Positron–lithium-atom collisions using the two-state approximation

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The two-state approximation is applied to positron–lithium-atom collisions considering only the elastic scattering and the ground-state positronium formation. Taking the effect of the adiabatic polarization potential into account in both the direct and rearrangement channels, results for the differential, total, and momentum-transfer cross sections are computed at incident positron energies 0.5–10 eV. While for the elastic scattering the present data show satisfactory agreement with other available calculations, for positronium formation the present results are quite new and give us an idea of the order of the cross section. It is found that the differential cross section for both the elastic scattering and positronium formation shows a deep minimum at low energies of positron impact in agreement with available earlier findings.

I. INTRODUCTION

The importance of positron scattering of gas atoms and molecules and also the recent experimental measurements of the total cross section stimulate work on this problem. Extensive studies have been performed for elastic positron scattering from hydrogen and helium atoms. A few calculations have been carried out on the scattering of positrons by alkali atoms. Bui and Stauffer[1] (see also Bui[2]) applied a polarized orbital method to investigate the low-energy elastic scattering in positron-lithium collisions and computed total and momentum-transfer cross sections for incident positron energies 0–7 eV. They also calculated the annihilation parameter Z_{eff}. A detailed study of the system covering a wider range of incident energies was later performed by Sarkar *et al.*[3] by using the first Born approximation (FBA), the polarized FBA, and the modified eikonal method. Their results for the total cross section are in substantial agreement with the earlier findings of Bui and Stauffer. The elastic differential cross sections as computed by them show, however, a deep minimum at some scattering angle at low energies. More recently Bordonare *et al.*[4] and Ferrante *et al.*[5] employed the semiclassical JWKB approximation to study the positron-alkali atom scattering. Their results for the differential cross section for these atoms predict a deep minimum near the scattering angle 90° at low energies in conformity with the calculation of Sarkar *et al.* in the case of a lithium atom.

In none of these theoretical investigations has the Ps-formation (positronium-formation) channel been taken into account explicitly. It is important to note that, in the case of alkali atoms, Ps formation is possible even at zero positron incident energy. It is also well known that the effect of Ps formation influences the elastic cross section appreciably in the vicinity of the pickup threshold. The results for the elastic cross section calculated without taking the effect of Ps formation is not at all expected to be reliable at very low energies.

The motivation of the present paper is twofold. Firstly we are interested to find out the effect of the Ps-formation channel on the elastic-scattering parameters. The effect of the Ps-formation channel is attractive in nature. The adiabatic dipole polarization is also attractive in nature whereas the static potential is repulsive. Therefore, it is worthwhile to study this effect. The determination of scattering parameters for Ps formation is the second aim of this paper. The absence of any results, rather, warrants this investigation. In the present paper, we use a polarized orbital method[6] (POM) to investigate the positron-lithium collision problem with the inclusion of the Ps-formation channel explicitly. This prescription of Temkin and Lamkin[6] is found to be suitable in atomic and molecular collision problems. The present calculations include the effect of the adiabatic dipole polarization in both channels. Owing to the adiabatic approximation, this method is suitable in the energy region where the effect of nonadiabatic potentials is negligible. That is to say that the present model is suitable at very low incident energies.

We visualize the many-electron target atom as essentially a one-electron system with the consideration of a core potential. From an independent-particle model we can determine the parameters of the core potential as has been done by Walters,[7] previously. It is assumed at the outset that Ps formation is possible only by the capture of the most "active" valence electron while the other two atomic electrons are mere spectators.

II. THEORY

Let the particles 1 and 2 be the positron and the valence electron of the lithium atom, respectively, and particle 3 the lithium ion; we assume that the center of mass lies with the lithium core. The interacting potentials $v_{\beta\alpha}$ $(\alpha,\beta=1,2,3)$ are expressed in atomic units as

$$v_{13}=1/r_1\,,\quad v_{23}=-1/r_2\,,\quad v_{12}=-1/|\vec{r}_1-\vec{r}_2|\,.$$

