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Generalized oscillator strengths and excitation cross sections for forbidden transitions in lithium

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Generalized oscillator strengths and integrated cross sections from threshold to 1000 eV are calculated in the Glauber approximation for $2s$-$3s$ and $2s$-$3d$ excitations. The calculations are carried out using the Hartree-Fock wave function of Weiss. The results are compared with the Born calculations using the same wave function and available experimental data.

I. INTRODUCTION

In a recent paper (hereafter referred to as I), Tayal and Tripathi[1] have studied the behavior of the generalized oscillator strength (GOS) as a function of momentum transfer for allowed transitions in lithium using Glauber approximation. We have shown that the Glauber approximation predicts the occurrence of the minima and maxima in the GOS and the positions of these extrema shift with the energy of the projectile, in contrast to the results of the Born approximation. It has been known for some time that the Glauber approximation gives a good account of the experimentally well-known departures from the first Born approximation for the excitation cross sections. Although several theoretical calculations of the electron-excitation cross section for the $2s$-$2p$ transition of lithium have been carried out, there have been relatively few studies for the excitation to higher states. Experimental data for electron-impact excitation of the lithium S and D states over a wide range of energy have recently become available.[2,3] Recently Tripathi[4] carried out a systematic calculation of the GOS and total cross sections for several transitions in lithium in the first Born approximation using the Hartree-Fock (HF) wave function of Weiss.[5] Greene and Williamson[6] used Born, Bethe, and Ochkur approximations in their calculations on the electron impact excitation of lithium, while McCavert and Rudge[7] used variation principle in their low-energy calculations. In this paper we have extended the work of I to study the GOS and excitation cross sections for optically forbidden transitions $2s$-$3s$ and $2s$-$3d$ in the Glauber approximation. We have used the Hartree-Fock wave functions of Weiss[5] to describe the initial and final states of lithium. In Sec. II, we give a brief description of the theoretical method and the details of calculation. The results are presented and discussed in Sec. III.

II. THEORY

The details of the theory are given elsewhere. However, we shall rewrite some of the equations of I in order to derive explicitly the Glauber amplitude for $s \rightarrow s$ and $s \rightarrow d$ transitions. We use throughout the notation of I. The Glauber amplitude for the scattering of a charged particle with an atom is written as

$$F^{\rm GA}=\frac{iK_i}{2\pi}\left\langle \psi_f(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)\left|1-\prod_{j=1}^{N}\exp\left(-i\eta\int_{-\infty}^{+\infty}v(r,S_j,Z_j)\,dz_j\right)\right|\psi_i(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)\right\rangle e^{i\vec{K}\cdot\vec{b}}\,db\ , \tag{1}$$

$$\vec{K}=\vec{K}_i-\vec{K}_f,\ \ \text{and}\ \ \eta=1/K_i\ ,$$

where $\vec{K}_i$, $\vec{K}_f$, and $\vec{K}$ denote, respectively, the initial and final wave vectors and momentum transferred to the target as a result of the collision. The product of the bound-state wave function is assumed to have the form

$$\psi_f^*\psi_i=\prod_{j=1}^{3}P_j\ , \tag{2}$$

where

$$P_j=a_j\left(\sum_{k=1}^{N_j}C_{k,j}r_j^{n_{k,j}}e^{-\alpha_{k,j}r_j}\right) \tag{3}$$

with

$$a_1=a_2=a_3=1/4\pi$$

for $s \rightarrow s$ transitions or

$$a_1=a_2=1/4\pi\ ,$$

and

$$a_3=Y_{2m_3'}(\theta_3,\phi_3)/\sqrt{4\pi}$$

for $s \rightarrow d$ transitions. Use of Eq. (2) in Eq. (1) gives

$$F^{\rm GA}=\frac{K_i}{2\pi i}\int d\vec{b}\,e^{i\vec{K}\cdot\vec{b}}\prod_{j=1}^{3}P_j\left(\frac{|\vec{b}-\vec{s}_j|}{b}\right)^{2i\eta}d\vec{r}_j\ . \tag{4}$$

