Elastic scattering of electrons and positrons by lithium atoms

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A two-potential approach is used to study the elastic scattering of electrons and positrons by lithium atoms in the intermediate-energy region. Within the framework of the two-potential method, the effect of close coupling is considered by including the closely lying $2p$ state in the distorted-wave representation of the total scattering wave function. Differential and integrated cross sections are calculated for the elastic electron and positron scattering. The differential spin asymmetry and ratio R of the triplet-to-singlet cross section are also calculated to study the effect of exchange for electron scattering. The results thus obtained are compared with available experimental data and other available theoretical calculations.

I. INTRODUCTION

The study of spin dependence in electron-atom scattering has been receiving considerable attention in recent years both theoretically and experimentally. The measurement of spin asymmetry in the scattering of spin-polarized electrons with spin-polarized low-Z atoms provides useful information about the exchange contribution to the scattering. With the development of polarized electron beams,[1,2] it has become possible to measure the spin asymmetries in the elastic and inelastic scattering of polarized electron with polarized atoms. The measurements of differential spin asymmetry are, however, at present limited to a few scattering angles only. Theoretically, several studies have been performed on electron-hydrogen elastic and inelastic spin asymmetry;[3] however, measurements on hydrogen have so far been reported for elastic scattering only.[4] For the helium atom Mathur *et al.*[5] have studied theoretically the spin dependence in the inelastic scattering of electrons from the triplet metastable $2\,^3S$ state. In electron-lithium resonant excitation measurements of spin asymmetry have been reported by Baum *et al.*[6] Theoretical calculations for this process have been performed by Mathur,[7] and Burke and Taylor.[8] For electron-sodium resonant scattering, Mathur and Purohit[9] have recently reported theoretical calculations on spin asymmetry. McClelland, Kelly, and Celotta[10] have reported measurements on elastic and superelastic scattering of polarized electrons with polarized sodium atoms.

Recently Baum *et al.*[11] have studied the energy dependence of spin asymmetry in the elastic scattering of polarized electrons from polarized lithium atoms at three scattering angles 65°, 90°, and 107.5° for incident electron energies from 1 to 30 eV. In this paper we report a theoretical calculation for the differential spin asymmetry in the polarized electron-polarized lithium-atom elastic scattering at energies from 10 to 60 eV, and compare these results with the above experimental data[11] and other theoretical calculations.[8,12,13] The results for the differential and total elastic cross sections are compared with the experimental[14] and theoretical results.[12,15,16] We use a two-potential localized-exchange approach. Within the framework of this two-potential approach, we also consider the effects of close coupling by including the closely lying $2p$ state in the distorted-wave representation of the total scattering function.

Recent developments in the experimental measurements on the positron-atom scattering and the comparative study of electron and positron scattering stimulate us to study the positron elastic scattering with the lithium atom. Stein *et al.*[17,18] and Kwan *et al.*[19] have reported measurements for the positron alkali-metal (K,Na,Rb,Cs) atom scattering, and Smith *et al.*[20] for the elastic scattering of positrons with inert gases (Ar and Ne). Theoretically the close-coupling calculations for the positron-lithium scattering have been reported recently by Ward *et al.*;[21] Sarkar and co-workers;[22] and Khan, Dutta, and Ghosh.[23] The eikonal Born series and the modified Glauber approximation have also been used for the electron and positron alkali-metal scattering.[24] Dai and Stauffer[25] calculated the e^+-Li elastic scattering using the modified polarized-orbital method. Tayal, Tripathi, and Srivastava[26] studied the elastic scattering of positron by the lithium atom using the two-potential eikonal approximation, and corrected static, and the modified corrected static approximations. Mukherjee and Sural[16] used the integral approach to the second-order potential method for $e^{\pm}$ scattering by H, He, and Li. Guha and Ghosh[27] calculated the elastic scattering of positrons with the lithium atom using the polarized-orbital method in an adiabatic coupled static method.

In addition to the electron scattering we also report here our results, based on the two-potential approach with the inclusion of the effect of coupling to the closely lying state, for the positron-lithium scattering. We have calculated the differential and the total cross sections between 10 and 60 eV, where some other theoretical calculations are also available for comparison with the present results. Since the positronium formation in the positron alkali-metal scattering begins even at zero energy, the positronium formation cross section would be very small for the intermediate energies studied here. In view of this, we have neglected the positronium formation channel in the present calculation.

