Positron-lithium scattering at low and intermediate energies

Madhumita Basu and A. S. Ghosh
Department of Theoretical Physics, Indian Association for the Cultivation of Science, Jadavpur, Calcutta 700 032, India
(Received 18 April 1990)

Positron-lithium scattering has been investigated using the three-state [Li($2s$), Li($2p$), and Ps($1s$)] close-coupling approximation. Calculations have also been carried out by using the static, coupled static, and Born approximations. Elastic ($2s$-$2s$), excitation ($2s$-$2p$), and Ps-formation cross sections are reported up to an incident energy of 100 eV. The effect of the Ps-formation channel on elastic scattering is found to be pronounced at low incident energies, and this effect is not negligible even up to 50 eV. The positronium formation cross section is reduced appreciably in the energy region 1.0–20.0 eV when the $2p$ state is included in the expansion scheme.

I. INTRODUCTION

Measured data of positron–alkali-metal-atom scattering have become recently available. Kwan and coworkers[1] have reported the total cross sections of K, Na, Rb, and Cs atoms and the same for other alkali-metal atoms are expected in the near future. These stimulate the theoretical works on e^+–alkali-metal-atom scattering. Investigations have been carried out recently by Khan, Dutta, and Ghosh,[2] Sarkar, Basu, and Ghosh,[3] and Ward *et al.*[4] using the close-coupling approximation (CCA). In these calculations, the maximum number of eigenstates retained in the expansion scheme is five. Apart from CCA calculations a polarized orbital method has also been employed by Ward *et al.*[4] None of these calculations includes the Ps-formation channel.

Our recent studies[5,6] on e^+-H scattering at low and intermediate energies led to the conclusion that to predict reliable scattering parameters, both the effects of atomic distortion and the rearrangement channel must be included simultaneously. In the case of alkali-metal atoms, the effect of Ps formation is expected to be more pronounced as the Ps-formation channel is open even at zero incident energy. The only existing calculation to investigate e^+-Li scattering in which both these effects are included is due to Guha and Ghosh.[7] They have employed a polarized orbital method using a very simple wave function. Moreover, their polarization potential is subject to refinement.

The alkali-metal atom is a highly polarizable target. Therefore, reliable estimates of the effect of distortion of the alkali-metal target is rather essential to predict scattering parameters. In the CCA, the effect of distortion of the target atom is taken into account reliably by including the p orbitals in the expansion scheme. Inclusion of the $2p$ state is expected to be a good representation of the long-range effect since 98% of the polarizability of the lithium atom is given by the $2p$ state alone.

Here, we investigate e^+-Li scattering using the three-state CCA [Li($2s$), Li($2p$), Ps($1s$)]. However, to have knowledge of the relative importance of the individual states the expansion schemes

(i) Li($2s$) (static),

(ii) Li($2s$),Ps($1s$) (coupled static),

(iii) Li($2s$),Li($2p$) (two-state CCA)

have also been used. Two- and three-state CCA will be denoted as $2s$-$2p$ and $2s$-$2p$-Ps CCA, respectively.

II. THEORY

The total wave function for the e^+-Li system is expressed as

$$\Psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3,\mathbf{X})=\sum_i \Phi_i(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)F_i(\mathbf{X}) + \sum_\nu \Phi^+_{1s}(\mathbf{r}_1,\mathbf{r}_2)\eta_\nu(\boldsymbol{\rho})G_\nu(\mathbf{R})$$

with

$$\boldsymbol{\rho}=|\mathbf{X}-\mathbf{r}_3|, \quad R=\left|\frac{\mathbf{r}_3+\mathbf{X}}{2}\right| .$$

Here, $\Phi_i(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)$ and $\eta_\nu(\boldsymbol{\rho})$ are the ith and νth eigenstates of the lithium and positronium atoms, respectively. The ground-state wave function of the lithium ion is denoted by $\Phi^+_{1s}(\mathbf{r}_1,\mathbf{r}_2)$. $F_i(\mathbf{X})$ describes the motion of the incident positron and G_ν is the motion of the positron atom relative to the lithium nucleus.

