Elastic Scattering of Electrons and Positrons by Lithium Atoms

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The eikonal approximation has been used to investigate $e^{\pm}$-Li scattering in the energy region $E=0.8$ to 500 eV. In addition to the static potential, the effect of the polarization potential has been included explicitly. Our results for the total cross section of e^--Li scattering in the energy region $4 \leq E \leq 10$ eV are in close agreement with the recent experimental findings as well as with the theoretical results obtained by various authors using the close-coupling approximation. In the energy region $10 < E \leq 500$ eV, the present approach yields higher values than first Born approximation (FBA). Our results for the total cross section for e^+-Li scattering in the eikonal approximation are displayed and compared with the corresponding polarized FBA results and the results obtained by the polarized-orbital method. Results for the differential cross sections for both the systems $e^{\pm}$-Li in the eikonal approximation are also presented together with the corresponding polarized FBA results.

I. INTRODUCTION

Investigations into the collision processes between electrons and alkali-metal atoms have, of late, assumed much importance in view of the applications proposed for alkali-metal vapors and plasmas. Karule[1] has calculated the total cross sections for the elastic scattering of electrons by atomic Li, Na, K, and Cs below the first excited state threshold by close-coupling (CC) exchange approximation, taking into consideration the effect of the first excited state $2p$. Using the same approximation, Karule and Peterkop[2] have further obtained the total cross sections of elastic scattering and $2s$-$2p$ excitation of the lithium atom for the incident electron energy E ranging from 2 to 3 eV. They have shown that allowance for the atomic $2p$ state permits the calculation of 98% of the observed polarizability of lithium. Marriott and Rotenberg[3] also have carried out CC exchange calculations of the same problem with the further inclusion of $3s$ and $3p$ states. Their results are in close agreements with those of Karule and Peterkop[2] when coupling with the Li ($2p$) state alone is retained. Burke and Taylor,[4] who have extended the $2s$, $2p$ CC method to higher energies, have also analyzed the resonances that occur at low energies. The results of Burke and Taylor do not agree well with the experimental findings of Perel *et al.*[5] Burke and Taylor[4] have questioned the normalization of the experimental findings. Bederson and Kieffer[6] have renormalized the experimental values of Perel *et al.*[5] Recently Kasdan *et al.*[7] have measured the total cross section for this system, and their values are in close agreement with Burke and Taylor.[4] The various close-coupling calculations agree well with each other. Vinkalns *et al.*[8] have calculated the total cross sections for elastic scattering of electrons with energies from 0 to 12 eV by lithium atoms. They have employed three different approaches in their investigation: (i) the polarization-exchange approximation, (ii) the distorted-wave approximation, and (iii) an approximation which takes polarization into account, but not exchange. Their calculated results using approximation (i) are in better agreement with the experiment than those using (ii) and (iii).

The polarized-orbital method, originally introduced by Temkin,[9] has been applied to the e^--Li problem by several authors.[10–14] Marked differences have been noted in the results of various polarized-orbital calculations. The results obtained by Garrett[10] are higher than the experimental values, whereas Stone's[11] results are much below those of Garrett.[10] The results of Feautrier and Lan[12] lie between those of Stone[11] and Garrett.[10] The calculated values of Lan[13] are in close agreement with those of Burke and Taylor[4] below 2 eV. The reason may be attributed to the variety of approximations used by different authors in their calculations. The results obtained by the polarized-orbital method do not agree with the CC results.

In the high-energy region, Mathur *et al.*[15] have applied the Glauber approximation[16] to calculate the elastic scattering of the lithium atom by electron impact, taking the one-electron wave function of Clementi[17] of the lithium atom. Their results do not agree with the experimental observations. The same problem has also been investigated by Mathur *et al.*[18] using the Born approximation with and without the inclusion of the polarization potential. The polarized Born results obtained by them are too high in the low-energy region, whereas the first-Born-approximation (FBA) results are close to those obtained by Burke and Taylor[4] at $E \gtrsim 10$ eV.