On retaining only two bound states (the ground state of the target atom in the entrance channel and the ground-state Ps atom in the exit channel) in the eigenfunction expansion of the total wave function of the system, the integral form of the close-coupling equations in the two-state approximation may be written as[8,9]

$$\langle\vec{k}_1'2s\,|Y_{11}\,|\vec{k}_1 2s\rangle=\langle\vec{k}_1'2s\,|Y_{11}^B\,|\vec{k}_1 2s\rangle+\int d\vec{k}_1''\frac{\langle\vec{k}_1'2s\,|Y_{11}^B\,|\vec{k}_1''2s\rangle\langle\vec{k}_1''2s\,|Y_{11}\,|\vec{k}_1 2s\rangle}{E-E_1''}$$
$$+\int d\vec{k}_3''\frac{\langle\vec{k}_1'2s\,|Y_{31}^B\,|\vec{k}_3''\mathrm{Ps}\rangle\langle\vec{k}_3''\mathrm{Ps}\,|Y_{31}\,|\vec{k}_1 2s\rangle}{E-E_3''}\,, \tag{1}$$

$$\langle\vec{k}_3'\mathrm{Ps}\,|Y_{31}\,|\vec{k}_1 2s\rangle=\langle\vec{k}_3'\mathrm{Ps}\,|Y_{31}^B\,|\vec{k}_1 2s\rangle+\int d\vec{k}_1''\frac{\langle\vec{k}_3'\mathrm{Ps}\,|Y_{31}^B\,|\vec{k}_1''2s\rangle\langle\vec{k}_1''2s\,|Y_{11}\,|\vec{k}_1 2s\rangle}{E-E_1''}$$
$$+\int d\vec{k}_3''\frac{\langle\vec{k}_3'\mathrm{Ps}\,|Y_{33}^B\,|\vec{k}_3''\mathrm{Ps}\rangle\langle\vec{k}_3''\mathrm{Ps}\,|Y_{33}\,|\vec{k}_1 2s\rangle}{E-E_3''}\,, \tag{2}$$

where $2s$ and Ps stand for the ground states of lithium and Ps atoms, respectively. We are treating the lithium atom as a one-electron atom. Under this assumption, the center of charge and center of mass of positronium coincides in the positronium channel. Therefore, we have omitted the self-coupling term arising from the static interaction in this channel. For the vanishing of the self-coupling term, a one-electron wave function is not necessary. If one excludes exchange, the self-coupling term also vanishes. The self-coupling term arising in Eq. (2) is therefore due to the presence of the polarization potential in the rearrangement channel, i.e., $Y_{33}^B=V_p^{\mathrm{Ps}}$. Here k_1, k_1', and k_3' denote the wave numbers of the incident positron, the elastically scattered positron, and the moving Ps, respectively, and satisfy the total energy conservation relation

$$E=\tfrac{1}{2}k_1^2-\epsilon_{2s}=\tfrac{1}{4}k_3'^2-\epsilon_{\mathrm{Ps}}\,,$$

where ϵ_{2s}, ϵ_{Ps} stand for the binding energies of lithium and Ps atoms, respectively.

The matrix elements for the potential operators Y_{11}^B and Y_{31}^B can be expressed in terms of the two-body scattering amplitudes $f_{11}^B(\vec{k}_1',\vec{k}_1)$ and $f_{31}^B(\vec{k}_3',\vec{k}_1)$ as

$$-[1/(4\pi^2\mu_\beta)]f_{\beta\alpha}^B(\vec{k}_\beta',\vec{k}_\alpha)=\langle\vec{k}_\beta'\,|Y_{\beta\alpha}^B\,|\vec{k}_\alpha\rangle \qquad (\alpha=1\,,\ \beta=1,3)\,, \tag{3}$$

where μ_β is the reduced mass in channel β. We may obtain similar expressions for the three-body operators in terms of the unknown scattering amplitudes $f_{\beta\alpha}(\vec{k}_\beta',\vec{k}_\alpha)$. Following Guha and Ghosh[10] we can now perform the partial-wave analysis of Eqs. (1) and (2) with the help of Eq. (3) and reduce these coupled three-dimensional integral equations to a set of coupled one-dimensional integral equations which are then solved numerically for the partial-wave scattering amplitudes $f_l^{(\beta\alpha)}(k_\beta',k_\alpha)$.

The differential cross section $d\sigma_{\beta\alpha}/d\Omega$ is obtained from

$$\frac{d\sigma_{\beta\alpha}}{d\Omega}=\frac{v_\beta}{v_\alpha}\left|\frac{1}{(k_\alpha k_\beta')^{1/2}}\sum_{l=0}^{\infty}(2l+1)f_l^{(\beta\alpha)}(k_\beta',k_\alpha)\right.$$
$$\left.\times P_l(\hat{k}_\beta'\cdot\hat{k}_\alpha)\right|^2 Q_0^2\,, \tag{4}$$

with $v_\beta=k_\beta/\mu_\beta$ and $v_\alpha=k_\alpha/\mu_\alpha$, $\alpha=1$, $\beta=1,3$. $f_l^{(\beta\alpha)}(k_\beta',k_\alpha)$ denotes the scattering amplitude for the partial wave l, and $P_l(t)$ the Legendre polynomial of the first kind. The total cross section $\sigma_{\beta\alpha}$ is finally obtained by the integration of $d\sigma_{\beta\alpha}/d\Omega$ over the solid angle.