II. THEORY

We assume the lithium atom to be a one-valence-electron system with a core. The total Hamiltonian of the projectile plus the lithium-atom system is then written (in a.u.) as

$$H=-\tfrac{1}{2}(\nabla_1^2+\nabla_2^2)-\frac{1}{r_1}+V_c(r_1)+V_c(r_2)-\frac{Z'}{r_{12}}+\frac{Z'}{r_2}\ ,$$
$$H=H_0+V \quad \text{with} \quad V=-\frac{Z'}{r_{12}}+\frac{Z'}{r_2}+V_c(r_2)\ , \tag{1}$$

where $\mathbf{r}_1$ and $\mathbf{r}_2$ are the position coordinates of the valence electron and the incident particle, respectively; $V_c(r)$ is the core potential; Z' is -1 for electron scattering and $+1$ for positron scattering. ∇_1^2 and ∇_2^2 are the kinetic-energy operators. In the two-potential approach, the T matrix for the elastic scattering is given by[1]

$$T=\langle\phi|U|\chi^+\rangle+\langle\chi^-|W|\mathcal{A}\psi^+\rangle\ . \tag{2}$$

$\mathcal{A}$ is the antisymmetrization operator. For the positron scattering $\mathcal{A}$ is ignored. The interaction potential between the incident particle and the lithium atom is divided as

$$V=U+W\ . \tag{3}$$

Since we assume U to be dependent on the incident particle coordinate only, it will not contribute to exchange scattering. Therefore the antisymmetrization operator $\mathcal{A}$ does not appear in the first term of Eq. (2). The functions ϕ, χ, and ψ satisfy the Schrödinger equations

$$(H_0-E)\phi(\mathbf{r}_1,\mathbf{r}_2)=0\ ,$$
$$(H_0+U-E)\chi(\mathbf{r}_1,\mathbf{r}_2)=0\ , \tag{4}$$
$$(H-E)\psi(\mathbf{r}_1,\mathbf{r}_2)=0\ ,$$

where E is the total energy of the system. Considering close coupling effects and making the usual distorted-wave approximation, we write

$$\psi^+(\mathbf{r}_1,\mathbf{r}_2)=\chi_i^+(\mathbf{r}_1,\mathbf{r}_2)+\chi_n^+(\mathbf{r}_1,\mathbf{r}_2)\ , \tag{5}$$

where i denotes the initial ground state of the atom ($2s$) and n is an excited state. For lithium the state n is taken to be the closely lying $2p$ state which accounts for 98% of the polarizability of the lithium atom.

The direct (f) and the exchange (g) scattering amplitudes for the elastic scattering from the initial state i are then given by

$$f=-(2\pi)^{-1}\{\langle\phi_i(\mathbf{r}_1,\mathbf{r}_2)|U_i|\chi_i^+(\mathbf{r}_1,\mathbf{r}_2)\rangle+\langle\chi_i^-(\mathbf{r}_1,\mathbf{r}_2)|W_i|[\chi_i^+(\mathbf{r}_1,\mathbf{r}_2)+\chi_n^+(\mathbf{r}_1,\mathbf{r}_2)]\rangle\} \tag{6}$$

and

$$g=-(2\pi)^{-1}\{\langle\chi_i^-(\mathbf{r}_1,\mathbf{r}_2)|W_i|[\chi_i^+(\mathbf{r}_2,\mathbf{r}_1)+\chi_n^+(\mathbf{r}_2,\mathbf{r}_1)]\rangle\}\ . \tag{7}$$

We express

$$\chi_j^\pm(\mathbf{r}_1,\mathbf{r}_2)=F_j^\pm(\mathbf{r}_2)v_j(\mathbf{r}_1),\quad j=i \text{ or } n \tag{8}$$

where $F_j(\mathbf{r}_2)$ is the scattered particle wave function and $v_j(\mathbf{r}_1)$ the bound-state atomic wave function. $\mathbf{k}_j$ is the momentum of the scattered particle. The scattering function $F_j(\mathbf{r}_2)$ satisfies the equation

$$[\tfrac{1}{2}\nabla_2^2-U_j(r_2)+\tfrac{1}{2}k_j^2]F_j(\mathbf{r}_2)=0\ . \tag{9}$$

For the evaluation of the exchange term in Eq. (7), we use the local exchange approximation (Bransden *et al.*,[28] Furness and McCarthy,[29] and Mathur[3]) and obtain

$$g=-\left\langle F_i^-(\mathbf{r}_2)v_i(\mathbf{r}_2)\left|\frac{1}{K_{i,n}^2}+\frac{1}{K_i^2}\right|[F_i^+(\mathbf{r}_2)v_i(\mathbf{r}_2)+F_n^+(\mathbf{r}_2)v_n(\mathbf{r}_2)]\right\rangle\ , \tag{10}$$

where $K_j^2=k_j^2-2U_j$, $j=i$ or n.