In our previous work[19] (to be referred to as Paper I), we have applied the eikonal approximation[20] to $e^{\pm}$-He and $e^{\pm}$-H elastic scattering systems with

satisfactory results. We have taken account of the effect of the polarization potential in addition to the static potential in Paper I. In this paper we have extended our previous approach in order to calculate the scattering of electrons and positrons by the lithium atom. We have neglected the exchange effects in e^--Li calculations. In the framework of potential scattering, these effects could be taken into account, to some extent, by introducing a suitable pseudopotential. However, this pseudopotential acts only on s-wave electrons. Therefore, it is expected that inclusion of such potential will not be of much importance in our case. The same problem has also been investigated by Dai and Stauffer[21] using the polarized-orbital method.

II. THEORY

We consider the target nucleus to be infinitely heavy and the origin of the coordinate system to be placed at the position of the nucleus. Let $\vec{b}$ be the impact-parameter vector relative to the origin. In the eikonal approximation[20] the scattering amplitude is given by

$$F(\theta)=\frac{k}{2\pi i}\int d^2b\, e^{i\vec{q}\cdot\vec{b}}(e^{-i\chi(\vec{b})}-1), \tag{1}$$

where $\vec{q}$ is the momentum transfer vector and is written as $\vec{q}=\vec{k}-\vec{k}_0$, where $\vec{k}$ and $\vec{k}_0$ represent, respectively, the incident and the final momentum. The phase-shift function $\chi(\vec{b})$ corresponding to the impact parameter $\vec{b}$ may be expressed as

$$\chi(\vec{b})=\frac{1}{\hbar v}\int_{-\infty}^{\infty}V(\vec{r})\,dz, \tag{2}$$

where v is the velocity and $\vec{r}$ denotes the position vector of the incident particle and is given by

$$\vec{r}=\vec{b}+\hat{k}z.$$

Here $\chi(\vec{b})$ represents the combined effect of the static potential (V_s) as well as the polarization potential (V_p). Hartree–Fock screening factors[22] for lithium atom can be expressed analytically in the form

$$f(r)=\sum_{j=1}^{6}\alpha_j e^{-\gamma_j r},$$

so that the static potential in e^--Li scattering may be written as

$$V_s(\vec{r})=(Ze^2/r)f(r), \tag{3}$$

where $Z=3$ for lithium. We have taken the polarization potential of the lithium atom obtained by Gupta.[23] He obtained a value of the polarizability which is less than the experimental value by a factor 1.25. He augmented his value by the above factor following Crown and Russek.[24] The augmented expression for the polarization potential of lithium atom is as follows:

$$V_p(r)=-1.25\,\alpha(r)/2r^4, \tag{4}$$

where

$$\alpha(r)=\frac{2}{3}\left(a_0-\sum_{i=0}^{8}a_i r^i e^{-2\beta r}\right),$$

with

$$a_0=221.99,\quad a_1=340.53,\quad a_2=261.18,$$
$$a_3=133.56,\quad a_4=51.29,\quad a_5=13.64,$$
$$a_6=7.65,\quad a_7=-0.67,\quad a_8=0.084$$

and

$$\beta=0.767.$$

Substituting $V_s(r)$ and $V_p(r)$ in Eq. (2), we have

$$\chi(\vec{b})=(1/\hbar v)(I_s+I_p),$$

with

$$I_s=\int_{-\infty}^{\infty}V_s(\vec{b}+\hat{k}z)\,dz \tag{5}$$

and

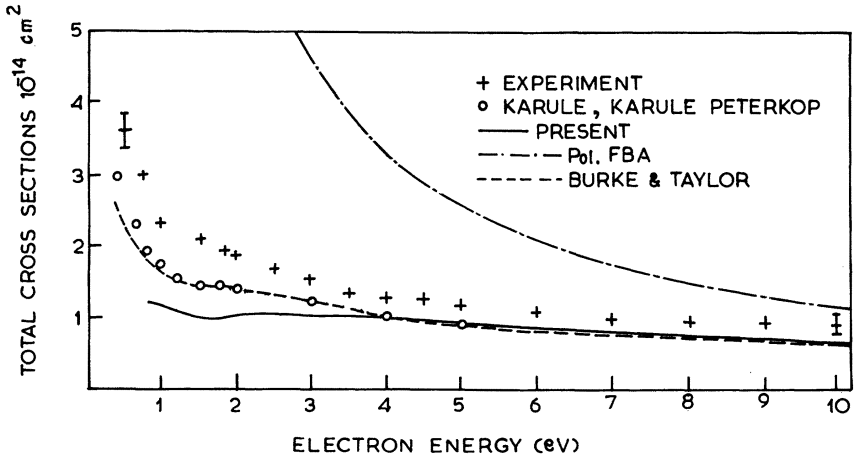

FIG. 1. Total cross section for e^--Li scattering.

