Possible resonance in positron-lithium scattering

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The possible appearance of resonances in the partial cross sections of the inelastic collisions of positrons with lithium atoms at energies below 5 eV is investigated. It is assumed that only elastic and rearrangement channels are open, while excitation channels are closed. A coupled static formalism, in which the polarization potentials of the lithium and positronium are switched on, is employed. The basis set of Clementi and Roetti [At. Data Nucl. Data Tables **14**, 177 (1974)] is used for describing the target model. Comparison between the resulting total cross sections and those obtained by other authors is presented.

Inelastic collisions of positrons with alkali-metal atoms have generated intense interest among positron physicists recently. Although the positronium (Ps) formation channel is open even at zero incident energy, very few works[1] explicitly considering the effect of this channel and treating the rearrangement process properly have appeared. The reason lies in two points: (i) There have been no experimental investigations of the effect, and (ii) most experimental and theoretical studies of these collisions have been restricted to energies above 10 eV, where excitation may play the dominant role rather than the Ps formation. In the work reported here, we concentrated on an investigation of the inelastic scattering of positrons from the ground state of lithium within the energy region 0–5 eV, which is the most interesting range for Ps formation, (i.e., the region where the Ps channel cannot be ignored). Our purpose was to calculate the partial and total elastic and Ps formation cross sections using an elaborate but still tractable algorithm, and to study the possible appearance of resonances. For this purpose, we used a restricted coupled static approximation (RCSA) in which reactance matrices are symmetrized so that unitarity of the scattering matrices and fulfillment of Mott and Massey's bounds[2] on partial cross sections are guaranteed. (The coupled static approximation (CSA) was employed some years ago by Bransden and Jundi[3] for treating e^+-H scattering below the Ps threshold, where virtual Ps-proton bound states have been identified. In Ref. 1, the authors applied the same method to e^+-Li scattering using Walters's wave functions.) Also both lithium- and positronium-polarization potentials (the polarization potentials of the first and second channels, respectively) were switched on. The most important step in this algorithm is the solution of the coupled integro-differential equations

$$\left[\frac{d^2}{dx^2}-\frac{l(l+1)}{x^2}+k_1^2\right]f_l(x) = U_x f_l(x)+\int_0^\infty K_{12}(\sigma,x)g_l(\sigma)d\sigma \ , \quad (1)$$

$$\left[\frac{d^2}{d\sigma^2}-\frac{l(l+1)}{\sigma^2}-k_2^2\right]g_l(\sigma) = U_\sigma g_l(\sigma)+\int_0^\infty k_{21}(\sigma,x)f_l(x)dx \ , \quad (2)$$

where x and σ are, respectively, the position vectors of the incident positron and the center of mass of the positronium, both taken relative to an infinitely heavy nucleus located at the origin of our configuration space. Correspondingly, k_1 and k_2 are the momenta and $f_l(x)$ and $g_l(\sigma)$ are the partial scattering wave functions of the first and second channels associated with the total angular momentum l. The potentials U_x and U_σ are defined by

$$U_x = V_{\rm ST}^{\rm Li}(x)+V_{\rm pol}^{\rm Li}(x) \quad (3)$$

and

$$U_\sigma = V_{\rm st}^{\rm Ps}(\sigma)+V_{\rm pol}^{\rm Ps}(\sigma) \ , \quad (4)$$

where $V_{\rm st}^{\rm Li}(x)$ and $V_{\rm pol}^{\rm Li}(x)$ are the static and polarization potentials of the lithium atom and $V_{\rm st}^{\rm Ps}(\sigma)$ and $V_{\rm pole}^{\rm Ps}(\sigma)$ are those of the positronium atom. The kernels $k_{12}(\sigma,x)$ and $k_{21}(\sigma,x)$ are defined at Eqs. (24) and (25) in Ref. 4 in terms of the Ps wave function and the target wave function which was chosen in the form developed by Clementi and Roetti.[5]

The final forms of the potentials $V_{\rm st}^{\rm Li}(x)$ and $V_{\rm st}^{\rm Ps}(\sigma)$ are given in Ref. 4, while $V_{\rm pol}^{\rm Ps}(\sigma)$ is expressed in Ref. 6 [Eqs. (21)–(24)] for the collisions of positrons with lithium-isoelectronic sequence in terms of $Z_{\rm eff}$, the net charge of the ionized target in the second channel. (In our case $Z_{\rm eff}=1$). $V_{\rm pol}^{\rm Li}(x)$ is chosen in the same form presented by Peach.[7]

In order to calculate the reactance and transition matrices ($\underline{R}$ and $\underline{T}$, respectively) required for the evaluation of the partial and total cross sections of the first and second channels we employed the iterative Green-function partial-wave expansion technique described in

TABLE I. Comparison between present partial elastic cross sections (in units of πa_0^2), calculated with the Clementi-Roetti basis set, and those of Khan, Dutta, and Ghosh (Ref. 9) obtained using the five-state close-coupling method.

	Present work					Khan, Dutta, and Ghosh (Ref. 9)				
k_1^2 (eV)	$l=0$	$l=1$	$l=2$	$l=3$	$l=4$	$l=0$	$l=1$	$l=2$	$l=3$	$l=4$
0.005	386.712	0.132	0.000	0.000	0.000					
0.01	377.742	0.506	0.000	0.000	0.000					
0.05	323.675	9.178	0.013	0.000	0.000					
0.1	273.665	26.164	0.157	0.000	0.000					
0.5	104.071	115.638	14.196	0.555	0.004					
1.0	32.441	118.748	39.029	5.422	0.204					
4.0	0.001	24.685	34.021	24.362	7.813	0.165	12.254	21.651	17.087	9.187
5.0	0.002	17.030	24.882	20.565	8.234	0.500	6.989	13.697	11.981	7.383
7.0	2.946	10.679	13.118	11.977	6.569	1.015	2.854	6.313	6.573	4.827
10.0	4.363	6.102	5.550	4.817	3.375	1.359	1.302	2.955	3.204	2.714

detail in Refs. 4 and 6 within the framework of the RCSA discussed in Ref. 8.

