Glauber cross sections for the $2s \rightarrow 2p$ resonance excitation in lithium by electron impact*

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The cross sections for the electron-impact-induced resonance transition ($2s \rightarrow 2p$) in lithium are calculated in the Glauber approximation using Franco's method of explicitly involving all the electrons of the many-electron target. Our results are always a bit smaller than the frozen Glauber results, but approach them as the energy increases. However, these differences are not very significant, indicating that the inner electrons (those in $1s$ state) are rather inert. Both of the Glauber results are found to be in good agreement above 15 eV with the recent experimental results of Leep and Gallagher.

I. INTRODUCTION

The Glauber approximation[1] has been quite widely used during the past few years to study electron-impact excitation and elastic scattering by atomic hydrogen and helium.[2-8] 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 effectively one-electron system.[9,10] The complication in calculations with many-electron targets (atomic number Z) arises because of the occurrence of a $(3Z+2)$-dimensional integral which must first be sufficiently reduced. Franco[11] has recently formulated the Glauber approximation for many-electron atoms in such a way that this $(3Z+2)$-dimensional integral is reduced to a one-dimensional integral without any further approximation. This method has been used by Franco[12] to study the electron-impact excitation of helium and by the authors[13] to study the elastic scattering of electrons by lithium. An alternative expression for reducing the Glauber amplitude for charged-particle many-electron-atom collisions to a one-dimensional integral representation involving modified Lommel functions has been proposed by Thomas and Chan.[14] It has been used to calculate the electron-impact excitation of helium.[15,16] The primary usefulness of these methods is that the contribution of the inner electrons is explicitly taken into account and can be analyzed, in contrast to the frozen-core approximation.

The purpose of this paper is to use Franco's procedure[11] to calculate the Glauber cross section for the resonance transition $\mathrm{Li}(2s) \rightarrow \mathrm{Li}(2p)$ and compare the results with the recent experimental findings of Leep and Gallagher.[17] On the procedural side we show that Franco's procedure is numerically tractable even when non-spherically-symmetric states ($2p$ state in lithium) are involved.

Section II of this paper sketches an outline of Franco's method applied to our problem. Section III contains the details of the calculation. The results are presented and discussed in Sec. IV.

II. METHOD

The amplitude $F_{fi}(\vec{q})$ for the scattering of a charged 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, in the Glauber approximation, by the expression[11]

$$F_{fi}(\vec{q}) = \frac{ik_i}{2\pi} \int \Phi_f^*(\vec{r}_1, \ldots, \vec{r}_Z)\Gamma(\vec{b}, \vec{r}_1, \ldots, \vec{r}_Z) \times \Phi_i(\vec{r}_1, \ldots, \vec{r}_Z) e^{i\vec{q}\cdot\vec{b}} d^2b\, d^3r_1 \cdots d^3r_Z, \tag{1}$$

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 vector $\vec{q}$ is assumed to lie in the plane of the impact parameter $\vec{b}$. The profile function Γ is given by

$$\Gamma(\vec{b}, \vec{r}_1, \ldots, \vec{r}_Z) = 1 - \exp[i\chi_{\mathrm{tot}}(\vec{b}, \vec{r}_1, \ldots, \vec{r}_Z)] = 1 - \prod_{j=1}^{Z} \left(\frac{|\vec{b} - \vec{s}_j|}{b}\right)^{2i\eta}, \tag{2}$$

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, and $\vec{s}_j$ is the projection of $\vec{r}_j$ onto the plane of $\vec{b}$. The first term in Eq. (2) does not contribute in the case of inelastic scattering since Φ_f is orthogonal to Φ_i. Following Ref. 11, we assume that the wave functions Φ_f and Φ_i are such that the product $\Phi_f^*\Phi_i$ may be expressed as

$$\Phi_f^*\Phi_i = \prod_{j=1}^{Z} \left(\sum_{k=1}^{N_j} C_{k,j} r_j^{\eta_{k,j}} e^{-\alpha_{k,j} r_j}\right) \times Y_{l_j m_j}(\theta_j, \phi_j) Y^*_{l'_j m'_j}(\theta_j, \phi_j). \tag{3}$$