We have also calculated the momentum-transfer cross section $\sigma_{\beta\alpha}^M$ which is given by

$$\sigma_{\beta\alpha}^M=\left(\frac{d\sigma_{\beta\alpha}}{d\Omega}^M\right)d\Omega\,,$$

with

$$\frac{d\sigma_{\beta\alpha}^M}{d\Omega}=\left(1-\frac{v_\beta}{v_\alpha}\cos\theta_s\right)\frac{d\sigma_{\beta\alpha}}{d\Omega}\,,$$

θ_s being the scattering angle.

We compute cross sections after solving the close-coupling equations with and without consideration of the adiabatic dipole polarization potential. For the elastic scattering, we use the form of this potential.[11] The dipole polarizability of a Ps atom is eight times that of atomic hydrogen.

The adiabatic polarization potential for the Ps-formation channel is exactly the same as that of the hydrogen atom multiplied by eight. For the elastic case, evaluation of the partial-wave amplitudes $f_l^{B(11)}(k_1', k_1)$ is simple and may be obtained in closed analytic form. This we show in the Appendix along with the Ps-formation scattering amplitude $f_{31}^B(\vec{k}_3', \vec{k}_1)$ and its partial-wave analysis.

III. RESULTS AND DISCUSSION

We have computed total and differential cross sections for the elastic scattering and ground-state Ps formation at several incident energies in the range 0.5–10 eV. Before commenting on our results in which long-range forces are included in both channels, we would like to compare our results in the very low energies with or without the long-range forces. This discussion is required due to the fact that Bransden and Jundi[12] found s-wave resonance in the case of a hydrogen atom just below the Ps-formation threshold. In the case of alkali atoms Ps formation is possible even at zero incident energy. P-wave resonance has been noticed by Kraidy and Fraser[13] and Mandal *et al.*[14] in the Ps-formation channel near the Ps-formation threshold. At a limited number of incident energies we have run our program. Therefore, in our case it is not possible to predict any possible resonance in any channel. S-wave resonance as obtained by Bransden and Jundi is spurious.[15] In view of this fact we have run our program neglecting the polarization potential in the Ps-formation channel, i.e., by omitting the last term on the right-hand side of Eq. (2) (Table I). We have obtained cross sections neglecting long-range forces in both channels. The elastic S- and P-wave partial cross sections without polarization are always greater than the corresponding cross-section values with polarization taking either one or both channels. These results are in conformity with the findings of Bransden and Jundi.[12]

TABLE I. Partial elastic cross sections (in units of πa_0^2) in e^+-Li atom collisions. a: Partial cross sections without polarization. b: Partial cross sections without Ps polarization. c: Partial cross sections with polarization in both channels.

Energy (eV)		Partial cross sections $l=0$	$l=1$	$l=2$	$l=3$
0.1	a	170.07	11.13		
	b	103.67	7.522		
0.2	a	134.68	126.29		
	b	112.12	46.59		
0.4	a	90.06	51.72		
	b	97.09	17.51		
0.5	a	75.34	58.17	3.30	0.024
	b	86.76	21.20	10.20	4.127
	c	79.87	4.20	8.33	3.632

TABLE II. Partial Ps-formation cross sections (in units of πa_0^2) in e^+-Li atom collisions. a: Partial cross sections without polarization. b: Partial cross sections without Ps polarization. c: Partial cross sections with polarization in both channels.