$$I_p = \int_{-\infty}^{\infty} V_p(\vec{b} + \hat{k}z)\, dz. \tag{6}$$

The integration in expression (6) for I_p has been carried out numerically. The integral I_s may be written analytically as

$$I_s = Ze^2 \sum_{j=1}^{6} \alpha_j K_0(\gamma_j b), \tag{7}$$

where K_0 is the Bessel function of the third kind. Equation (1) thus can be expressed as

$$F(\theta) = \frac{k}{i} \int_0^{\infty} J_0(qb) \left(\exp \frac{i}{\hbar v} (I_s + I_p) - 1 \right) b\, db,$$

where the symbols have their usual significance. The scattering amplitude $F(\phi)$ has been obtained by numerical integration over the impact parameter $\vec{b}$.

For comparison we have also calculated the elastic scattering amplitudes F_{PB} in the Born approximation by including the polarization potential. The expression for the scattering amplitude for the e^--Li scattering in the polarized FBA is given by

$$F_{PB} = Ze^2 \sum_{j=1}^{6} \frac{\alpha_j}{\gamma_j + q^2} + 2a_0 \left[\frac{\beta}{3} + \frac{q}{6} \tan^{-1}\left(\frac{q}{2\beta} \right) - \frac{\pi q}{12} \right]$$

$$- 4a_0 \left[\frac{2\beta^3}{9D} + \frac{4\beta^5}{9D^2} + \frac{a_5(12\beta^2 - q^2)}{3a_0 D^3} + \frac{8a_6\beta(4\beta^2 - q^2)}{a_0 D^4} + \frac{4a_7}{a_0} \left(\frac{80\beta^4 - 40\beta^2 q^2 + q^4}{D^5} \right) + \frac{80\beta a_8}{a_0} \left(\frac{48\beta^4 - 40\beta^2 q^2 + 3q^4}{D^6} \right) \right],$$

where $D = 4\beta^2 + q^2$, and α and γ are constants. The values of α and γ are as follows:

$$\alpha_1 = 1.2197, \quad \alpha_2 = -0.2197, \quad \alpha_3 = 1.6368, \quad \alpha_4 = 0.9508, \quad \alpha_5 = -1.6368, \quad \alpha_6 = -0.9508$$

and

$$\gamma_1 = 0.8776, \quad \gamma_2 = 7.951, \quad \gamma_3 = 2.4948, \quad \gamma_4 = 3.9701, \quad \gamma_5 = 1.4948, \quad \gamma_6 = 2.9701.$$

The standard relations are employed to calculate the differential as well as the total cross sections.

For the case of positron-lithium scattering, the sign of the static potential is to be reversed.

III. RESULTS AND DISCUSSION

We have calculated the total and the differential cross sections for the elastic $e^{\pm}$-Li atom scattering in the energy region $E = 0.8$ to 500 eV.

In Fig. 1 we show our curve for the total cross sections of e^--Li scattering along with the polarized FBA results and have compared them with the experimental findings due to Kasdan *et al.*[7] for $E = 0$ to 10 eV. The curve of Burke and Taylor and the values of Karule[1] and of Karule and Peterkop[21] (all these results are as quoted by Kasdan *et al.*[7]) are also displayed in the same figure. The values of Burke and Taylor, Karule, and Karule and Peterkop are the sum of the $2s$-$2s$ and $2s$-$2p$ total cross sections, whereas we have considered only the elastic scattering. From 4 eV and onwards, our curve is in very close agreement with the theoretical results of Burke and Taylor[4] and Karule and Peterkop.[2] Our values are slightly greater than the other theoretical values obtained by CC methods and lie between the experimental findings and these theoretical results. Below 4-eV incident energy our curve shows a slight fluctuation similar to that of Burke and Taylor. From 1 to 4 eV our curve lies below the experimental and other theoretical values given in the figure. In this energy region the discrepancy of the present results with the other theoretical values and the experimental findings may be due to the fact that we have ignored exchange effects in our approach. A

TABLE I. Calculated total cross sections for elastic e^--Li scattering.