The assumption regarding the form [Eq. (3)] of $\Phi_f^* \Phi_i$ is really no restriction since the wave functions usually employed in describing atoms can easily be put in that form. Since we are concerned here with the electron-impact resonance transition $1s^2 2s^1 \rightarrow 1s^2 2p^1$ in lithium atoms, we have

$$\begin{aligned} &l_1 = l_2 = l_3 = m_1 = m_2 = m_3 = 0, \\ &l_1' = l_2' = m_1' = m_2' = 0, \\ &l_3' = 1, \quad m_3' = 0, \pm 1. \end{aligned} \tag{4}$$

In the present case Eq. (3) simplifies to

$$\Phi_f^* \Phi_i = \prod_{j=1}^{3} a_j \left(\sum_{k=1}^{N_j} C_{k,j} r_j^{n_{k,j}} e^{-\alpha_{k,j} r_j} \right) \tag{5a}$$

$$= \prod_{j=1}^{3} P_j, \tag{5b}$$

where

$$a_1 = a_2 = 1/4\pi \tag{5c}$$

$$a_3 = Y_{1m_3'}^*(\theta_3, \phi_3)/\sqrt{(4\pi)}. \tag{5d}$$

Using Eqs. (5) in Eq. (1) gives

$$F_{fi}(\vec{q}) = \frac{-ik_i}{2\pi} \int d^2b \, e^{i\vec{q}\cdot\vec{b}} \prod_{j=1}^{3} \int P_j \left(\frac{|\vec{b} - \vec{s}_j|}{b} \right)^{2i\eta} d^3 r_j. \tag{6}$$

The terms P_1 and P_2 also appear in the case of elastic scattering and have been evaluated in Ref. 13 [Eqs. (9), (10), and (12]:

$$\int P_j \left(\frac{|\vec{b} - \vec{s}_j|}{b} \right)^{2i\eta} d^3 r_j = \frac{1}{4\pi} \sum_{k=1}^{N_j} C_{k,j} (-1)^{1+n_{k,j}} \left(\frac{\partial}{\partial \alpha_{k,j}} \right)^{1+n_{k,j}} I(\alpha_{k,j}, b) = \frac{1}{4\pi} T_j(b), \quad j = 1, 2 \tag{7}$$

where

$$I(\alpha_{k,j}, b) = -2b^2 E(\eta) \int_0^\infty dt \, \frac{t^{-2i\eta} [J_1(t) + 2t J_0(t)/(t^2 + \alpha_{k,j}^2 b^2)]}{(t^2 + \alpha_{k,j}^2 b^2)}, \tag{8a}$$

and

$$E(\eta) = -\pi 2^{1+2i\eta} \frac{\Gamma(1 + i\eta)}{\Gamma(1 - i\eta)}. \tag{8b}$$

We now calculate the contribution to Eq. (6) from the factor P_3:

$$\begin{aligned} \int P_3 \left(\frac{|\vec{b} - \vec{s}_3|}{b} \right)^{2i\eta} d^3 r_3 &= \frac{1}{\sqrt{(4\pi)}} \int \sum_{k=1}^{N_3} C_{k,3} r_3^{n_{k,3}} e^{-\alpha_{k,3} r_3} \left(\frac{|\vec{b} - \vec{s}_3|}{b} \right)^{2i\eta} Y_{1m_3'}^*(\theta_3, \phi_3) \, d^3 r_3 \\ &= \frac{1}{4\pi} \left(\frac{3(1 - m_3')!}{(1 + m_3')!} \right)^{1/2} (-1)^{m_3'} \int \sum_{k=1}^{N_3} C_{k,3} (s_3^2 + z_3^2)^{n_{k,3}/2} \, e^{-\alpha_{k,3} (s_3^2 + z_3^2)^{1/2}} \left(\frac{|\vec{b} - \vec{s}_3|}{b} \right)^{2i\eta} \\ &\quad \times P_{1m_3'} \left(\frac{z_3}{(s_3^2 + z_3^2)^{1/2}} \right) e^{-im_3' \phi_3} s_3 \, ds_3 \, d\phi_3 \, dz_3. \end{aligned} \tag{9}$$