Energy (eV)		Partial cross sections $l=0$	$l=1$	$l=2$	$l=3$
0.1	a	39.25	28.85		
	b	20.24	78.53		
0.2	a	25.80	83.72		
	b	11.85	39.42		
0.4	a	16.46	20.86		
	b	6.68	50.17		
0.5	a	13.94	18.86	23.66	4.17
	b	5.49	44.70	46.06	5.99
	c	11.66	9.43	19.78	6.60

Our Ps-formation partial cross-section results in the energy region 0.1 to 0.5 eV are given in Table II. Table II does necessarily show the effect

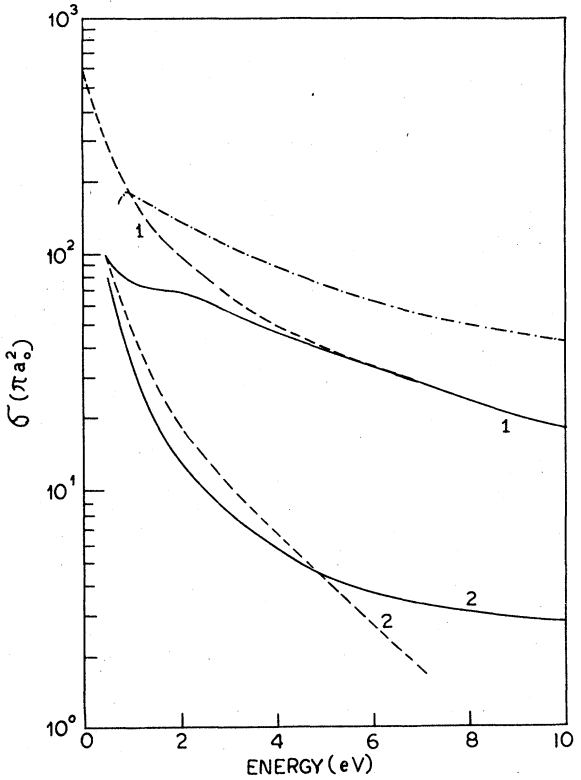

FIG. 1. Total cross section for elastic positron–lithium-atom collisions. The solid line, the present calculation; the broken line, Bui and Stauffer calculation; the dotted chain line, Sarkar *et al.* calculation. 1 represents total cross section and 2 the momentum cross section.

of long-range forces in the Ps-formation channel. From the table it is apparent that the effect of long-range forces in this channel dies out with the increase of l.

Our values of the POM total elastic and momentum-transfer cross sections σ_{11} and σ_{11}^{M} are plotted in Fig. 1, where we also include the results from Sarkar *et al.*[3] and Bui and Stauffer[1] at incident energies for which these are available. It may be seen that the eikonal cross sections of Sarkar *et al.* are much higher than the present results at all the energies. The single-channel polarized orbital calculation of Bui and Stauffer predicts elastic cross sections in quite good accord with our present study in the energy range $4 \leq E \leq 7$ eV. However, at lower energies, the difference between these two calculations is much more pronounced as is evident from the graph. The effect of Ps formation which is attractive in nature is expected to be maximum near the threshold. Bui and Stauffer[1] have neglected this effect completely. The inclusion of the Ps-formation channel is found to influence the elastic results appreciably in the low-energy region. This effect should be included for meaningful results.

In Fig. 2 we display our POM results of the elastic differential cross sections $d\sigma_{11}/d\Omega$ at incident energies 2 and 10 eV and compare them with the elastic-scattering calculation of Sarkar *et al.*[3] using the eikonal approximation. The present differential cross-section curve becomes minimum at around the scattering angle 120° at an incident energy of 2 eV, while for 10-eV positrons, the curve shows a narrow minimum around an angle of 36° and a broad secondary minimum around 140°. The findings of Sarkar *et al.*, however, predict only one minimum at positron energy 10 eV and no minimum for 2-eV positrons. Although this minimum occurs at around the same scattering angle 36° as in our calculation, its value is much higher.

We may mention here that Ferrante *et al.*[5] in the investigation of the low-energy elastic scattering of positrons from alkali atoms Na, K, Rb, and Cs have also reported a similar structure in the dif-