We assume that the $1s^2$ core of the lithium atom is frozen. Since the valence electron lies well outside the core, this assumption introduces only a small error. The same assumption is used by Burke and Taylor[8] in the case of e^--Li scattering and by Khan, Dutta, and Ghosh,[2] Sarkar, Basu, and Ghosh,[3] and Ward *et al.*[4] in e^+-Li scattering. The wave function $\Psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3,\mathbf{x})$ must satisfy the following Schrödinger equation:

$$(H-E)\Psi=0 ,$$

where H is the total Hamiltonian of the system and is

 ©1991 The American Physical Society

given by

$$H=\sum_{i=1}^{3}\left[-\frac{1}{2\mu}\nabla_{r_i}^2-Z/r_i\right]+\sum_{i<j=1}^{3}\frac{1}{r_{ij}}+H_T$$

with

$$H_T=-\frac{1}{2\mu}\nabla_x^2+\frac{z}{x}-\sum_{i=1}^{3}\frac{1}{|\mathbf{X}-\mathbf{r}_i|}\ .$$

The ground- and excited-state wave functions of the target lithium atom are taken from Weiss.[9]

Instead of solving the conventional coupled integrodifferential equations, coupled integral equations for the scattering amplitudes in the momentum space have been solved following Basu, Mukherjee, and Ghosh.[5] The cross sections have been obtained by using the standard relations.

III. RESULTS AND DISCUSSIONS

The calculations using the static, coupled static, 2*s*-2*p*, and 2*s*-2*p*-Ps CCA in the incident positron energy range 0.1–100 eV have been performed by us. Guha and Ghosh[7] carried out the first coupled static calculations of e^+-Li scattering using very simple wave functions. Recently, Abdel-Raouf[10] performed a nearly coupled static calculation for positron–alkali-metal system. Khan, Dutta, and Ghosh,[2] Sarkar, Basu, and Ghosh,[3] and Ward *et al.*[4] predicted the cross sections employing 2*s*-2*p* CCA. The present elastic results using the 2*s*-2*p* CCA are in close agreement with the previous two sets of results. However, present results at 0.5 eV differ by about 2.9% from those of Ward *et al.*

Our main motivation is to study the effect of atomic distortion as well as the effect of the Ps-formation channel on the direct one. In the case of the alkali-metal atom, these two effects are expected to be very significant at low incident energies. Figure 1 presents the present elastic integrated cross sections obtained using the static, coupled static, and 2*s*-2*p* close-coupling approximation. The dramatic enhancement of the elastic cross section obtained by using the two-state (2*s*, 2*p*) CCA over the corresponding static (2*s*) results has been noticed at low incident energy. This confirms the fact that the lithium atom is a highly polarizable target. This effect of atomic distortion decreases rapidly with the increase of energy, and at about 30 eV the difference between the two results is marginal. In the energy range 0.5–30 eV, coupled static results are also found to be significantly greater than the corresponding static predictions. At very low energies, coupled static results are comparable with those using the 2*s*-2*p* CCA. However, the difference between the coupled static and static results decreases with the in-

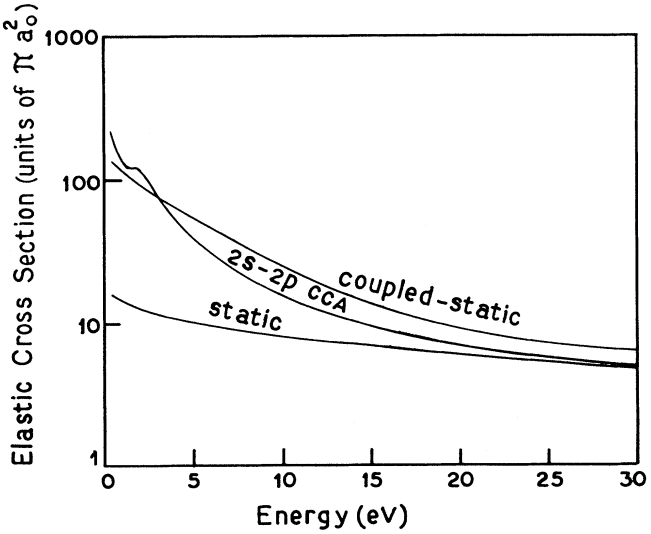

FIG. 1. Elastic (2*s*-2*s*) integrated cross section (πa_0^2) using the static, coupled static, and 2*s*-2*p* close-coupling approximations.