Electron energy E (eV)	Q (πa_0^2)[a] FBA	Polarized FBA	Present
0.8	1.16122 (2)	1.56760 (3)	1.37384 (2)
1.0	1.08143 (2)	1.30235 (3)	1.30535 (2)
1.6	8.940 (1)	8.45917 (2)	1.14650 (2)
2.0	8.0006 (1)	6.92717 (2)	1.15514 (2)
4.5	4.7811 (1)	3.14545 (2)	1.07536 (2)
6.3	3.695 (1)	2.25960 (2)	9.70323 (1)
10.0	2.5188 (1)	1.43593 (2)	7.6427 (1)
30.0	9.39399	4.8826 (1)	3.58687 (1)
70.0	4.23696	2.11903 (1)	1.77002 (1)
100.0	3.01096	1.48990 (1)	1.29382 (1)
500.0	6.25269 (−1)	2.98041	2.89932

[a]The number in the parentheses in each entry is the power of 10 by which the cross-section value should be multiplied.

similar discrepancy has also been noted in the case of e^--H and e^--He scattering (Paper I). Further investigations with the inclusion of exchange effects will be of interest to ascertain the ranges of energy and angles for which these effects will be appreciable. The polarized FBA curve is too high in the said energy region. In Table I we tabulate our present values along with the polarized FBA and FBA results. From the table it is evident that even at an incident energy as high as 500 eV, our results differ appreciably from those of FBA. However, the polarized FBA are in close agreement with the present results in the high-energy region. Exactly similar discrepancies among the values of FBA and those obtained by the present method have been noted for both the e^--H and e^--He systems (Paper I).

Figure 2 represents the results of the differential cross sections of the present approach for (a) $E = 2$ eV and (b) $E = 10$ eV along with the corresponding