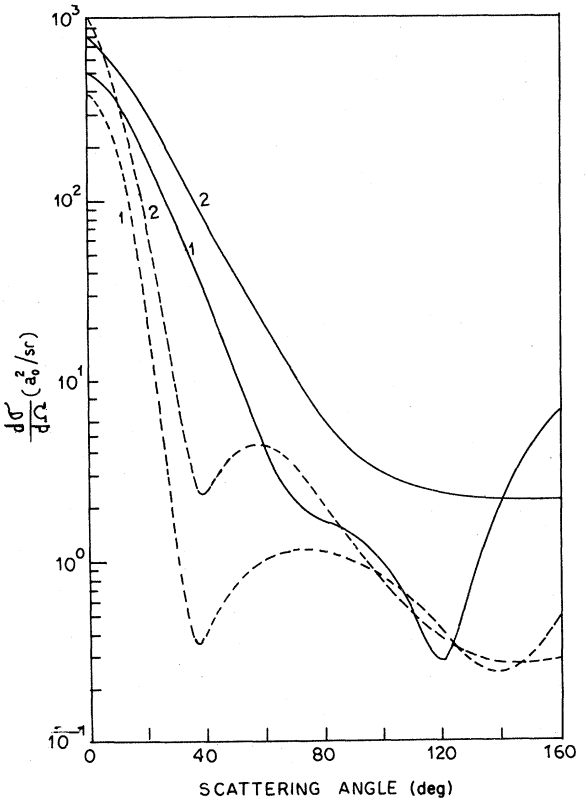

FIG. 2. Differential cross section for elastic positron–lithium-atom collisions at incident energies 2 eV (solid lines) and 10 eV (broken lines). 1 represents present results; 2 represents the result of Sarkar *et al.*

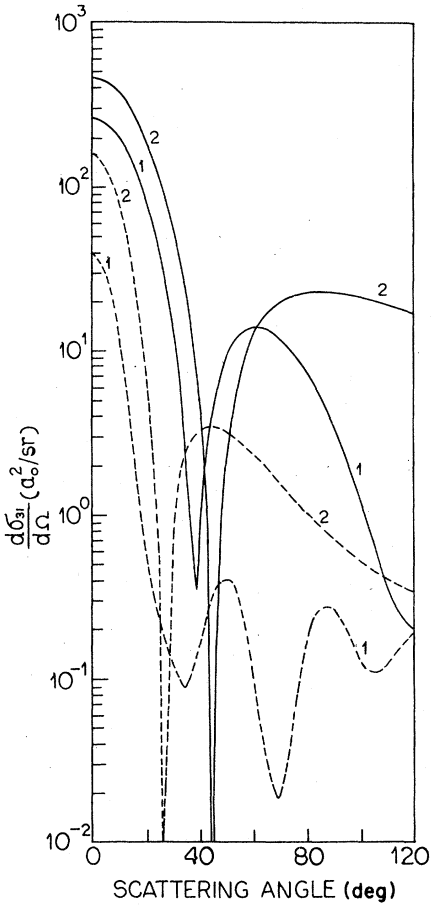

FIG. 3. Differential cross section for Ps formation in positron–lithium-atom collisions at incident energies 2 eV (solid line) and 10 eV (broken line). 1 represents present results and 2 represents present FBA results.

TABLE III. Total Ps-formation cross section σ_{31} in units of πa_0^2 in e^+-Li atom collisions at energies 0.5–10 eV. The symbol $X+Y$ denotes $X\times10^{+Y}$. The superscripts M and B denote, respectively, the momentum-transfer and FBA cross sections. a: Cross section with polarization. b: Cross section without polarization.

Energy (eV)		0.5	1.0	2.0	5.0	10.0
σ_{31}	a	4.787+1	4.997+1	4.171+1	1.380+1	1.613+0
	b	6.095+1		4.691+1	2.619+1	9.626+0
σ_{31}^M	a	3.576+1	3.582+1	2.692+1	8.202+0	1.087+0
	b	5.159+1		3.313+1	1.725+1	5.892+0
σ_{31}^B		1.990+2	1.739+2	1.164+2	4.033+1	1.075+1

ferential cross section. In the absence of any other calculations using rigorous methods, it is not possible to ascertain the exact behavior of the differential cross section.

The present values of the Ps-formation cross sections are quite new, and by comparing them with the elastic cross section we shall be able to get an idea of the relative importance of this rearrangement collision process in positron-lithium atom scattering. In Fig. 3 we show our POM values of the formation differential cross sections $d\sigma_{31}/d\Omega$ at positron energies of 2 and 10 eV and in Fig. 4, the total and momentum-transfer cross sections σ_{31} and σ_{31}^M throughout the entire energy range. In these figures we also include the FBA cross sections for comparison. The present feature of the differential cross section for Ps formation has also been observed in earlier calculations for other systems, namely, e^+-H and e^+-He atom collisions.[16,17] The existence of 3 minima at