To evaluate f and g we make the partial-wave expansion of $F_j^\pm(\mathbf{r}_2)$. The function $F_j^\pm(\mathbf{r}_2)$ can be expanded in partial waves as

$$F_j^\pm(\mathbf{r}_2)=k_j^{-1/2}r_2^{-1}\sum_{l=0}^{\infty}(2l+1)i^l\exp[\pm i\delta_l(k_j^2)]\times u_l(k_jr_2)P_l(\cos(\hat{k}_j\cdot\hat{r}_2))\ , \tag{11}$$

where δ_l is the phase shift of the lth partial wave, u_l are the radial functions, and P_l are the Legendre polynomials. The resulting infinite sums over partial waves in Eqs. (6)–(11) are performed by replacing the matrix elements for high l values by the corresponding full Born values.[30]

The distorting potential U_j is expressed as

$$U_j=V_c+V_s^j+V_p^j\ , \tag{12}$$

where V_c is the core potential[30]

$$V_c(r_2)=2Z'\left[\frac{1}{r_2}+2.7\right]e^{-5.4r_2}\ . \tag{13}$$

The static potential V_s^j is given by

$$V_s^j=\langle v_j(\mathbf{r}_1)|V|v_j(\mathbf{r}_1)\rangle\ . \tag{14}$$

The polarization potential V_p^j is taken to be the nonadiabatic polarization potential (V_p^{na}), which is expressed as[30]

$$V_p^{\rm na}=\frac{V_p^a}{(1+6k_j^2/\omega^2 r_2^2)} \ ; \tag{15}$$

ω is the average excitation energy. For evaluating the adiabatic polarization potential V_p^a, we follow the polarized-orbital approach of Stone.[31] In this approach V_p^a is given by

$$V_p^a=\langle v_j(\mathbf{r}_1)|V|v_j^{\rm pol}(\mathbf{r}_1,\mathbf{r}_2)\rangle \ . \tag{16}$$

The first-order perturbed wave function for the *ns* and *np* states, respectively, is written as[5]

$$\begin{aligned} v_{ns}^{\rm pol}(\mathbf{r}_1,\mathbf{r}_2)&=\beta_{ns}(r_2)\sum_m Y_{lm}^*(\hat{\mathbf{r}}_2)v_{\rm npm}(\mathbf{r}_1) \ , \\ v_{npm}^{\rm pol}(\mathbf{r}_1,\mathbf{r}_2)&=\beta_{np}(r_2)Y_{lm}(\hat{\mathbf{r}}_2)v_{ns}(\mathbf{r}_1) \ . \end{aligned} \tag{17}$$

The functions β are obtained by solving the following pair of equations which result from minimizing the energy of the atom:

$$\begin{aligned} \langle v_{ns}(\mathbf{r}_1)|H_A+V-E|[v_j(\mathbf{r}_1)+v_j^{\rm pol}(\mathbf{r}_1,\mathbf{r}_2)]\rangle&=0 \ , \\ \langle v_{npm}(\mathbf{r}_1)|H_A+V-E|[v_j(\mathbf{r}_1)+v_j^{\rm pol}(\mathbf{r}_1,\mathbf{r}_2)]\rangle&=0 \ , \end{aligned} \tag{18}$$

where H_A is the atomic Hamiltonian.

The spin-averaged differential cross section for the electron scattering is obtained from the following equation:

$$\sigma=\tfrac{1}{4}|f+g|^2+\tfrac{3}{4}|f-g|^2 \ . \tag{19}$$

The differential cross section for the positron scattering is obtained from

$$\sigma=|f|^2 \ . \tag{20}$$

The differential spin asymmetry parameter A for the electron scattering is defined by

$$A=\frac{\sigma(\uparrow\downarrow)-\sigma(\uparrow\uparrow)}{\sigma(\uparrow\downarrow)+\sigma(\uparrow\uparrow)} \ , \tag{21}$$

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

$$\begin{aligned} \sigma(\uparrow\downarrow)&=|f|^2+|g|^2 \ , \\ \sigma(\uparrow\uparrow)&=|f-g|^2 \ . \end{aligned} \tag{22}$$

The total cross sections are evaluated by integrating the differential cross sections over the entire angular region

$$Q=\int \sigma \, d\Omega \ . \tag{23}$$

III. RESULTS

Figure 1 shows the spin-averaged differential cross section [Eq. (19)] for the elastic scattering of electron with the lithium atoms at 20 eV energy. In this figure we have compared our results with the only available experimental data of Williams, Trajmar, and Bozinis.[14] The other available theoretical calculations of the differential cross section have not been plotted in this figure for brevity and also to see the suitability of the present theory with respect to the experiment. From the figure it is seen that the present theory yields results which are in reasonable accord with the experimental data of Williams, Trajmar, and Bozinis. In this figure we have also shown our results (dotted curve) obtained by dropping the second term in Eq. (5), i.e., by the neglect of the coupling effects. We notice that the neglect of the coupling effects leads to poor results in the low-angle region.