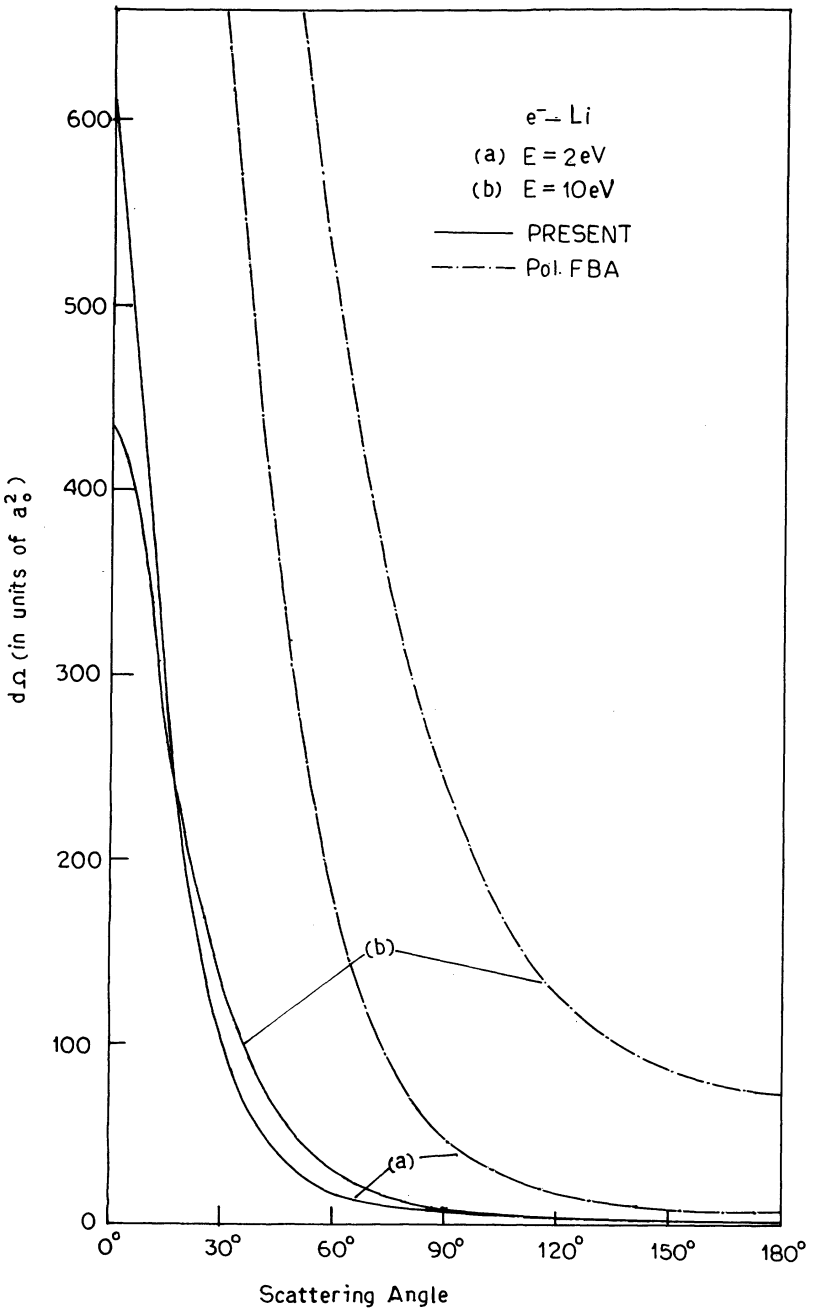

FIG. 2. Differential cross sections for e^--Li scattering at (a) $E = 2$ eV and (b) $E = 10$ eV.

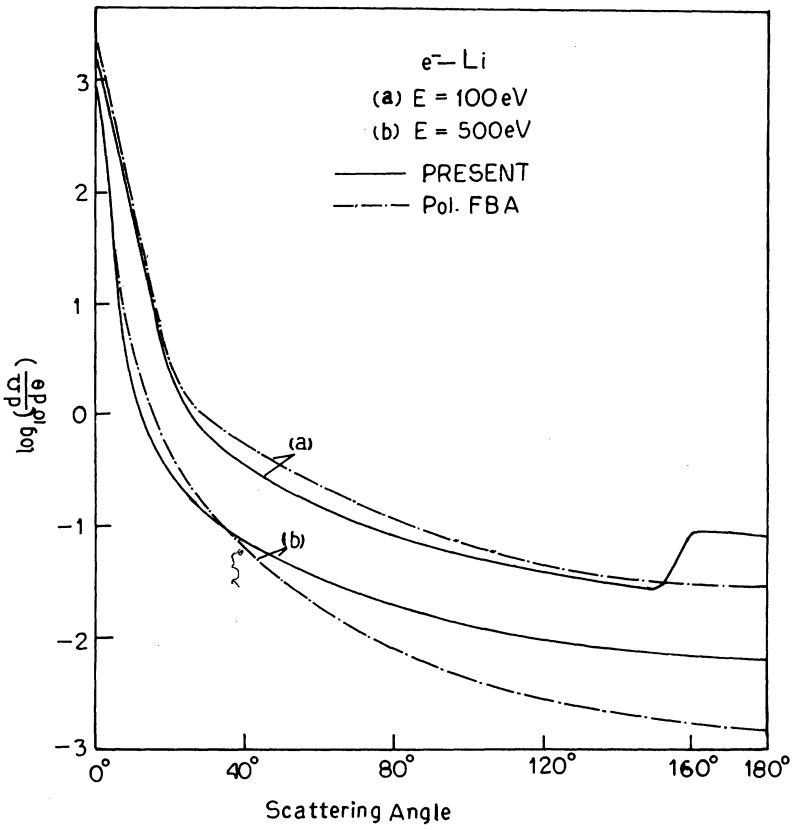

FIG. 3. Differential cross sections for e^--Li scattering at (a) $E=100$ eV and (b) $E=500$ eV.