For $m_3' = 0$, the associated Legendre polynomial $P_{1m_3'}$ is an odd function of z_3 and therefore the integral over over z_3 vanishes. For $m_3' = \pm 1$, Eq. (9) can be written as

$$\begin{aligned} &\int P_3 \left(\frac{|\vec{b} - \vec{s}_3|}{b} \right)^{2i\eta} d^3 r_3 \\ &= \mp \frac{\sqrt{6}}{2(4\pi)} \left[2 \int_0^\infty ds_3 \, s_3^2 \int_0^{2\pi} d\phi_3 \, e^{\mp i\phi_3} \left(\frac{|\vec{b} - \vec{s}_3|}{b} \right)^{2i\eta} \sum_{k=1}^{N_3} C_{k,3} (-1)^{n_{k,3}} \left(\frac{\partial}{\partial \alpha_{k,3}} \right)^{n_{k,3}} \int_0^\infty \frac{dz_3 \exp[-\alpha_{k,3} (s_3^2 + z_3^2)^{1/2}]}{(s_3^2 + z_3^2)^{1/2}} \right]. \end{aligned} \tag{10}$$

The integral over z_3 gives $K_0(\alpha_{k,3} s_3)$. Expression (10) can now be evaluated in a straightforward way [Ref. 11, Eqs. (11)–(21)] to yield

$$\mp \frac{\sqrt{6}}{2(4\pi)} e^{\mp i\phi_b} \left[8i\eta E(\eta) b^3 \sum_{k=1}^{N_3} C_{k,3} (-1)^{n_{k,3}} \left(\frac{\partial}{\partial \alpha_{k,3}} \right)^{n_{k,3}} H(\alpha_{k,3}, b) \right] = \mp \frac{\sqrt{6}}{2(4\pi)} e^{\mp i\phi_b} T_3(b), \tag{11a}$$

where

$$H(\alpha_{k,3}, b) = \int_0^\infty \frac{J_1(t)t^{-2i\eta}}{(t^2+\alpha_{k,3}^2 b^2)^2}\, dt . \tag{11b}$$

We have evaluated the integrals in Eqs. (8a) and (11b) numerically rather than expressing them as a sum of two hypergeometric functions (Eq. 22 of Ref. 11). These hypergeometric functions are divergent for large b. Our procedure, as pointed out in Ref. 13, although it leads to a final expression involving two-dimensional integrals, avoids the problems associated with the calculation of the differences between divergent functions. The integrands in these integrals [Eqs. (8a) and (11b)], except for the factor $t^{-2i\eta}$, need be evaluated only once at mesh points and can be stored.

The scattering amplitude can now be obtained by putting together the contributions P_1, P_2, and P_3 [Eqs. (7) and (11)] in Eq. (6). Integrating it with respect to ϕ_b gives

$$F_{fi}(\vec{q}, m_3' = \pm 1) = \frac{\sqrt{6}k_i}{2(4\pi)^3} e^{\mp i\phi_q} \int_0^\infty db\, bJ_1(qb) \prod_{j=1}^{3} T_j(b). \tag{12}$$

The oscillations of the Bessel functions in the integrals in Eqs. (8a), (11b), and (12) can be accounted for accurately by combining Simpson's rule with the standard Bessel-function integrals.[18]

III. CALCULATIONS

The ground-state wave function Φ_i of a lithium atom with electronic configuration $1s^2 2s^1$ has been obtained by taking the antisymmetric combination of the $1s$ and $2s$ orbitals of the form given by Clementi.[19] Similarly the final-state wave function Φ_f is the antisymmetric combination of the $1s$, $1s$, and $2p$ orbitals. This leads to

$$\begin{aligned}\Phi_f^* \Phi_i &= (1/3!)[\det(\Psi_{1s\uparrow}, \Psi_{1s\downarrow}, \Psi_{2p})]^* \\ &\quad \times [\det(\Psi_{1s\uparrow}, \Psi_{1s\downarrow}, \Psi_{2s})] \\ &= |\Psi_{1s}(1)|^2 [\,|\Psi_{1s}(2)|^2 \Psi_{2p}(3)^* \Psi_{2s}(3) \\ &\quad - \Psi_{2p}(2)^* \Psi_{1s}(2) \Psi_{1s}(3)^* \Psi_{2s}(3)\,] .\end{aligned} \tag{13}$$