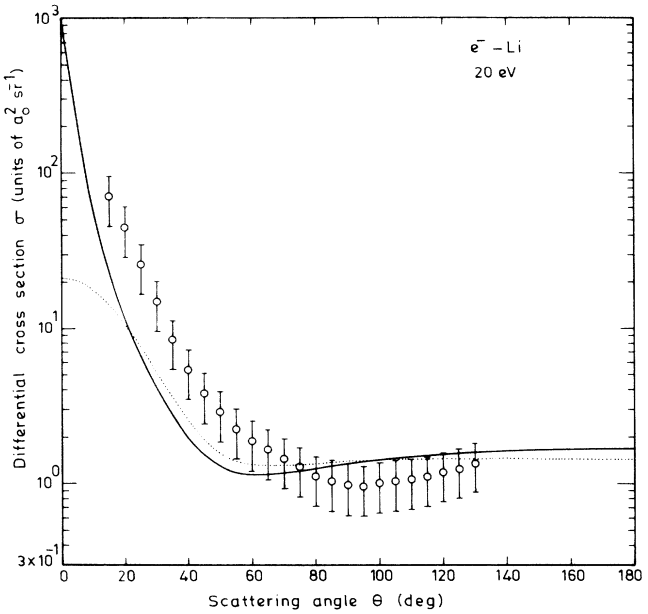

FIG. 1. The spin-averaged differential cross section for electron-lithium elastic scattering at 20 eV. ——, present calculation; . . ., present calculation with neglect of coupling; $\bar{\Phi}$, experimental data of Williams, Trajmar, and Bozinis (Ref. 14).

Figure 2 shows the variation of the total elastic cross section Q for incident electron scattering energies up to 60 eV. The present results are compared with other theoretical calculations, viz. the two-state close-coupling calculation of Issa,[15] the five-state close-coupling calculation of Moores,[12] the integral approach to the second-order potential method by Mukherjee and Sural,[16] and the experimental data of Williams, Trajmar, and Bozinis.[14] It is noticeable from the figure that our calculation agrees well with the close-coupling calculations of Issa and Moores. However, we notice that almost all the theoretical calculations differ with the experimental data. This may be due to the fact that experimentally it is very difficult to distinguish the elastically scattered electrons in the forward direction that significantly contribute to the total cross section.

Figure 3 shows our results for the differential spin asymmetry parameter A at three scattering angles, viz. 65°, 90°, and 107.5° for electron energies between 10 and 60 eV. In this figure we compare our results with the recent measurements of Baum *et al.*[11] and with the other available calculations, viz. the two-state close-coupling calculation of Burke and Taylor,[8] the five-state close-coupling calculation of Moores,[12] and the modified polarized-orbital calculation of Bhatia *et al.*[13]

From Fig. 3(a) at 65° scattering angle, we see that our calculations are in very good agreement with the experi-

mental data at 30 eV and also with the calculations of Burke and Taylor from 30 to 54.4 eV. At 20 eV Burke and Taylor's calculation gives higher asymmetries compared to our calculations. At lower energies our calculations agree well with the calculation of Bhatia *et al.* and are also quite close to the calculation of Moores. The experimental asymmetries are quite low in the region 10–20 eV.

From Fig. 3(b) at 90° scattering angle, we again notice that our results are quite close to the experimental data at 30 eV energy. The agreement of our results with the Burke and Taylor calculation is also good in the energy range beyond 20 eV. In the 10-eV region our results agree well with the calculation of Moores. Also at this angle the experimental data yield lower values of asymmetries up to 20 eV energy.

From Fig. 3(c) at 107.5° scattering angle, we see that the measured asymmetry at 10.6 eV is lower than our calculation. The agreement between our calculations and Burke and Taylor's calculation is again very good for energies beyond 30 eV.

Since the data are available only at three scattering angles, it is very difficult to draw any conclusions about the validity of the various theories in comparison to experiment. More experimental and theoretical work is needed to overcome the present gaps between experiment and theory. In Fig. 4 we give full angular variation of asymmetry at 10, 10.6, 19.9, and 29.8 eV energies for comparison with future measurements.