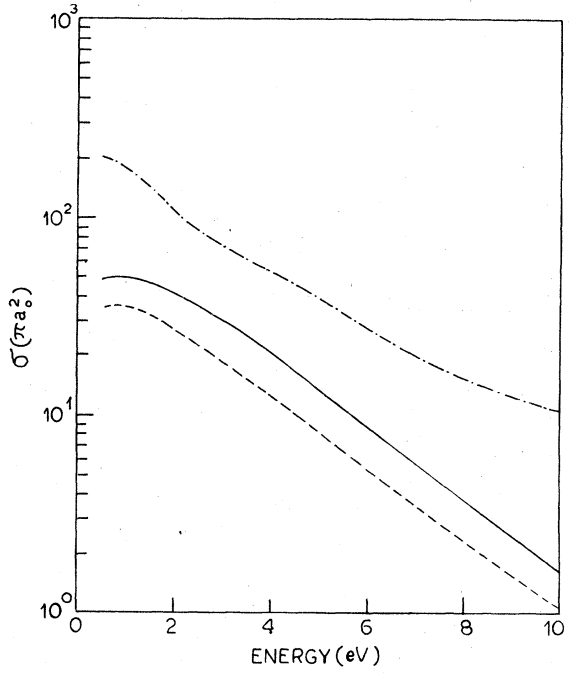

FIG. 4. Total cross section for Ps formation in positron–lithium-atom collisions. The solid line, present result; the broken line, present momentum cross-section results; the dotted chain, the present FBA results.

TABLE IV. Differential cross sections in units of a_0^2/sr for the elastic scattering and Ps formation in e^+-Li atom collisions at incident positron energy 5 eV. The symbol $X\pm Y$ denotes $X\times10^{\pm Y}$. The superscript B denotes the FBA cross sections.

Angles[a] (degree)	Elastic $d\sigma_{11}/d\Omega$	Ps formation $d\sigma_{31}/d\Omega$	$d\sigma_{31}^B/d\Omega$
0.00	5.650+2	1.422+2	3.262+2
4.52	5.070+2	1.308+2	2.996+2
10.37	3.260+2	9.077+1	2.078+2
10.26	1.612+2	4.514+1	1.052+2
22.15	7.070+1	1.419+1	3.579+1
28.05	2.986+1	1.875+0	5.760+0
33.95	1.115+1	9.745−1	3.320−2
39.85	3.065+0	3.315+0	3.301+0
45.75	4.836−1	4.726+0	7.388+0
51.65	8.185−2	4.599+0	9.741+0
57.55	2.846−1	3.707+0	1.035+1
63.45	5.875−1	2.761+0	9.875+0
69.35	7.717−1	2.035+0	8.890+0
75.25	8.025−1	1.517+0	7.766+0
81.15	7.691−1	1.116+0	6.690+0
87.05	7.105−1	7.719−1	5.741+0
92.95	6.188−1	4.830−1	4.937+0
98.85	5.269−1	2.754−1	4.273+0
104.75	4.814−1	1.561−1	3.729+0
110.65	4.775−1	1.014−1	3.286+0
116.55	4.893−1	7.835−2	2.927+0
122.45	3.262−1	6.368−2	2.636+0
128.35	6.044−1	4.638−2	2.400+0
134.25	7.003−1	2.764−2	2.209+0
140.15	7.892−1	1.868−2	2.055+0
145.05	8.953−1	2.683−2	1.932+0
151.95	1.034+0	4.207−2	1.835+0
157.85	1.170+0	4.639−2	1.761+0
163.74	1.274+0	3.445−2	1.706+0
169.63	1.383+0	1.831−2	1.670+0
175.48	1.494+0	9.083−3	1.650+0

[a] The angles correspond to 30 Gauss-Lagendre quadrature points. The zero angle, however, does not belong to this family of mesh points.

TABLE V. Total elastic cross section σ_{11} in units of πa_0^2 in e^+-Li atom collisions at incident energies 0.5–10 eV. The symbol $X+Y$ denotes $X\times 10^{+Y}$. The superscript M denotes momentum-transfer cross sections. a: Cross section with polarization. b: Cross section without polarization.

Energy (eV)		0.5	1.0	2.0	5.0	10.0
σ_{11}	a	9.757+1	7.544+1	6.932+1	4.167+1	1.826+1
	b	1.368+2	1.063+2	9.309+1	5.383+1	3.489+1
σ_{11}^M	a	7.862+1	3.805+1	1.354+1	4.380+0	2.788+0
	b	6.982+1	6.221+1	3.529+1	1.584+1	3.841+0

10 eV may be due to the alkali target. We may also note from Fig. 3 that, at small angles of scattering, the values of $d\sigma_{31}^B/d\Omega$ are much larger than the present cross sections. And in effect the FBA total formation cross section σ_{31}^B is always found to overestimate the present values of σ_{31} (Table III). This is shown graphically in Fig. 4 along with the momentum-transfer cross sections σ_{31}^M.