The $1s$ and $2s$ orbitals of Clementi are of the form

$$\Psi_{ns}(\vec{r}) = R_{ns}(r) Y_{00}(\theta, \phi), \quad n = 1, 2, \tag{14a}$$

with

$$R_{ns}(r) = \sum_{i=1}^{2} A_{in} e^{-\xi_{in} r} + \sum_{i=3}^{6} A_{in} r e^{-\xi_{in} r} . \tag{14b}$$

The $2p$ orbital has been taken to be of the form given by Stone,[20]

$$\Psi_{2p}(\vec{r}) = R_{2p}(r) Y_{1m}(\theta, \phi), \tag{15a}$$

with

$$R_{2p}(r) = A r e^{-\xi r}, \tag{15b}$$

where

$$A = 0.228\,205, \tag{15c}$$

$$\xi = 0.5227 . \tag{15d}$$

Both of the terms in Eq. (13) for $\Phi_f^* \Phi_i$ with Φ's of the form (14a) and (15a) lead to the expression (5a), with

$$N_j = 21, \quad n_{k,j} = \begin{cases} 0, & k \leq 3, \\ 1, & 3 < k \leq 11, \\ 2, & 11 < k \leq 21, \end{cases} \tag{16a}$$

for the products of the type $|\Psi_{1s}|^2$ and $\Psi_{2s}^* \Psi_{1s}$, and

$$N_j = 6, \quad n_{k,j} = \begin{cases} 1, & k \leq 2, \\ 2, & 2 < k \leq 6, \end{cases} \tag{16b}$$

for $\Psi_{2p}^* \Psi_{1s}$ and $\Psi_{2p}^* \Psi_{2s}$. The values of $C_{k,j}$ and $\alpha_{k,j}$ appearing in Eq. (5a) are obtained from the value of the parameters A_{in} and ξ_{in} given by Clementi[19] and the values of A and ξ given in Eqs. (15c) and (15d).

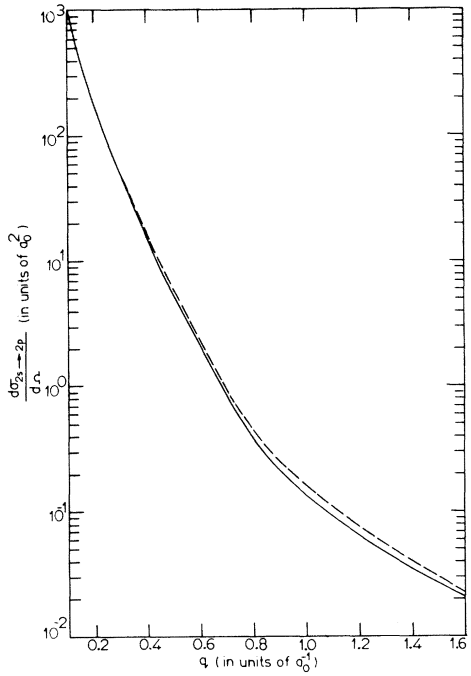

FIG. 1. Differential cross section $d\sigma_{2s\rightarrow 2p}/d\Omega$ (in units of a_0^2 vs momentum transfer $q(a_0^{-1})$ at an electron energy of 54.38 eV ($k = 2$ a.u.). Dashed curve: calculation in the frozen-core Glauber approximation; continuous curve: present calculation.

