Spin asymmetry, alignment, and coherence in electron-lithium resonant excitation

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A two-potential localized exchange approach is used to study the coherence and alignment in electron-lithium resonant (2*s*-2*p*) excitation processes at intermediate electron energies of 10, 15, and 20 eV. Furthermore, the total and differential spin asymmetry in the resonant scattering of spin-polarized electrons with spin-polarized lithium atoms is also investigated.

The study of alignment and coherence in electron-atom collision processes provides significant information about the shape and dynamics of the states excited in collision. Two types of experiments (coherence and correlation experiments) have been performed[1] to obtain the above information experimentally. In the correlation experiments one measures the angular distribution of photons in coincidence with scattered electrons, while in coherence experiments the polarization of the emitted photons is determined in coincidence with scattered electrons. The information obtained by these experiments can be characterized in various ways. A detailed discussion about the same experiment has been given by Andersen *et al.*[2] They have shown that parameters such as the alignment angle (γ) of the charge cloud with respect to the incident electron direction provide characteristic insight into the dynamics of the collision process. The alignment angle is directly related to the experimentally measured components of polarization (P_1,P_2,P_3) of the emitted photon, in a plane perpendicular to the scattering plane, viz.,

$$\gamma=\tfrac{1}{2}\tan^{-1}(P_2/P_1) . \tag{1}$$

The coherence of excitation is implied by

$$|P|=(P_1^2+P_2^2+P_3^2)^{1/2}=1 . \tag{2}$$

In recent years it has been possible to develop polarized electron beams and polarized targets.[3,4] The study of spin asymmetry in the scattering of spin-polarized electrons with spin-polarized targets provides useful information about the contribution of exchange to the scattering process. The spin asymmetry A is defined as,

$$A=[\sigma(\uparrow\downarrow)-\sigma(\uparrow\uparrow)]/[\sigma(\uparrow\downarrow)+\sigma(\uparrow\uparrow)] , \tag{3}$$

where $\sigma(\uparrow\downarrow)$ and $\sigma(\uparrow\uparrow)$ are the differential cross sections for spin-antiparallel and spin-parallel scattering, respectively, and are given by

$$\begin{aligned}\sigma(\uparrow\downarrow)&=|f|^2+|g|^2 ,\\ \sigma(\uparrow\uparrow)&=|f-g|^2 ,\end{aligned} \tag{4}$$

where f and g are the direct and exchange scattering amplitudes, respectively.

Recently, I have studied[5] the parameters of Eqs. (1)–(3) for electron-hydrogen inelastic scattering. In the present paper I extend the above study to electron-lithium resonant (2*s*-2*p*) scattering. We use the two-potential approach, which has been found in our earlier studies[5–7] to yield reliable results for the differential cross sections, angular correlation parameters, and spin asymmetries at intermediate electron energies. In this energy regime the close-coupling approach will not be suitable as many channels would become open and to account for them all would be very difficult.

Since the alkali-metal atoms behave more or less like one-electron systems, we assume the lithium atom to be a one-valence-electron system with a frozen core. It is assumed that during scattering from an initial atomic state to a final atomic state, the core orbitals remain fixed and only the valence-electron state undergoes a change. The effect of core electrons is taken into consideration in the form of a core potential. The total Hamiltonian of the electron-lithium system is given by

$$\begin{aligned}H&=-\tfrac{1}{2}(\nabla_1^2+\nabla_2^2)-\frac{1}{r_1}+V_c(r_1)+\frac{1}{r_{12}}-\frac{1}{r_2}+V_c(r_2)\\ &=H_0+V ,\end{aligned} \tag{5}$$

with

$$V=\frac{1}{r_{12}}-\frac{1}{r_2}+V_c(r_2) ,$$

where $V_c(r)$ is the core potential given by[6,8]