Lastly, we list our present POM values of the differential cross section in Table IV for the elastic scattering and ground-state Ps formation at a single positron energy of 5 eV. The total elastic and Ps-formation cross sections are shown in Tables V and III. In these tables, the cross section without polarization values are also included. From a close look at the numbers we can see the effect of the inclusion of the long-range forces in the calculations. We may now be interested in comparing the contribution of the ground-state Ps formation to the total scattering cross section with that coming from the elastic positron scattering at low energies of impact below 5 eV. Thus for example, at 0.5 eV, we find that the total elastic cross section is 97.6 πa_0^2, while the corresponding formation cross section is 47.9πa_0^2. Thus the Ps-formation cross section is comparable to that of the elastic one in the low energies. In FBA, the Ps-formation cross section is 192.9πa_0^2. As there is no other calculation, the validity of the present results for the Ps-formation channel may be settled by further calculations.

It may be pointed out that for a highly polarizable target, adiabatic approximation may not be valid for the energy range considered here. The inclusion of a nonadiabatic effect which is repulsive in nature is expected to influence the results to some extent.[18] Further investigation is warranted.

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APPENDIX

The two-body amplitude for the elastic positron scattering may be written as

$$f_{11}^B(\vec{k}_1',\vec{k}_1)=-\frac{\mu_1}{2\pi}\int e^{i\vec{q}\cdot\vec{r}_1}|\Phi_{2s}(r_2)|^2[V_{13}+V_{12}+V_p(r_1)+V_c(r_1)]d\vec{r}_1 d\vec{r}_2\,, \tag{A1}$$

with $\mu_1=1$. The interaction potentials V_{12} and V_{13} are as defined earlier and V_c is the core potential obtained by following Walters[7] (1973) and is given as

$$V_c(r)=2(1/r+\lambda/2)e^{-\lambda r}\,,\quad \lambda=5.4\,. \tag{A2}$$

$V_p(r)$ is the polarization potential [Gupta (1967), Guha and Ghosh (1979)] and $\Phi_{2s}(\vec{r})$ denotes the wave function of the active valence electron

$$\Phi_{2s}(\vec{r})=De^{-\lambda_1 r}+Are^{-\lambda_2 r}\,, \tag{A3}$$

with $\lambda_1=2.7$, $\lambda_2=0.65$, $D=-0.422\,045\,05$, and $A=0.112\,521\,41$. We, however, show below the reduction of the integrals in the expression of $f_{11}^B(\vec{k}_1,\vec{k}_1)$, setting $V_p=0$. The integration over $d\vec{r}_1$ and $d\vec{r}_2$ in (A1) is performed very easily to get finally

$$f_{11}^{B}(\vec{k}_1',\vec{k}_1)=-16\pi\left[\left(\frac{D^2}{\alpha_1^3}+\frac{3AD}{\alpha_2^4}+\frac{12A^2}{\alpha_3^5}\right)\left(\frac{1}{q^2}-\frac{2}{(q^2+\lambda^2)}+\frac{2\lambda^2}{(q^2+\lambda^2)^2}\right)\right.$$
$$\left.-\frac{1}{q^2}\left(D^2 I_{\alpha_1}-AD\frac{\partial}{\partial\alpha_2}I_{\alpha_2}+A^2\frac{\partial^2}{\partial\alpha_3^2}I_{\alpha_3}\right)\right], \tag{A4}$$

with $I_\alpha=\alpha/(q^2+\alpha^2)^2$, $\alpha_1=2\lambda_1$, $\alpha_2=\lambda_1+\lambda_2$, $\alpha_3=2\lambda_2$. The partial-wave elastic-scattering amplitude $f_l^{B\,(11)}(k_1',k_1)$ may now be obtained from the relation

$$f_l^{B\,(11)}(k_1',k_1)=\frac{(k_1k_1')^{1/2}}{2}\int_{-1}^{+1}f_{11}^{B}(\vec{k}_1',\vec{k}_1)P_l(t)dt\,. \tag{A5}$$

We now define the two-body Ps-formation scattering amplitude as

$$f_{31}^{B}(\vec{k}_3',\vec{k}_1)=-\frac{\mu_3}{2\pi}\int e^{-i\vec{k}_3'\cdot(\vec{r}_1+\vec{r}_2)/2}\Phi_{Ps}(\vec{r}_{12})[V_{23}+V_{13}+V_c(r_1)+V_c(r_2)]e^{i\vec{k}_1\cdot\vec{r}_1}\Phi_{2s}(r_2)d\vec{r}_1\,d\vec{r}_2\,. \tag{A6}$$