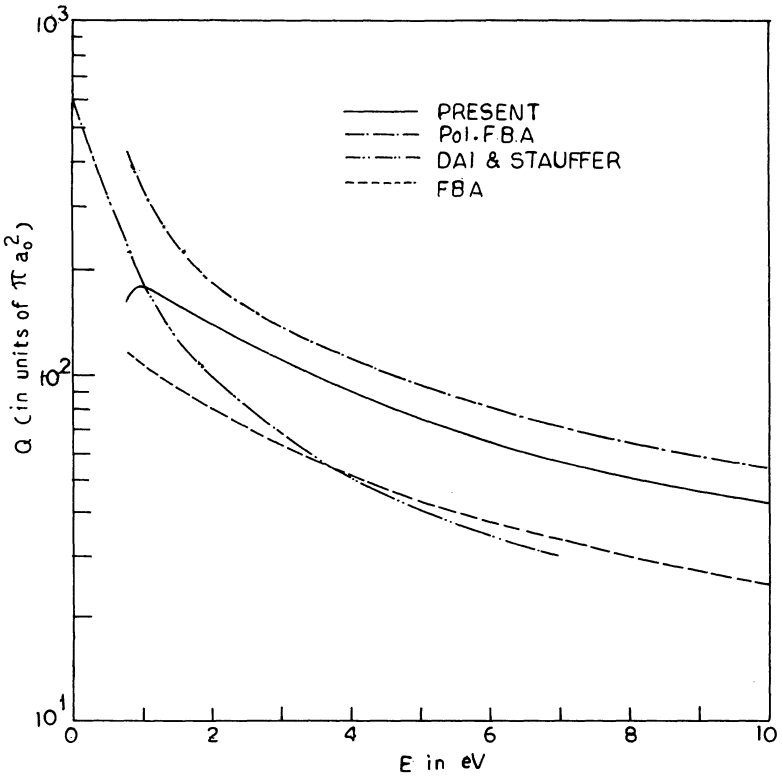

FIG. 4. Total cross sections for e^+-Li scattering.

polarized FBA values. It is apparent from the figure that the polarized FBA results are too high for small scattering angles. The difference between the values obtained by the polarized FBA and those obtained by the present approach decreases with the increase of the scattering angle. In the high-energy region the feature is reversed. In Fig. 3 we show our results for the differential cross section for the incident energies (a) $E = 100$ eV and (b) $E = 500$ eV together with the corresponding polarized FBA results. Near the forward direction the difference between the two results is negligible for both of the incident energies, whereas in the backward direction the difference between the two curves is maximum. In the eikonal curve for $E = 100$ eV, there is a sudden rise in the value of the differential cross section at about 160° scattering angle. No kink was observed at 70 eV and below. With the increase of the incident energy, the position of the kink is shifted towards the forward direction and the magnitude of the sudden rise is decreasing. This kink in the differential cross section is rather uncommon and has not been noticed in e^--H and e^--He systems (Paper I). This feature may be due to the fact that the polarizability of Li is very large in comparison with the polarizabilities of He and H. However, it may be interesting to investigate the nature of the angular distributions in the cases of other alkali atoms.