Figure 5 shows the variation of the ratio R of the triplet $\sigma(\uparrow\uparrow)$ scattering cross section to the singlet $\sigma(\uparrow\downarrow)$ scattering cross section at electron energies 10, 10.6, 19.9, and 29.8 eV. At 10 and 10.6 eV we find that the singlet scattering dominates over the triplet scattering for scattering angles up to about 50°, beyond which the triplet scattering is more prominent up to about 140° scattering angle. Beyond 140° the singlet and the triplet scattering are nearly identical. For higher energies (19.9 and 29.8 eV) also, we find that at lower angles (up to about 35° at 19.9 eV, and up to about 30° for 29.8 eV) the singlet scattering dominates and at intermediate angles (40°–115° at 19.9 eV, and 35° and beyond for 29.8 eV) the triplet scattering dominates. Close to the backward direction the two scatterings tend to become equal, thereby giving nearly zero asymmetry. From these figures we notice that the maximum value of the ratio decreases with the increase in energy and its position is shifted towards

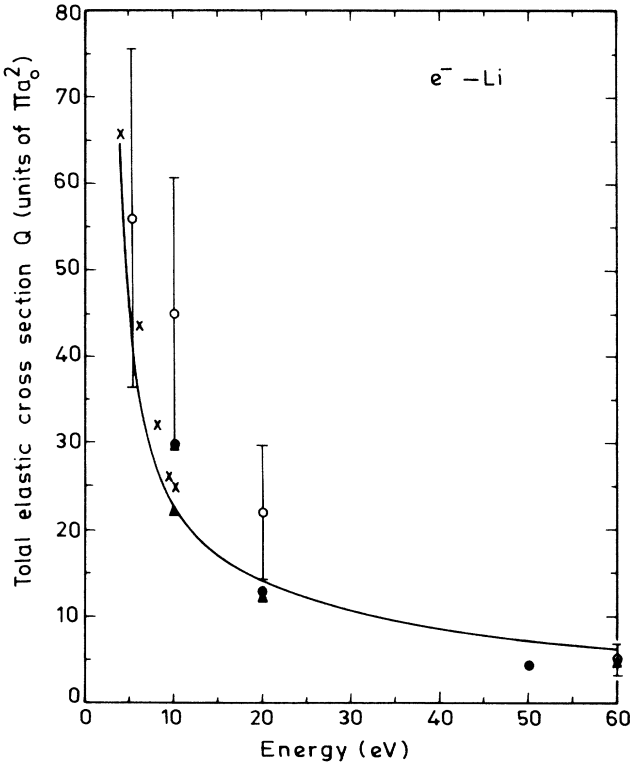

FIG. 2. Total elastic cross section for electron-lithium elastic scattering. ——, present calculation; ▲, two-state close-coupling calculation of Issa (Ref. 15); ×, five-state close-coupling calculation of Moores (Ref. 12); ●, results of Mukherjee and Sural (Ref. 16); ⊼, experimental data of Williams, Trajmar, and Bozinis (Ref. 14).

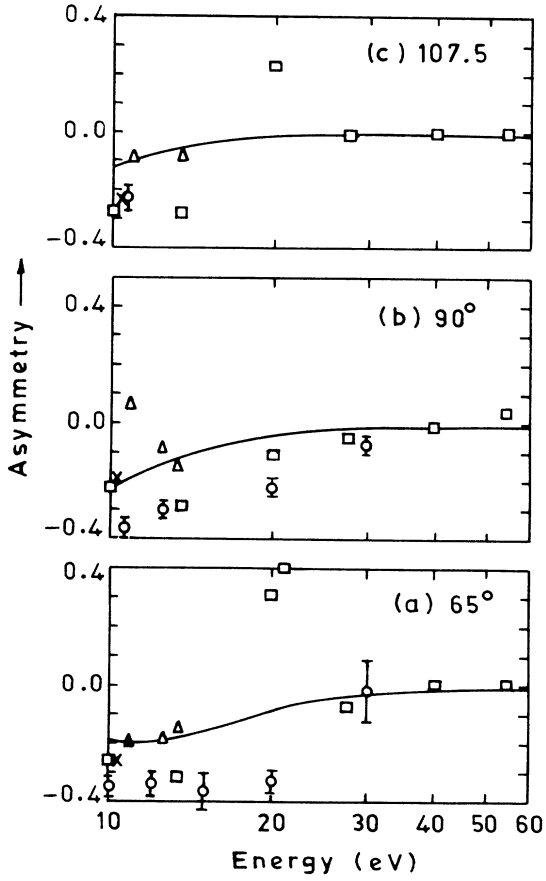

FIG. 3. Differential spin asymmetry A at (a) 65°, (b) 90°, and (c) 107.5° scattering angle for incident electron energies from 10 to 60 eV. ——, present calculation; □, two-state calculation of Burke and Taylor (Ref. 8); ×, five-state calculation of Moores (Ref. 12); △, modified polarized-orbital calculation of Bhatia *et al.* (Ref. 13); ⊼, experimental data of Baum *et al.* (Ref. 11).