TABLE I. Elastic (2*s*-2*s*) cross sections in e^+-Li scattering (in units of πa_0^2) using the FBA, static, coupled static, 2*s*-2*p*, and 2*s*-2*p*-Ps(1*s*) CCA.

Energy (eV)	FBA[a]	Static	2*s*-2*p*	Coupled static	2*s*-2*p*-Ps(1*s*)
0.1	147.51	17.17	655.75	181.29	147.17
0.5	125.39	15.81	234.58	137.62	103.88
1.0	104.95	14.60	140.47	117.09	94.82
1.5	89.84	13.71	116.92	114.13	95.74
1.8	82.57	13.27	120.41	97.26	99.83
2.0	78.30	13.00	119.80	93.45	107.19
3.0	62.02	11.91	77.65	77.90	87.93
5.0	43.52	10.38	40.42	57.43	65.15
10.0	24.84	8.15	15.95	26.14	38.85
20.0	13.46	5.91	7.04	9.21	16.67
30.0	9.28	4.71	4.96	5.77	8.01
50.0	5.76	3.40	3.40	3.59	3.91
100.0	2.98	2.05	1.95	2.04	1.97

[a]We recalculate the FBA using the wave function of Weiss (Ref. 9) with the following interaction potential:

$$V_{\text{int}}=\frac{Z}{X}-\sum_{i=1}^{3}\frac{1}{|x-r_i|}\ .$$

crease of energy, the rate of decrease being slower than the 2*s*-2*p* CCA. At the highest energy shown here (30 eV), this effect is about 20%, coupled static results being higher. However, at 100 eV, the difference between the two sets of results is negligible (Table I). In the case of e^+-H (Refs. 11 and 12) and e^+-He (Ref. 13) scattering, the effect of Ps formation is found to be less pronounced.

The effect of positronium formation on the elastic scattering can also be noticed by comparing the present 2*s*-2*p*-Ps and 2*s*-2*p* CCA (Fig. 2). Five-state CCA (Refs. 2–4) results are the most elaborate calculations so far reported in the case of e^+-Li scattering and have been included in the same figure as a reference. The effect of Ps formation is found to be very pronounced in the energy range considered. Present 2*s*-2*p*-Ps CCA results are always greater than the corresponding 2*s*-2*p* and five-state CCA results above 2.5 eV. These corroborate our earlier findings[5] that the inclusion of the Ps-formation channel in the expansion scheme enhances the elastic cross section. Below 2.5 eV, the present 2*s*-2*p*-Ps CCA results lie below the two- and five-state results and the position of the minima is shifted towards lower energy. There are differences between 2*s*-2*p* and 2*s*-2*p*-Ps CCA results even up to 100 eV (Table I) whereas the difference between the two- and five-state results is marginal beyond 30 eV.

In positron–alkali-metal-atom scattering, the contribution of inelastic scattering is dominant (Khan, Dutta, and Ghosh[2]). The major contribution to the inelastic scattering comes from the 2*s*-2*p* excitation process. The 2*s*-2*p* excitation cross section is expected to shape the total cross section at intermediate energies. Integrated 2*s*-2*p* excitation cross sections are presented in Fig. 3 up to the incident energy 30 eV. This figure also contains the results of the two- and five-state CCA. Below the incident energy 10 eV, our 2*s*-2*p*-Ps CCA results are always less than two- and five-state predictions, five-state results being highest. Moreover, the position of the maximum is shifted towards the higher energy when the positronium-formation channel is included in the expansion scheme.