$$V_c(r)=-2\left[\frac{1}{r}+2.7\right]e^{-5.4r} . \tag{6}$$

$\mathbf{r}_1$ and $\mathbf{r}_2$ are the position vectors of the valence and incident electrons, respectively. H_0 is the unperturbed Hamiltonian. The above model of the lithium atom is similar to that used by Walters[8] in electron–alkali-metal-atom scattering. Dividing the total interaction potential V into two parts, viz.,

$$V=U_i+W_i \tag{7a}$$

in the initial channel and

$$V=U_f+W_f \tag{7b}$$

in the final channel, the T matrix in the two-potential approach for inelastic scattering with exchange included is given by[6,9]

$$T_{\pm}=\langle\chi_f^-(\mathbf{r}_1,\mathbf{r}_2)|W_f|(\psi_i^+(\mathbf{r}_1,\mathbf{r}_2)\pm\psi_i^+(\mathbf{r}_2,\mathbf{r}_1))\rangle$$
$$=-2\pi(f\pm g)\ , \tag{8}$$

where, to the first order, the direct and exchange scattering amplitudes are given by

$$f=-(2\pi)^{-1}\langle\chi_f^-(\mathbf{r}_1,\mathbf{r}_2)|W_f|\chi_i^+(\mathbf{r}_1,\mathbf{r}_2)\rangle\ , \tag{9}$$

$$g=-(2\pi)^{-1}\langle\chi_f^-(\mathbf{r}_1,\mathbf{r}_2)|W_f|\chi_i^+(\mathbf{r}_2,\mathbf{r}_1)\rangle\ . \tag{10}$$

The functions χ and ψ satisfy the Schrödinger equations,

$$\begin{aligned}&(H_0+U_i-E)\chi_i^+(\mathbf{r}_1,\mathbf{r}_2)=0\ ,\\&(H_0+U_f-E)\chi_f^-(\mathbf{r}_1,\mathbf{r}_2)=0\ ,\\&(H-E)\psi_i^+(\mathbf{r}_1,\mathbf{r}_2)=0\ .\end{aligned} \tag{11}$$

As in our earlier work[6] we choose the distorting potentials U_i and U_f to be

$$\begin{aligned}&U_i=V_s^i+V_c+V_p^{\mathrm{na}}\ ,\\&U_f=V_s^f+V_c\ ,\end{aligned} \tag{12}$$

where V_s^j is the static potential in the channel j and V_p^{na} is the nonadiabatic polarization potential. Explicit expressions for the same are given in our earlier paper.[6]

The χ's are obtained by solving Eq. (11) along with the use of Eq. (12). These are then used in Eqs. (9) and (10) to obtain the direct and exchange amplitudes. The nonlocal character of Eq. (10), however, makes its numerical evaluation, difficult and time-consuming. Therefore, in practice, local approximations have been developed in the literature to evaluate Eq. (10). A comparative numerical study of the various types of local approximations has been made by Bransden *et al.*[10] and Bransden and McDowell.[11] They have concluded that the local approximations suggested by Furness and McCarthy[12] and Riley and Truhlar[13] provide a fairly accurate representation to Eq. (10) even up to lower energies. In view of the above we use the local approximation to evaluate the exchange amplitude.

Following Bransden *et al.*[10] and Furness and McCarthy,[12] and writing $\chi_j(\mathbf{r}_1,\mathbf{r}_2)=F_j(\mathbf{r}_2)v_j(\mathbf{r}_1)$, we obtain the local approximation to Eq. (10) as[7]

$$g=-\left\langle F_f^-(\mathbf{r}_2)v_f(\mathbf{r}_2)\left|\left[\frac{1}{K_i^2}+\frac{1}{K_f^2}\right]\right|F_i^+(\mathbf{r}_2)v_i(\mathbf{r}_2)\right\rangle\ , \tag{13}$$

with

$$K_j^2=k_j^2-2U_j\ ,$$

where $\mathbf{k}_j$ is the momentum vector of the scattered electron. The spin-averaged differential cross section is given by