The contribution of the integrals over r_j appearing in Eq. (4) is written as

$$\int P_j\left(\frac{|\vec{b}-\vec{s}_j|}{b}\right)^{2i\eta} dr_j = b^2E(\eta)\sum_{k=1}^{N_j} C_{k,j}(-1)^{1+n_{k,j}}\left(\frac{\partial}{\partial\alpha_{k,j}}\right)^{1+n_{k,j}}\int_0^\infty dt\frac{t^{-2i\eta}[J_1(t)+2tJ_0(t)/(t^2+\alpha_{k,j}^2b^2)]}{(t^2+\alpha_{k,j}^2b^2)} = T_j(b) \quad . \tag{5}$$

$T_1(b)$, $T_2(b)$, and $T_3(b)$ for $s\rightarrow s$ transitions are given by Eq. (5), while for $s\rightarrow d$ transitions $T_1(b)$ and $T_2(b)$ with factors P_1 and P_2 are given by Eq. (5) and $T_3(b)$ with P_3 can be written as

$$\int P_3\left(\frac{|\vec{b}-\vec{s}_3|}{b}\right)^{2i\eta} d\,\vec{r}_3 = \frac{1}{\sqrt{4\pi}}\left(\frac{2l_3'+1}{4\pi}\frac{(l_3'-m_3')!}{(l_3+m_3')!}\right)^{1/2}(-1)^{m_3'}\int\sum_{k=1}^{N_3} C_{k,3}(s_3^2+z_3^2)^{n_{k,3}/2}e^{-\alpha_{k,3}(s_3^2+z_3^2)^{1/2}}$$
$$\times\left(\frac{|\vec{b}-\vec{s}_3|}{b}\right)^{2i\eta}P_{l_3'm_3'}\left(\frac{z_3}{(s_3^2+z_3^2)^{1/2}}\right)e^{-im_3'\phi_3}s_3ds_3d\phi_3dz_3 \ , \tag{6}$$

where $l_3'=2$ and $m_3'=0,\ \pm1,\ \pm2$. For $m_3'=0$,

$$P_{20}=\left(1-\frac{3/2s_3^2}{(s_3^2+z_3^2)}\right) \ . \tag{7}$$

For $m_3'=\pm1$, $P_2\pm1$ is an odd function of z_3 and, therefore, the integral over z_3 vanishes. For $m_3'=\pm2$, the contribution corresponding to $m_3'=2$ is the same as for $m_3'=-2$ and

$$P_{22}=\frac{3s_3^2}{(s_3^2+z_3^2)} \ . \tag{8}$$

Finally, the scattering amplitude is obtained by putting T_1, T_2, and T_3 in Eq. (4) and carrying out integration over ϕ_b,

$$F^{\rm GA}=iK_i\int_0^\infty db\,bJ_0(Kb)\left(1-\prod_{j=1}^{3}T_j(b)\right) \tag{9}$$

for $s\rightarrow s$ transitions and

$$F^{\rm GA}=-iK_ie^{-2i\phi_k}\int_0^\infty db\,bJ_2(Kb)\prod_{j=1}^{3}T_j(b) \tag{10}$$

for $s\rightarrow d$ transitions. The GOS is obtained from the Glauber differential cross section $(d\sigma/d\Omega)^{\rm GA}$ using the relation

$$f_{i\rightarrow f}^{\rm GA}(\vec{K})=\frac{\Delta E_{i\rightarrow f}}{2}K^2\frac{K_i}{K_f}\left(\frac{d\sigma}{d\Omega}\right)^{\rm GA} \ , \tag{11}$$

where $\Delta E_{i\rightarrow f}$ is the excitation energy.