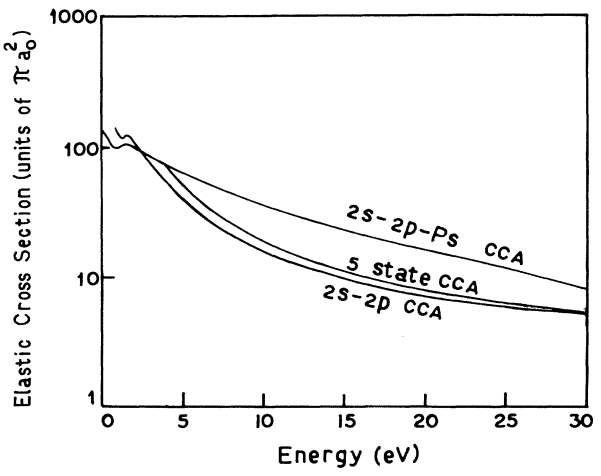

FIG. 2. Elastic (2*s*-2*s*) integrated cross section (πa_0^2) using the 2*s*-2*p*, five-state, and 2*s*-2*p*-Ps CCA.

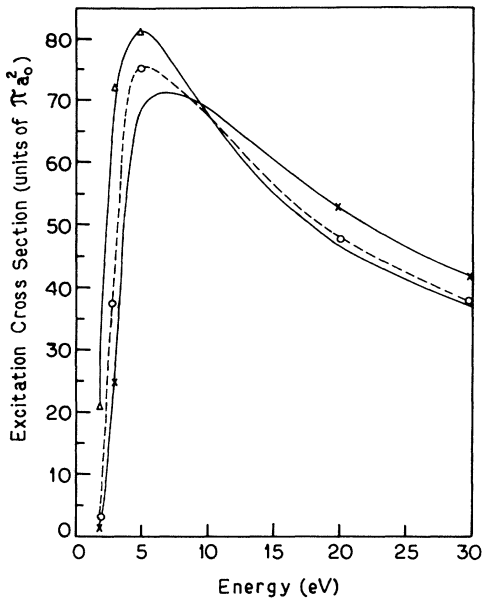

FIG. 3. Integrated excitation (2*s*-2*p*) cross section (πa_0^2): —*X*—, 2*s*-2*p*-Ps (CCA; —Δ—, five-state CCA; ——○——, 2*s*-2*p* CCA.

Above the incident energy 10 eV, the difference between the five- and two-state CCA predictions is not appreciable. On the other hand, we have noticed a significant difference between the three- and two-state (five-state) results, the three-state results being higher. With the increase of energy, the difference decreases (Table II). At incident energy 100 eV, the results nearly coalesce. The present 2*s*-2*p* results are in fair agreement with the earlier predictions of Khan, Dutta, and Ghosh[2] and Ward *et al.*[4] except at the two incident energies 2.0 and 3.0 eV.

It has already been shown by Guha and Ghosh[7] that the Ps-formation cross section in e^+-Li scattering is very sensitive to the model chosen. This feature is also clear from Table III, where we have presented a number of Ps-formation cross sections using the Born, coupled static, and the three-state CCA predictions. The FBA cross section is predominantly higher up to incident energy 5 eV. The results of coupled static and the three-state CCA predictions are nearly equal at 1 eV. Below this in-

TABLE II. Excitation (2*s*-2*p*) cross section (in units of πa_0^2) in e^+-Li scattering using the FBA, 2*s*-2*p*, and 2*s*-2*p*-Ps CCA.

Energy (eV)	FBA[a]	2*s*-2*p*	2*s*-2*p*-Ps
2.0	81.10	3.34	1.74
3.0	133.12	37.06	25.03
5.0	119.13	75.65	68.39
10.0	82.96	68.73	68.04
20.0	52.59	48.23	53.25
30.0	39.32	38.24	42.21
50.0	26.77	26.87	27.01
100.0	15.49	15.60	15.60

[a]Same as in Table I.

TABLE III. Ground-state capture cross section in e^+-Li scattering (in units of πa_0^2) using the FBA, coupled static, and 2*s*-2*p*-Ps CCA. Square brackets denote powers of 10.