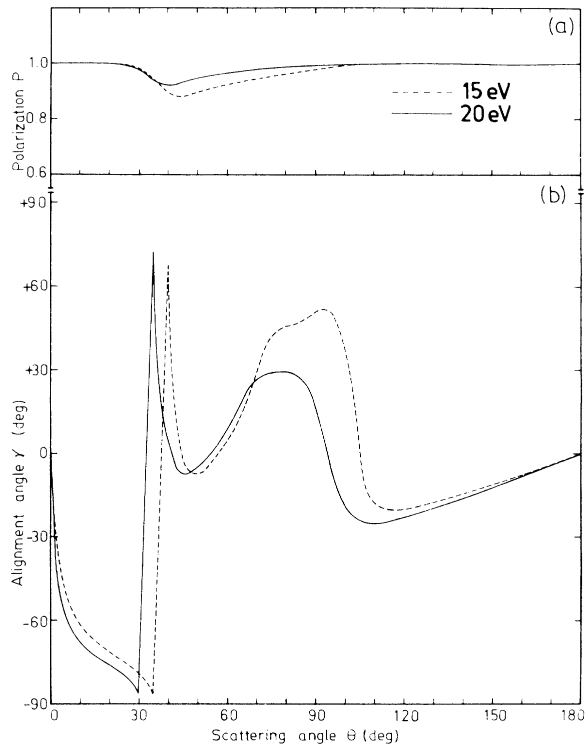

FIG. 1. Polarization P and alignment γ at 15- and 20-eV electron energy. — — —, present results at 15 eV; ——, present results at 20 eV.

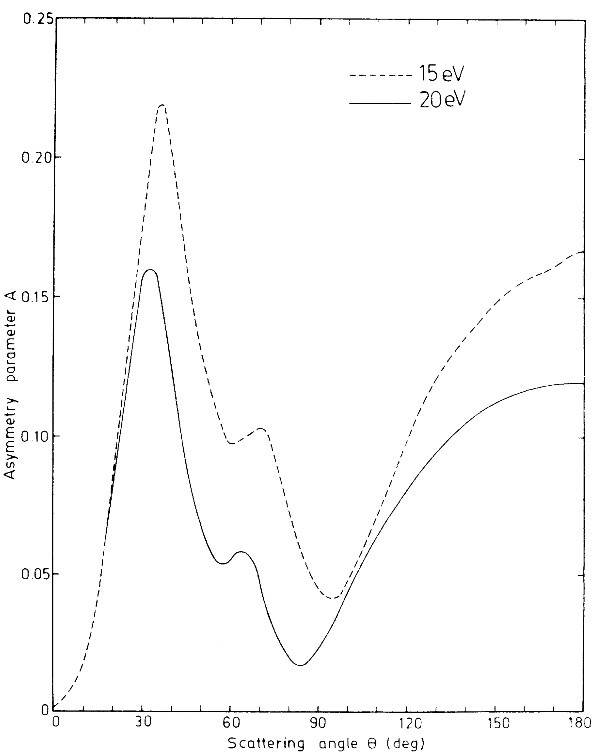

FIG. 2. Spin asymmetry A at 15- and 20-eV electron energy. Symbols mean the same as in Fig. 1.

TABLE I. Comparison of theoretical and experimental results for differential asymmetry.

	$E_i = 10$ eV			$E_i = 15$ eV			$E_i = 20$ eV		
θ (deg)	Experiment (Ref. 14)	Theory (Ref. 15)	Present results	Experiment (Ref. 14)	Theory (Ref. 15)	Present results	Experiment (Ref. 14)	Theory (Ref. 15)	Present results
65	-0.206 ± 0.019	0.10	0.225	-0.289 ± 0.037	0.06	0.100	-0.194 ± 0.046	0.01	0.058
90	-0.034 ± 0.042	0.12	0.215	$-0.31\ \pm0.049$	-0.08	0.045	-0.298 ± 0.065	0.25	0.022
107.5	-0.217 ± 0.045	-0.03	0.147		-0.16	0.065		0.45	0.059

$$\sigma = \frac{k_f}{k_i}\left(\tfrac{1}{4}|f+g|^2 + \tfrac{3}{4}|f-g|^2\right) . \tag{14}$$

The polarization components P_1, P_2, and P_3 are obtained following the procedure outlined in our earlier papers.[5,6] The alignment angle γ, coherence P, and spin asymmetry A are then calculated using Eqs. (1), (2), and (3), respectively.