The total wave function for the lithium atom in the ground state is expressed as a determinant of the one-electron spin-orbital function

$$\psi_i=\frac{1}{\sqrt{6}}\sum_{\rm cyc}\beta_1\alpha_2\alpha_3\phi_{1s}[\phi_i(2)\phi_{1s}(3)-\phi_i(3)\phi_{1s}(2)] \ , \tag{12}$$

where ϕ is the spatial part of the spin orbital; α and β refer to the components of the spin part. These orbitals are expanded in terms of one-electron Slater-type orbital basis functions; we have orthogonalized the excited-state wave function by the usual Schmidt orthogonalization procedure. The values of the parameters $C_{k,j}$ and $\alpha_{k,j}$ appearing in Eq. (3) are obtained from the coefficients and exponents of the wave function tabulated by Weiss.[5]

III. RESULTS AND DISCUSSION

Plots of the GOS as a function of the square of momentum transfer K^2 for optically forbidden $2s$-$3s$ and $2s$-$3d$ transitions are shown in Figs. 1 and 2. The GOS's for these

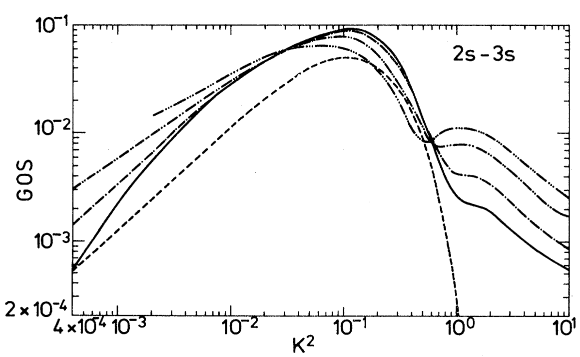

FIG. 1. Generalized oscillator strengths for the $2s$-$3s$ transition as a function of K^2. — — —, Born calculation; Glauber calculations: ——, at 1000 eV; —·—·—, at 500 eV; —··—··—, at 200 eV; —···—···—, at 100 eV.

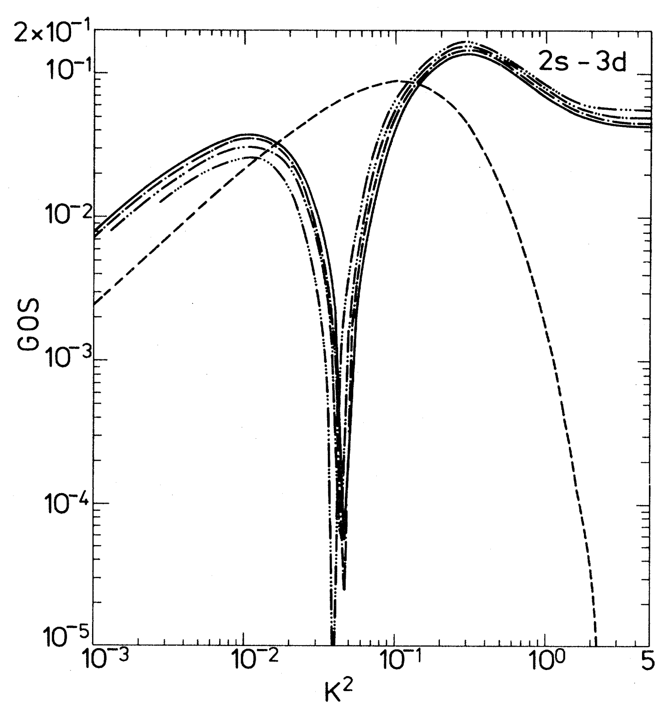

FIG. 2. Same as in Fig. 1 but for $2s$-$3d$ transition.

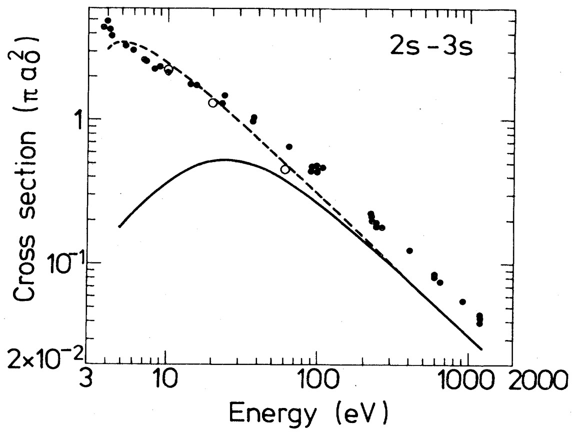

FIG. 3. Total electron impact excitation cross section for $2s$-$3s$ transition. — — —, Born calculation; ——, Glauber calculation; ●, experimental data of Zajone and Gallagher; ○, experimental data of Williams, Trajmar, and Bozinis.