Energy (eV)	FBA[a]	Coupled static	2*s*-2*p*-Ps CCA
0.1	137.68	68.76	158.61
0.5	192.76	56.91	81.89
1.0	170.28	51.94	51.32
1.5	139.96	47.25	33.81
1.8	123.88	44.66	24.13
2.0	114.23	43.17	18.78
3.0	78.50	36.96	6.97
5.0	39.15	24.94	3.43
10.0	10.19	9.28	1.34
20.0	1.34	1.25	1.32
30.0	2.47[−1]	2.58[−1]	3.76[−1]
50.0	1.74[−2]	2.32[−2]	2.82[−2]
100.0	4.01[−3]	4.02[−3]	2.60[−3]

[a]We recalculate the FBA using the wave function of Weiss with the post interaction.

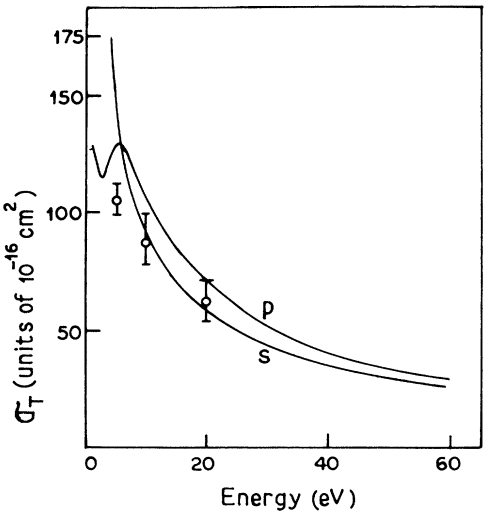

FIG. 4. Comparison of the total cross section for $e^{\pm}$-Li scattering (in 10^{-16} cm^2): ——*P*, present results (e^+-Li); —*S*, Sarkar, Basu, and Ghosh (Ref. 3) (e^+-Li). Φ, experimental results for e^--Li of Kasdan, Miller, and Bederson (Ref. 15).

cident energy, the three-state results are higher than the other two sets of results. Above this energy, the three-state results decrease faster than the coupled static results up to 20 eV. At an incident energy of 10 eV, the coupled static results are approximately sevenfold greater than the 2*s*-2*p*-Ps CCA predictions. This feature was also noticed by Guha and Ghosh when they included the polarization effect in the direct channel. From 20 eV and above, three sets of results are nearly equal.

The difference between the coupled static and three-state CCA prediction is due to the fact that the lithium atom is a highly polarizable target. The present coupled static results are in fair agreement with those of Guha and Ghosh. The results of Abdel-Raouf, who have performed a nearly coupled static calculation, differ from the present result at incident energies 3 and 5 eV, respectively.

It is instructive to compare the total positron cross section with the corresponding measured electron results. The total cross section σ_T is assumed as

$$\sigma_T=\sigma_{\rm el}+\sigma_{\rm Ps}+\sigma_{\rm exc}+\sigma_{\rm ion} .$$

Here, elastic ($\sigma_{\rm el}$) and Ps-formation ($\sigma_{\rm PS}$) cross sections are taken from the present studies. The excitation cross section ($\sigma_{\rm exc}$) consists of

$$\sigma_{\rm exc}=\sigma_{2s\text{-}2p}+\sigma_{2s\text{-}3s}+\sigma_{2s\text{-}3p}+\sigma_{2s\text{-}3d} ,$$

where the 2*s*-2*p* excitation cross section ($\sigma_{2s\text{-}2p}$) using the 2*s*-2*p*-Ps CCA is the present result and other results are taken from Khan, Dutta, and Ghosh and Sarkar, Basu, and Ghosh. The ionization cross section ($\sigma_{\rm ion}$) is taken from Basu and Ghosh.[14] Below the first electronic excitation threshold, the total cross section (σ_T) is the sum of elastic and Ps-formation cross sections. The present total cross sections for e^+-Li scattering thus defined is compared with the measured data of Kasdan, Miller, and Bederson.[15] (e^--Li) and the prediction of Sarkar, Basu, and Ghosh (e^+-Li) (see Fig. 4). Below the incident energy 5 eV, the present results lie below the prediction of Sarkar, Basu, and Ghosh, whereas above this incident energy the present results are always greater than those of Sarkar, Basu, and Ghosh. Moreover, the present positron results are greater than the measured values for e^--Li scattering; the difference is less than 10%. In the case of other alkali-metal atoms (Na,K), similar features have been observed by Stein *et al.*[16] The present total cross section has a kink below the incident positron energy 5 eV. This feature awaits experimental confirmation. The difference between the present total cross section and those of Sarkar, Basu, and Ghosh beyond 5 eV is due to the inclusion of the Ps-formation channel in the coupling scheme.