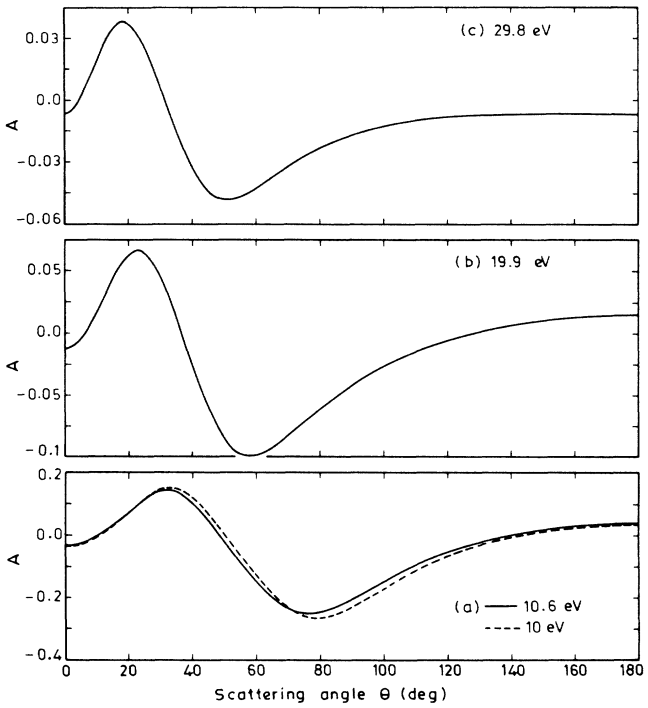

FIG. 4. Differential spin asymmetry A for electron-lithium elastic scattering. Present calculations: (a) — — —, 10 eV and ——, 10.6 eV; (b) ——, 19.9 eV; and (c) ——, 29.8 eV.

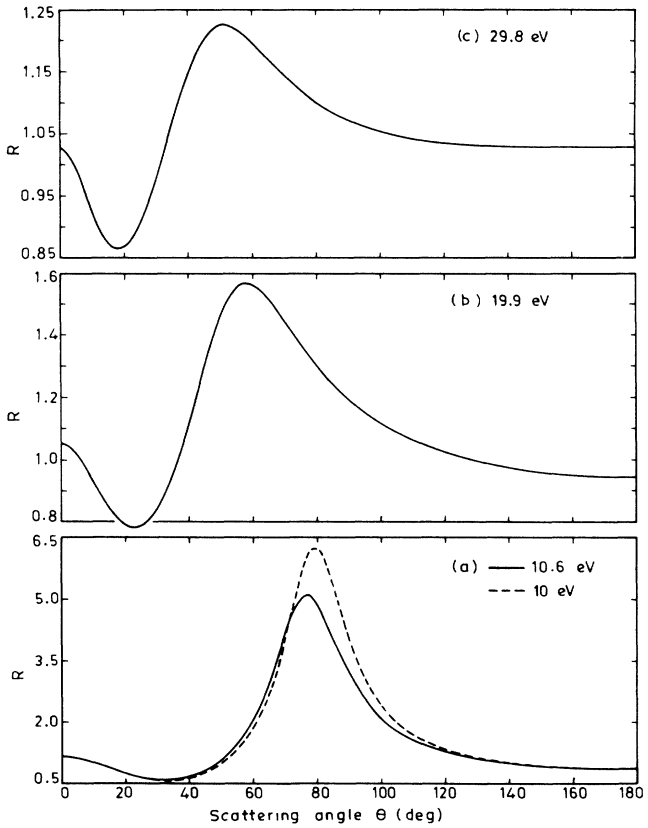

FIG. 5. The ratio R of the differential cross section for triplet and singlet scattering. Present calculations: (a) — — —, 10 eV, and ——, 10.6 eV; (b) ——, 19.9 eV; and (c) ——, 29.8 eV.

lower angle. No measurements of the ratio R are available at present.

Figures 6–8 show our results for the variation of the differential cross section of the elastic scattering of positron with the lithium atom at 20, 30, and 50 eV positron energies, respectively.

The absence of the exchange in positron-atom scattering and the presence of the exchange in the electron-atom scattering gives importance to the study of the positron-atom scattering. In addition to this, the positron-atom scattering differs from the electron-atom scattering with respect to the nature of the static interactions, which are attractive for the electron scattering and repulsive for the positron scattering.

The adiabatic polarization potential is attractive in both the cases, while the velocity-dependent nonadiabatic term [expressed by the denominator in Eq. (15)] is repulsive for both electrons and positrons. Thus during the scattering, the electrons will be accelerated more than the positrons. The effect of the dynamic term would therefore be different for electron and positron scattering. In the literature most of the work on electron and positron scattering with atoms and molecules has been reported using the same polarization potentials for electrons and positrons. However, some studies have been made recently (Nakanishi and Schrader;[32] Morrison, Gibson, and Austin;[33] Elza *et al.*;[34] and references therein) using different polarization potentials for electrons and positrons by taking different cutoff parameters which affect the short-range behavior of these potentials. The results from these studies indicate that the effect on the cross sections, by the use of different nonadiabatic polarization potentials in electron and positron scattering, is more prominent at low incident energies and less so at intermediate energies.