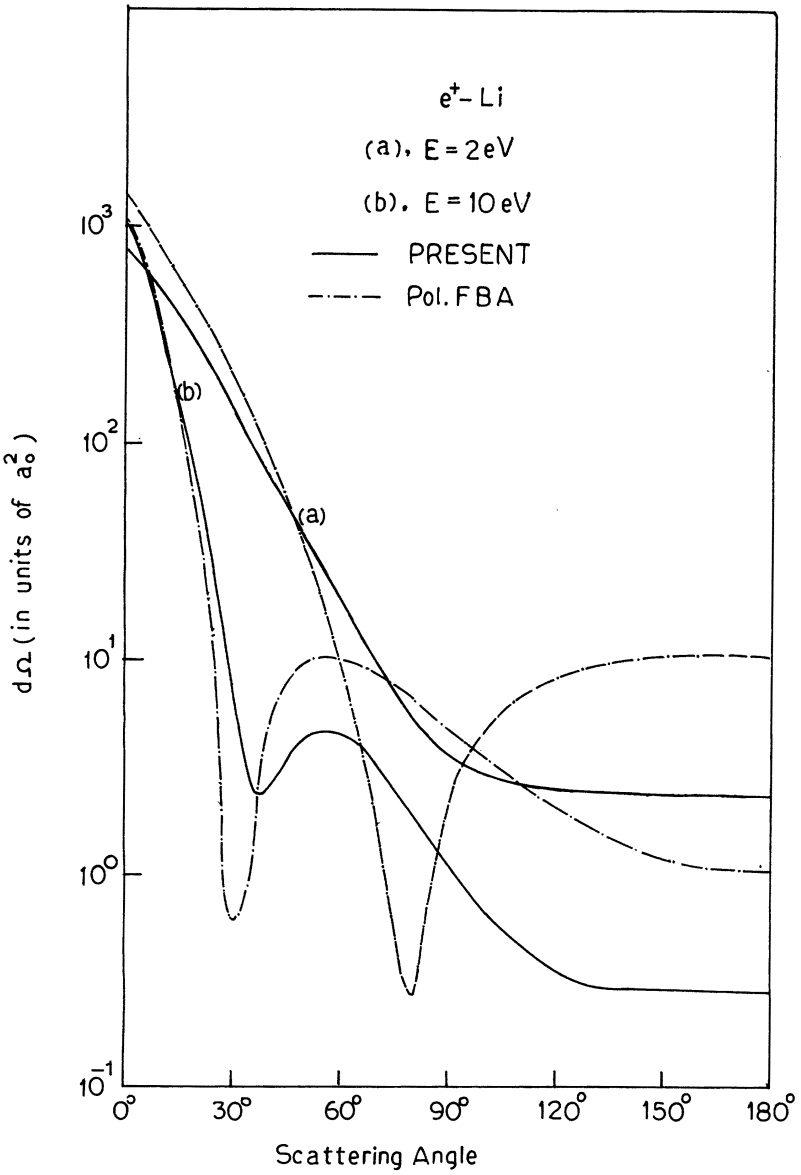

FIG. 5. Differential cross sections for e^+-Li scattering at (a) $E = 2$ eV and (b) $E = 10$ eV.