Here $\Phi_{Ps}(\vec{r}_{12})$ denotes the ground-state Ps wave function

$$\Phi_{Ps}(\vec{r}_{12})=(\lambda_f^3/\pi)^{1/2}\exp(-\lambda_f r_{12})\,,\quad \lambda_f=0.5 \tag{A7}$$

and μ_3 denotes the reduced mass in the final channel and is equal to 2.

Following Basu *et al.* (1976), the integration over $d\vec{r}_1$ and $d\vec{r}_2$ may be reduced to a one-dimensional integral from 0 to 1. The final form of this amplitude reads as

$$f_{31}^{B}(\vec{k}_3',\vec{k}_1)=-\frac{\mu_3}{2\pi}\left[\sqrt{\pi}\left(DI_0(\lambda_1)-A\frac{\partial}{\partial\lambda_2}I_0(\lambda_2)\right)+2D\left(J(a)-\frac{\lambda}{2}\frac{\partial}{\partial a}J(a)\right)+2A\left(-\frac{\partial}{\partial b}J(b)+\frac{\lambda}{2}\frac{\partial^2}{\partial b^2}J(b)\right)\right.$$
$$\left.-2D\left(I(\lambda_1)-\frac{\lambda}{2}\frac{\partial}{\partial\lambda_1}I(\lambda_1)\right)-2A\left(-\frac{\partial}{\partial\lambda_2}I(\lambda_2)+\frac{\lambda}{2}\frac{\partial^2}{\partial\lambda\,\partial\lambda_2}I(\lambda_2)\right)\right], \tag{A8}$$

where

$$I_0(\lambda_1)=\int e^{-i\vec{k}_3'\cdot(\vec{r}_1+\vec{r}_2)/2}\Phi_{Ps}(\vec{r}_{12})\left(\frac{1}{r_1}-\frac{1}{r_2}\right)e^{i\vec{k}_1\cdot\vec{r}_1}\Phi_{2s}(\vec{r}_2)d\vec{r}_1\,d\vec{r}_2$$
$$=\sqrt{2}\pi\left[\lambda_1\int_0^1 dx\,x(1-x)\left(\frac{3A_0^2+4\mu_0^2A_0+8\mu_0^4}{\mu_0^5A_0^3}\right)-8\int_0^1\frac{x\,dx}{A_0^3}\right],$$

$$J(a)=\int e^{-i\vec{k}_3'\cdot(\vec{r}_1+\vec{r}_2)/2}\Phi_{Ps}(\vec{r}_{12})\frac{\exp(-ar_2)}{r_2}e^{i\vec{k}_1\cdot\vec{r}_1}d\vec{r}_1\,d\vec{r}_2=8\pi\sqrt{2}\pi\int_0^1\frac{x\,dx}{A_1^3}\,,$$

$$I(\lambda_1)=\int e^{-i\vec{k}_3'\cdot(\vec{r}_1+\vec{r}_2)/2}\Phi_{Ps}(\vec{r}_{12})\frac{\exp(-\lambda_1 r_1)}{r_1}e^{i\vec{k}_1\cdot\vec{r}_1}d\vec{r}_1\,d\vec{r}_2$$
$$=2\pi\sqrt{2}\pi\lambda_1\lambda_f\int_0^1 dx\,x(1-x)\left(\frac{3A_0^2+2\mu_0A_0(3\lambda+2\mu_0)+8\mu_0^2\delta^2}{\mu_0^5A_0^3}\right),$$

with

$$\vec{\omega}=\vec{k}_1-\tfrac{1}{2}(2-x)\vec{k}_3'\,,\qquad A_0=\omega^2+\mu_0^2\,,$$
$$\mu_0^2=\tfrac{1}{4}x+\lambda_1^2(1-x)+x(1-x)\tfrac{1}{4}k_3'^2\,,\qquad A_1=\omega^2+\mu_1^2\,,\qquad b=\lambda+\lambda_2\,,$$
$$\mu_1^2=\tfrac{1}{4}x+a^2(1-x)+\tfrac{1}{4}x(1-x)k_3'^2\,,\qquad a=\lambda+\lambda_1\,,\qquad \delta=\mu_0+\lambda\,.$$

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