Since the present study is concerned with intermediate energies, the use of the same dynamic term in Eq. (15) for electron and positron scattering would not lead to much inaccuracy in the positron cross section. To test this we investigated the cross sections by replacing k_j^2 in Eq. (15) with the local energy $(k_j^2-2U_j)$, which is different for electrons and positrons. By doing so we found negligible change (less than 0.3%) in the cross sections at the intermediate energies studied here.

Figure 6 gives our results for the positron-lithium elastic differential cross sections at 20 eV. These are compared with the modified corrected static approximation results of Tayal.[26] We notice that our results differ with the calculation of Tayal beyond a 20° scattering angle. This may be due to the neglect of the contribution of core electrons in the calculation of the second-order Born terms in the calculation of Tayal.

Figure 7 shows our results for the positron-lithium elastic differential cross sections at 30 eV positron energy. Comparison is made with the recent results of Sarkar and Ghosh[22] based on the five-state close-coupling calculation. It is shown that our results agree well with the calculation of Sarkar and Ghosh in the angular region (0°–140°) studied by them.

Figure 8 shows our results for the positron-lithium scattering at 50 eV. Comparison with the five-state

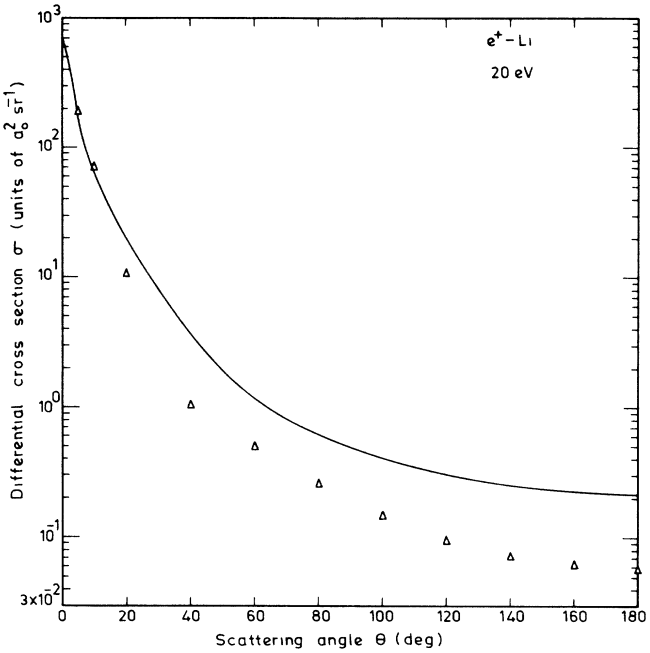

FIG. 6. Differential cross sections for positron-lithium elastic scattering at 20 eV. ——, present calculation; △, modified corrected static approximation of Tayal (Ref. 26).

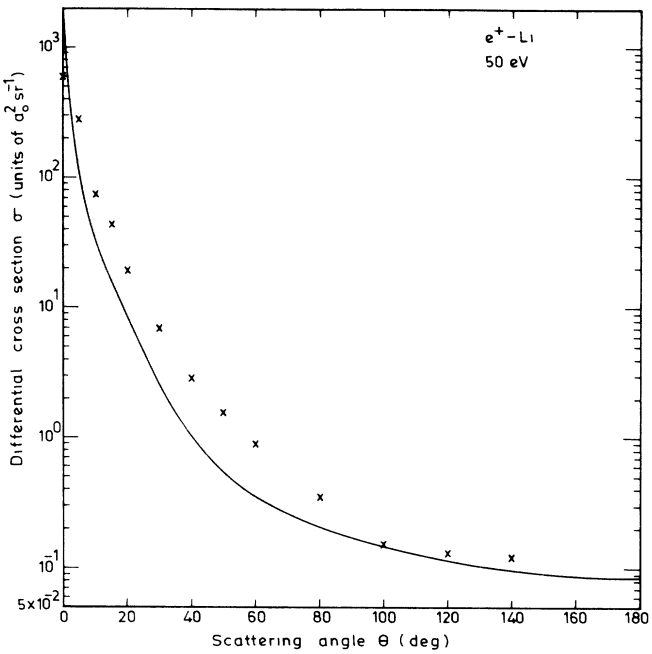

FIG. 8. Differential cross sections for positron-lithium elastic scattering at 50 eV. Symbols are the same as in Fig. 7.

close-coupling calculation of Sarkar and Ghosh shows that their calculation gives higher values of cross sections for scattering angle up to 80°. Beyond this the agreement between the two calculations is quite good.