Figures 1(a) and 1(b) show, respectively, the variation of coherence parameter P and the alignment angle γ with scattering angle at incident electron energies of 15 and 20 eV. From Fig. 1(a) it is seen that the minimum value of the coherence is obtained around a 45° scattering angle for 15-eV energy and around a 40° scattering angle for 20-eV energy. At both energies we find that for scattering angles below 20° and beyond 100° the value of $|P|$ is obtained nearly equal to unity, showing that in these angular regions the excitation process is completely coherent. Also we see that as the energy increases the excitation process becomes more coherent.

From Fig. 1(b) we see that the alignment angle goes on increasing in the negative direction and acquires its maximum negative value at around 35° for 15-eV energy and 30° for 20-eV energy. The negative value of γ signifies that the charge cloud is aligned away from the scattered electrons. A sudden jump in the alignment angle is noticed between 35° and 40° scattering angles for 15-eV and 30° and 35° for 20-eV energy. We have found that this sudden change in γ corresponds to those scattering angles where the angular momentum transfer is maximum during the collision process. It is also interesting to note that the minimum coherence is obtained in the region of maximum transfer of angular momentum. The variation of γ in the large-angle region follows the changes in the magnitude and sign of the angular momentum transferred.

Figure 2 shows our results for the variation of asymmetry parameter A with scattering angle at 15- and 20-eV incident electron energies. From the figure one sees that, for both the energies, there is a rapid increase in the asymmetry at low scattering angles. The maximum value of asymmetry is obtained between 30° and 40°, beyond which there is a rapid decrease. The minimum value of asymmetry is obtained at about 95° for 15-eV energy and 85° for 20-eV energy. In the entire angular region, the asymmetry is signficantly higher for 15-eV electron energy as compared to 20-eV electron energy.

TABLE II. Comparison of theoretical and experimental results for total asymmetry.

Energy (eV)	Present results	Experiment (Ref. 16)
10	0.054	0.026 ± 0.020[a]
15	0.028	0.035 ± 0.025
20	0.018	

[a]At 10.2 eV.

Recently, Baum *et al.*[14] have measured differential, asymmetries at three scattering angles 65°, 90°, and 107.5°. In Table I we compare our results at 10-, 15-, and 20-eV energies with the experimental data[14] and the two-state close-coupling calculation of Burke and Taylor[15] (obtained from the figures of Baum *et al.*[14]). From the table we notice that there is little agreement between either of the theories and the experimental data at these energies.

Besides the difference in the method of treating the exchange, the possible reason for the discrepancy between the two theories could be due to their different energy range of applicability. While the two-state close-coupling method would be good in an energy region close to the threshold, the two-potential approach is more suitable (see Figs. 1 and 2 of Saxena and Mathur[6]) in the intermediate-energy range, which is the region of interest in the present work.

Further, since the differential asymmetry data is available at present only at three scattering angles (65°, 90°, and 107.5°), it is difficult to draw any conclusions about the validity of the theory with respect to the experiment. It may, however, be mentioned that at the three angles where measurements have been reported, the differential cross sections for singlet and triplet scattering are small in magnitude and therefore the measurement of asymmetry is very difficult.

In Table II we compare our results for the total asymmetry (integrated over scattering angles) with the experimental data of Baum *et al.*[16] It is seen that our results for the total asymmetry are in reasonable accord with the experimental data.

It is concluded that more experimental and theoretical work is needed to obtain a better understanding of the differential and total asymmetry in electron-lithium scattering.

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