IV. CONCLUSION

We have investigated e^+-Li scattering using the three-state CCA in which Ps-formation channels have been included explicitly. This effect is not negligible even up to incident energy 50 eV. In the case of other atoms, this effect is less pronounced. Our assumption that in the case of alkali-metal atoms the effect of the Ps-formation channel is significant is corroborated here. Moreover, the lithium atom is a highly polarizable target. The effect of atomic distortion is also found to be significant, as expected. First-order Born approximation (FBA) results are not valid up to 100 eV. We conclude that to have a reliable result in e^+–alkali-metal-atom scattering the effect of the positronium channel and of atomic distortion have to be included with proper care.

The inclusion of the 3*d* state in the expansion scheme influences the cross section significantly below the incident energy 10 eV (Khan, Dutta, and Ghosh[2]). The present elastic and excitation cross sections are expected to be modified below 10 eV if the 3*d* state is included in the expansion scheme. Above this incident energy, we believe, present results are reliable.

[1]C. K. Kwan, M. S. Dababneh, W. E. Kauppila, R. A. Lukaszew, S. P. Parikh, T. S. Stein, Y. J. Wan, and S. Zhou, in *Abstracts of the Sixteenth International Conference on the Physics of Electronic and Atomic Collisions, New York, 1989,* edited by A. Dalgarno, R. S. Freund, M. S. Lubell, and T. B. Lucatorto (AIP, New York, 1990), p. 404; T. S. Stein, H. S. Dababneh, W. E. Kauppila, C. K. Kwan, and Y. J. Wan, in *Atomic Physics with Positrons,* edited by J. W. Humberston and E. A. G. Armour (Plenum, New York, 1987), p. 251.

[2]P. Khan, S. Dutta, and A. S. Ghosh, J. Phys. B **20**, 2927 (1987).

[3]K. P. Sarkar, M. Basu, and A. S. Ghosh, J. Phys. B **21**, 1649 (1988).

[4]S. J. Ward, M. Horbatsch, R. P. McEachran, and A. D. Stauffer, J. Phys. B **22**, 1845 (1989).

[5]M. Basu, M. Mukherjee, and A. S. Ghosh, J. Phys. B **22**, 2195 (1989).

[6]M. Mukherjee, M. Basu, and A. S. Ghosh, J. Phys. B **23**, 75 (1990).

[7]S. Guha and A. S. Ghosh, Phys. Rev. A **23**, 743 (1981).

[8]P. G. Burke and A. J. Taylor, J. Phys. B **2**, 869 (1969).

[9]A. W. Weiss, Astrophys. J. **138**, 1262 (1963).

[10]M. A. Abdel Raouf, J. Phys. B **21**, 2331 (1988).

[11]W. J. Cody, J. Lawson, H. S. W. Massey, and K. Smith, Proc. R. Soc. London Ser. A **278**, 479 (1964).

[12]D. Basu, G. Banerji, and A. S. Ghosh, Phys. Rev. A **13**, 1381 (1976).

[13]P. Mandal, A. S. Ghosh, and N. C. Sil, J. Phys. B **8**, 2377 (1975).

[14]M. Basu and A. S. Ghosh, J. Phys. B **19**, 1249 (1986).

[15]A. Kasdan, T. Miller, and B. Bederson, *Proceedings of the International Conference on Atomic Physics, Boulder, Colorado* (University of Colorado Press, Colorado, 1971), p. 120.

[16]T. S. Stein, W. E. Kauppila, C. K. Kwan, R. A. Lukaszew, S. P. Parikh, Y. J. Wan, S. Zhou, and M. S. Dababneh, in *Proceedings of the Workshop on Annihilation in Gases and Galaxies,* edited by R. J. Drachman (NASA Conference Publications, 1990), No. 3058, p. 13.