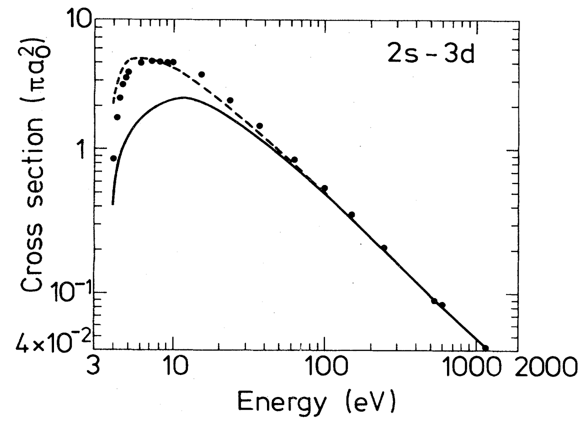

FIG. 4. Same as in Fig. 3 but for $2s$-$3d$ transition.

transitions approach zero as $K \rightarrow 0$. For comparison, we also present in these figures the Born GOS calculated in the length formulation by Tripathi[4] using the same wave functions. The Glauber GOS's clearly show minima and maxima in the K space. As K increases from zero, the Glauber GOS for both transitions at first increases, attaining a maximum value, and then decreases and passes through a series of minima. The importance of the minima has been discussed by Inokuti, Itikawa, and Turner[8] and is related to the nodal structure of the wave functions involved in the transition. We have plotted Glauber GOS at several energies (100–1000 eV). It is easily seen that the positions of the minima shift towards larger K values as incident energy is increased.

For the $2s$-$3s$ transition, the general trend of variation for the Born GOS and Glauber GOS at high impact energies is similar up to about $K = 0.7$ a.u., although the Born value is smaller by a factor of about 2. Beyond this K value the Born GOS falls off rapidly compared to Glauber GOS results. For $2s$-$3d$ transition (Fig. 2), the Born and Glauber calculations differ widely in shape and magnitude in the entire K region. It is seen that the Glauber GOS dominates over the Born GOS in the region of large K. This is due to the fact that the first Born approximation does not account for scattering by the nucleus while the Glauber approximation explicitly includes the nuclear potential contribution.

We have integrated the differential cross sections to obtain the total cross sections. In Figs. 3 and 4, we have displayed the integrated cross sections for the forbidden $2s$-$3s$ and $2s$-$3d$ transitions along with the Born results of Tripathi[4] and experimental data of Zajonc and Gallagher.[2] We have also shown the experimental results of Williams, Trajmar, and Bozinis[3] for $2s$-$3s$ transition in Fig. 3. For $2s$-$3s$ transition, it is seen that the Glauber predictions are lower than the Born results for energies less than 200 eV and thereafter the two results merge with each other. For $2s$-$3d$ transition, the Glauber values lie below the Born results from 50 eV down to threshold while for energies from 50 to 1000 eV they are in excellent agreement. The experimental data of Zajonc and Gallagher for $2s3s$ transition show a peak near threshold and remain higher throughout the energy region, whereas they agree better with the $2s$-$3d$ results. The data of Williams, Trajmar, and Bozinis also lie much above the present calculation and lie close to the Zajonc and Gallagher measurements. The convergence to the high-energy limit is obtained better for the $2s$-$3d$ transition than for the $2s$-$3s$ case. The poor agreement with experiment for the $2s$-$3s$ transition is rather disappointing and, therefore, further investigations are needed to clear the situation.

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