)/(t^2+\alpha_{k,j}^2 b^2)}{t^2+\alpha_{k,j}^2 b^2}\right] . \tag{12}$$

The integral in Eq. (12) can be easily evaluated numerically. We have used this form to avoid the problems associated with the calculation of the differences between strongly divergent functions appearing in Franco's expression [Eq. (11)].

The differentiations of I with respect to $\alpha_{k,j}$ in Eq. (7) can be done analytically.

III. CALCULATION

For elastic scattering by lithium atoms we need only Φ_i where the electrons are in $(1s)^2(2s)^1$ configuration. We have taken these orbitals of the form given by Clementi,[22] and Φ_i is obtained by taking their antisymmetric combination. This leads to

$$\Phi_f^*\Phi_i = (1/3!)|\det(\Psi_{1s_\uparrow}, \Psi_{1s_\downarrow}, \Psi_{2s})|^2$$

$$= |\Psi_{1s}(1)\Psi_{1s}(2)\Psi_{2s}(3)|^2$$

$$- |\Psi_{1s}(1)|^2\Psi_{1s}^*(2)\Psi_{2s}(2)\Psi_{1s}(3)\Psi_{2s}^*(3) . \tag{13}$$

The orbitals Ψ are of the form (Ref. 22)

$$\Psi(r) = R(r)Y_0^0(\theta, \varphi) , \tag{14a}$$

with

$$R(r) = \sum_{i=1}^{2} A_i e^{-\xi_i r} + \sum_{i=3}^{6} A_i r e^{-\xi_i r} . \tag{14b}$$

Both the terms in Eq. (13) for $\Phi_f^*\Phi_i$, with Ψ's of form (14) lead to expression (6a) with

$$N_j = 21$$

$$\eta_{k,j} = \begin{cases} 0, & k \leq 3 \\ 1, & 3 < k \leq 11 \\ 2, & 11 < k \leq 21 . \end{cases}$$

The values of the constants $c_{k,j}$ and $\alpha_{k,j}$ are obtained from the values of the parameters A_i and ξ_i given by Clementi.[22]

The integrals in Eqs. (7) and (12) were done by the Filon[23] method. The oscillations of the Bessel functions were accurately accounted for by

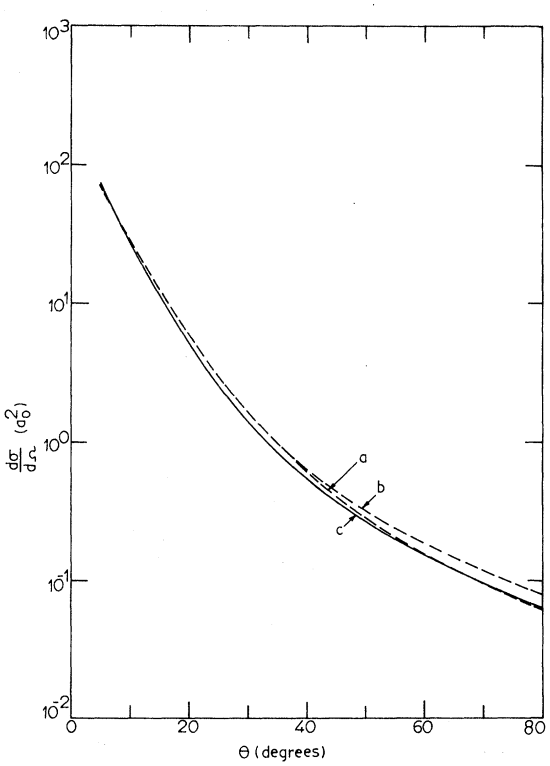

FIG. 1. Differential cross sections $(d\sigma_{el}/d\Omega)(a_0^2)$ vs scattering angle θ up to 80° at electron laboratory energy 54.38 eV ($k = 2$ a.u.). Curve a, frozen-core Glauber approximation without core potential; curve b, with core potential included; curve c, present calculation.

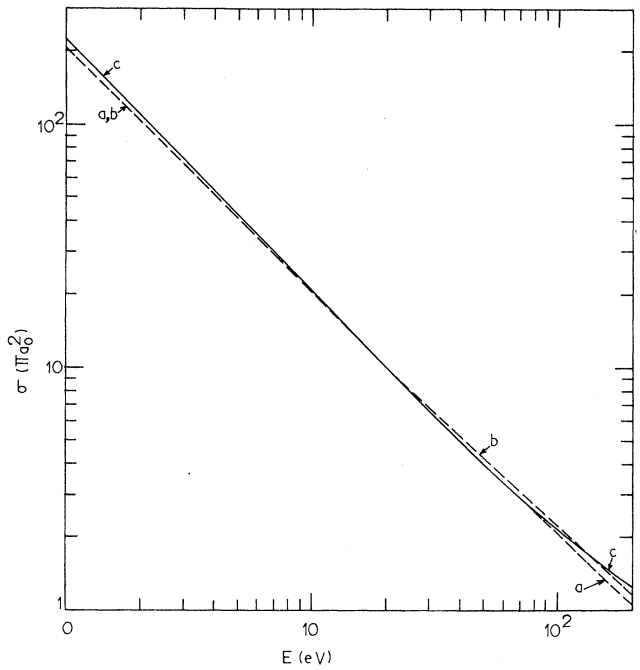

FIG. 2. Calculated total elastic cross sections $\sigma_{el}(\pi a_0^2)$ for energies up to 200 eV. Notation is same as in Fig. 1.

combining the Simpson rule with the standard Bessel-function integrals.[24]

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

$$d\sigma_{el}(q)/d\Omega = |F_{fi}(q)|^2 . \quad (15)$$

The total integrated cross section for elastic scattering is given by the expression

$$\sigma_{el} = \frac{2}{k_i^2}\int_0^{2k} \frac{d\sigma_{el}}{d\Omega} q\, dq . \quad (16)$$

IV. RESULTS

In Fig. 1 we have plotted the differential cross sections against the scattering angle θ up to 80° at an electron laboratory energy of 54.38 eV ($k = 2$ a.u.). The curves a and b correspond to the calculation in the frozen-core Glauber approximation without and with core potential, respectively. These are similar to those in Refs. 13–15. The curve c corresponds to the present calculation. Clementi wave functions have been used in all the calculations. All the curves show almost identical variation indicating that the inner electrons (those in the 1s state) are not very active. A more quantitative picture is given by Table I. The slight increase in cross section when the core potential is included is in agreement with the findings of Walters.[15] The differential cross sections with the present calculation differ little from those in the frozen-core approximation. Similar is the case with the total cross section for energies up to 200 eV.

TABLE I. Elastic differential cross sections in units of a_0^2 at $k = 2$ a.u.

Scattering angle (in deg)	Frozen-core Glauber approximation Without core potential	With core potential	Present calculation
10	27.11	27.06	26.90
20	5.59	5.52	5.01
30	1.58	1.57	1.37
40	0.61	0.63	0.54
50	0.29	0.31	0.27
60	0.16	0.18	0.16
70	0.10	0.12	0.10
80	0.06	0.08	0.06

It appears that nothing much is gained by including the inner electrons and the frozen-core Glauber calculation is good enough. It is expected that the same will be true in other systems.

On the procedural side, our calculations have further confirmed that Franco's procedure is numerically tractable.

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