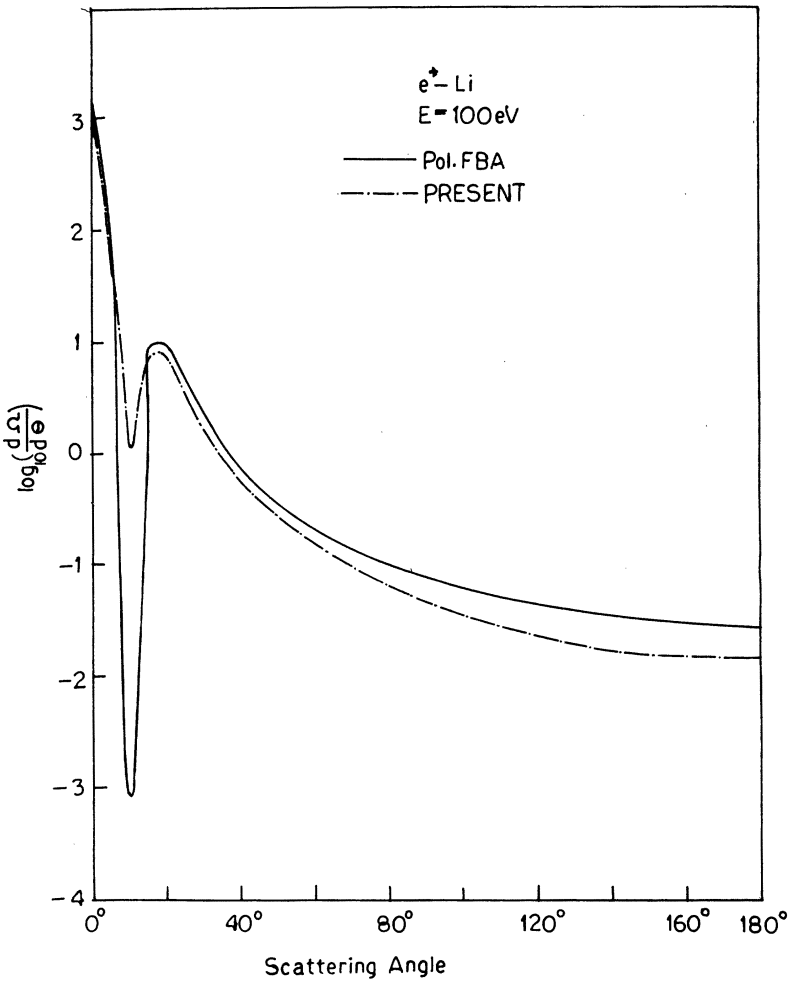

FIG. 6. Differential cross sections for e^+-Li scattering at $E = 100$ eV.

We plot our values for the total cross sections of e^+-Li scattering along with the polarized FBA and FBA results in Fig. 4. The curve of Dai and Stauffer[21] has also been displayed for comparison in the same figure. To our knowledge there is no other theoretical calculation. Experimental results are still unavailable on e^+-Li scattering. The FBA values are close to the results of Dai and Stauffer[21] beyond 3 eV, and both values are lower than the eikonal and the polarized FBA results. The polarized FBA curve is higher than the eikonal curve. Keeping in mind the results obtained for the total cross sections in the e^+-H and e^+-He scattering (Paper I), we may say that our method yields more or less reliable results for e^+-Li scattering also. Experimental measurements and some refined theoretical calculations are necessary to ascertain the actual nature of the cross-section curve for the e^+-Li system.

Figures 5 and 6 represent the differential cross-section curves for the incident energies 2, 10, and 100 eV with the polarized FBA results. At low incident energy (e.g., $E = 2$ eV), our eikonal curve is somewhat smooth, whereas the polarized FBA curve has a second peak. With the increase of energy ($E = 10$ eV), the eikonal curve gives a second peak similar to that in the polarized FBA curve, but the positions of the second peak are different for the two approaches. It is evident that at high incident energy ($E = 100$ eV), the positions of the second peak for both cases are almost the same. Moreover, with the increase of energy, the second peak is shifted towards the forward direction. A similar feature has also been observed in the case of e^+-H scattering (Paper I).

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Charge Exchange: Theory and Application to Proton-Hydrogen-Atom Collisions*†

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A theory of rearrangement collisions taking account of the nonorthogonality of initial and final states is presented. Detailed discussion of the range of validity of the theory is worked out. The method is applied to proton-hydrogen-atom charge exchange collisions. We find that at high energy the Jackson-Schiff results are obtained and that below 100 kev the cross section is raised significantly above the result of Jackson and Schiff. The new result is in better agreement with experimental results than the calculations based on the Jackson-Schiff formulation.

I. INTRODUCTION

I shall describe charge exchange collisions of the type $A+(B+e^-)\rightarrow(A+e^-)+B$, where A and B are cores which are difficult to excite. In the initial state ψ_i the electron is associated with core B and $(B+e^-)$ has a relative momentum $\vec{k}_i(\hbar=1)$ with respect to A. The final state that we shall consider is that of the electron associated with core A and $(A+e^-)$ having relative momentum $\vec{k}_f$ with respect to B.

There have been many different approaches to calculating charge exchange transition probabilities. In the energy range we are concerned with, relative velocities of 10^8 cm/sec or greater, there have been Born-approximation calculations carried out by Brinkman and Kramers,[1] by Saha and Basu,[2] and by Jackson and Schiff.[3] The last of these included the intercore potential and on the basis of their results, Jackson and Schiff claim that its neglect is not justified. Within the Born approximation no account has been taken of the nonorthogonality of initial and final states. Some attempts have been made at taking the nonorthogonality into account by Bassel and Gerjuoy[4] and by Grant and Shapiro[5] using a distorted-wave approximation. To first order the distorted-wave results tend asymptotically to the Brinkman–Kramers cross section. Cheshire[6] has also calculated the resonant charge exchange cross section using a distorted-wave approximation. McCarroll and Salin[7] obtain the same asymptotic result at large energies as Cheshire. Cheshire[8] has also calculated the charge exchange cross section into excited states using the results