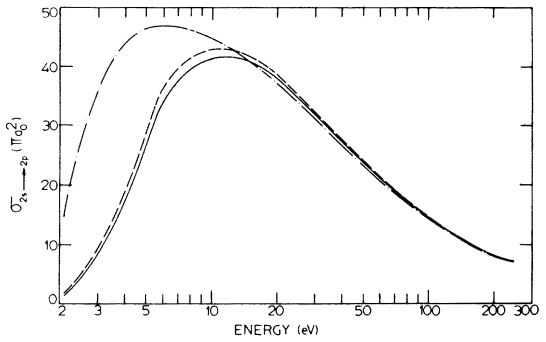

FIG. 2. Total cross sections $\sigma_{2s\rightarrow 2p}$ for electron energies up to 250 eV. Dashed curve: calculation in the frozen-core Glauber approximation; continuous curve: present calculation; dash-dot curve: experimental results of Leep and Gallagher, Ref. 17.

The differential and the total cross sections are given by

$$\frac{d\sigma_{2s\rightarrow 2p}}{d\Omega}=\frac{k_f}{k_i}\left[\,|F_{fi}(\vec{q},m_3'=1)|^2+|F_{fi}(\vec{q},m_3'=-1|^2\right]$$

$$=\frac{2k_f}{k_i}|F_{fi}(\vec{q})|^2 \qquad (17)$$

and

$$\sigma_{2s\rightarrow 2p}=\frac{4}{k_i^2}\int_{k_i-k_f}^{k_i+k_f}|F_{fi}(\vec{q})|^2 q\,dq\,. \qquad (18)$$

IV. RESULTS

In Fig. 1 we have plotted the differential cross section versus the momentum transfer q up to $1.6a_0^{-1}$ at an electron laboratory energy of 54.38 eV ($k=2$ a.u.). The dashed curve corresponds to the calculation in the frozen-core Glauber approximation. This is similar to the calculation by Walters.[10] The continuous curve corresponds to the present calculation. The same wave functions have been used in both calculations. Both curves show almost identical variation, indicating that the inner electrons (those in the $1s$ state) are rather inert, in agreement with our earlier observation in the case of e-Li elastic scattering.[13] In the forward direction, $q\leq 0.4a_0^{-1}$, the two curves overlap as expected. This region is dominated by large-b contributions and the incoming particle does not see much of the inner electrons.

Figure 2 shows the total $2s\rightarrow 2p$ cross sections in units of πa_0^2 for electron energies up to 250 eV. The results for both the frozen-core Glauber and the present calculations again show similar variation. Our results are always smaller than the frozen-core Glauber results and approach them as the energy increases. This is because the inner electrons are more tightly bound and their involvement decreases the calculated cross section. This difference in binding energies is naturally reflected more at lower energies. Both results are in very good agreement above 15 eV with the recent experimental data (dash-dot curve) of Leep and Gallagher.[17] However, at lower energies they appear to fail badly and give a cross-section peak at too high an energy. A more quantitative picture is provided by Table I. It appears that for any further improvement in the Glauber scattering amplitude one should look for corrections by including the exchange effect, polarization of the target, and the next term in the eikonal expansion.

On the procedural side our calculations have further confirmed that Franco's procedure presents no numerical problems.

TABLE I. Comparison of the $2s\rightarrow 2p$ total cross sections at different energies. σ_{FC} and σ are the total cross sections in units of πa_0^2 in the frozen-core Glauber approximation and present calculation, respectively, and σ_E are the experimental results of Leep and Gallagher (Ref. 17) corrected for cascade. The number in parentheses gives the uncertainty in the last place(s) of the preceding number.

Energy (eV)	σ_E	σ_{FC}	σ
2.10(1)	14.8	1.77	1.41
3.10(2)	37.1	10.57	9.15
5.00(3)	46.7	28.93	26.85
10.81(12)	44.3	43.12	41.67
15.64(12)	40.2	41.43	40.41
23.78(12)	34.5	35.99	35.40
38.60(12)	26.93	28.15	27.83
63.56(12)	19.79	20.55	20.40
99.15(15)	14.51	15.00	14.94
149.4(2)	10.67	10.99	10.98
249.9(2)	7.089	7.31	7.30

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