Figure 9 gives the variation of the total cross sections for the elastic scattering of positrons with lithium atom from 10 to 60 eV. In this figure the present results are compared with (i) the two-state close-coupling calculation

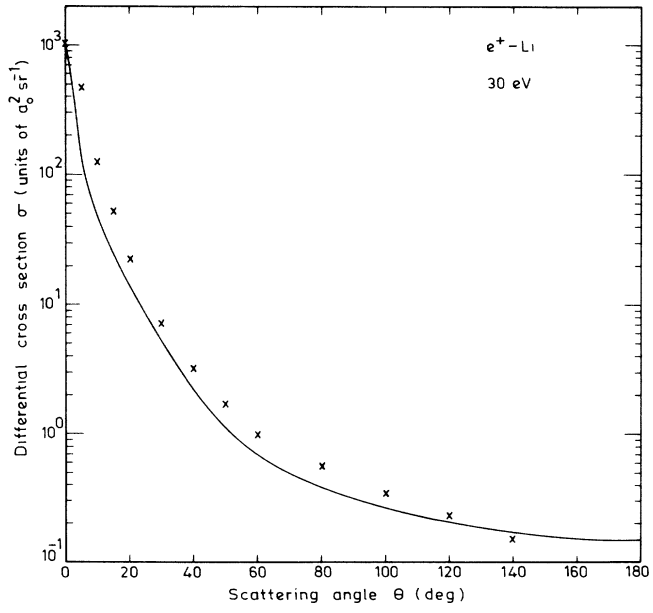

FIG. 7. Differential cross sections for positron-lithium elastic scattering at 30 eV. ——, present calculation; ×, five-state close-coupling calculation of Sarkar and Ghosh (Ref. 22).

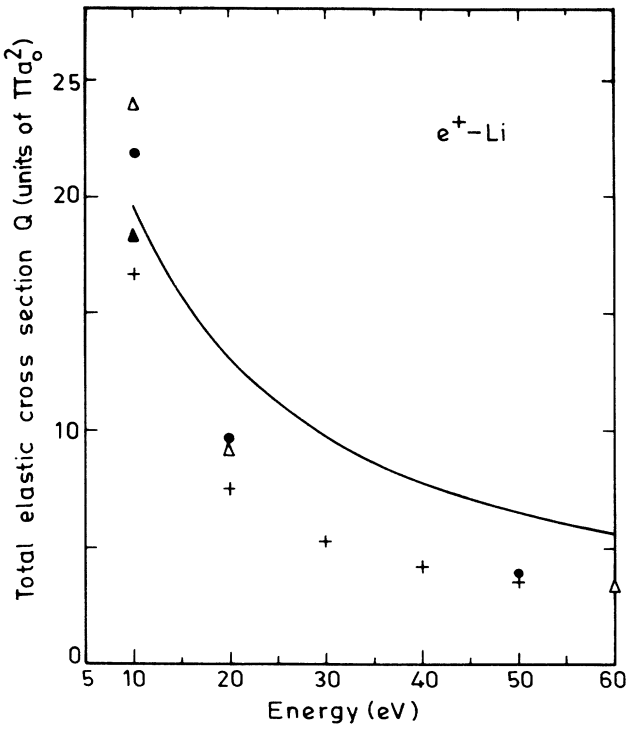

FIG. 9. Total elastic cross sections for positron-lithium elastic scattering. ——, present calculation; +, two-state close-coupling calculation of Ward *et al.* (Ref. 21); ●, results of Mukherjee and Sural (Ref. 16); ▲, datum of Guha and Ghosh (Ref. 27); △, modified corrected static approximation results of Tayal, Tripathi, and Srivastava (Ref. 26).

of Ward *et al.*;[21] (ii) the calculation of Mukherjee and Sural[16] using the integral approach to the second-order potential method; (iii) the modified corrected static approximation of Tayal, Tripathi, and Srivastava;[26] and (iv) the datum of Guha and Ghosh[27] at 10 eV using the polarized-orbital method. We find that the present results are qualitatively in reasonable accord with the other theoretical calculations, although quantitatively our results are somewhat higher in comparison to the above calcualtions for energies beyond 10 eV. However, on the basis of comparison of the differential cross sections in Figs. 7 and 8, it may be inferred that at 30 and 50 eV the recent five-state calculation of Sarkar and Ghosh would yield total elastic cross sections which will be in better agreement with our results.

Since no experimental measurements are available at present for the differential and the total elastic positron scattering with the lithium atom, it is difficult to judge the suitability of the various theories vis-à-vis experiment.

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