In order to investigate the possible appearance of resonances, we diagonalized the $\underline{R}$ matrix and calculated the eigenphases adherent to the two channels at each value of l and k_1^2, the energy of the incident positrons. Resonance states are identified in our units by the values of k_1^2 at which an eigenphase passes through $\pi/2$. The above algorithm was used in order to calculate the most accurate values of the elements of the $\underline{R}$ and $\underline{T}$ matrices, the elastic and rearrangement partial cross sections (σ_{11}^l and σ_{12}^l, respectively) at 40 values of k_1^2 between 0.005 and 20 eV and for eight values of the total angular momentum ranging from $l=0$ to $l=7$.

In Table I, we present examples for the S-, P-, D-, F-, and G-wave partial elastic cross sections obtained by our formalism. We also give the corresponding cross sections determined by Khan, Dutta, and Ghosh[9] at $k_1^2=4,5,7$, and 10 eV. The table emphasizes the dominant role played by the S wave at energies below 0.5 eV. Although the two sets of cross sections are based on different physical assumptions and, consequently, have rather different features, they show the same behavior with the increase of k_1^2 and support the increasing role played by the higher partial waves.

Figures 1 and 2 illustrate the behavior of σ_{11}^l and σ_{12}^l, respectively, at $l=0,1,2,3$, with the variation of the incident energy. Both figures demonstrate that the S-wave cross sections possess sharp maxima at k_1^2 close to zero and fall off rapidly beyond this energy. They also indi-

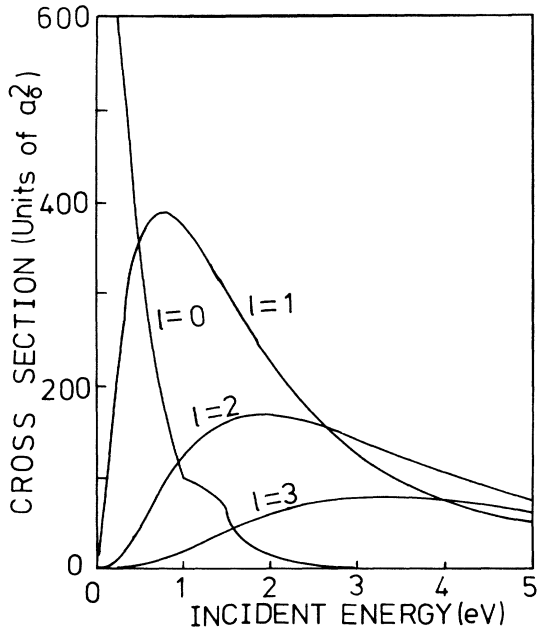

FIG. 1. Partial elastic cross sections (in units of a_0^2) of e^+-Li inelastic scattering determined using the Clementi-Roetti wave functions.

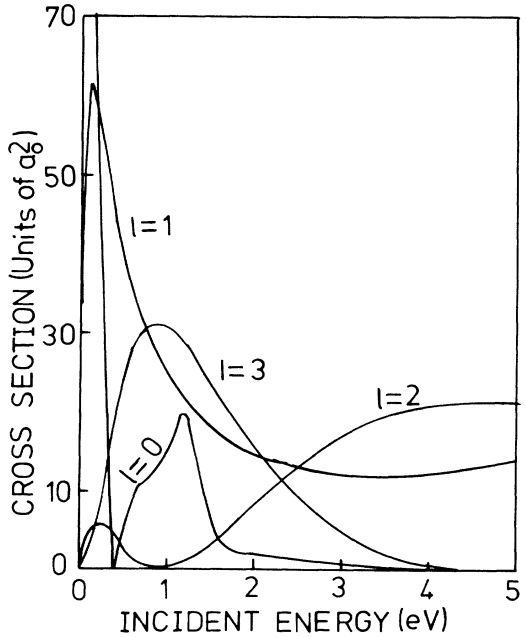

FIG. 2. Partial positronium-formation cross sections (in units of a_0^2) of e^+-Li inelastic scattering determined using the Clementi-Roetti wave functions.

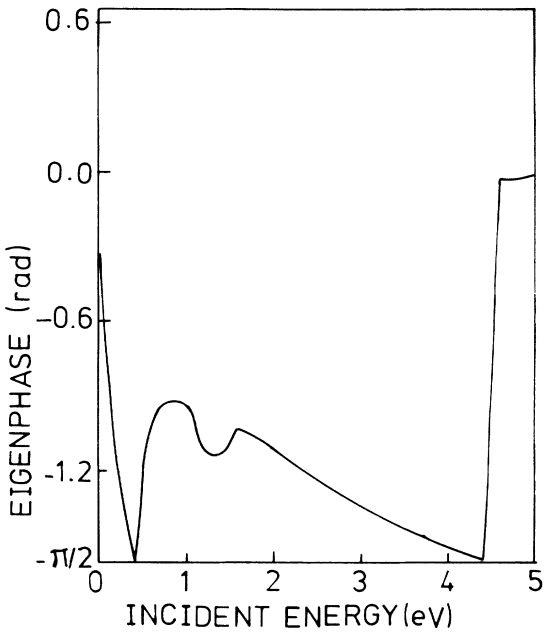

FIG. 3. Elastic eigenphases of e^+-Li scattering at $l=0$.

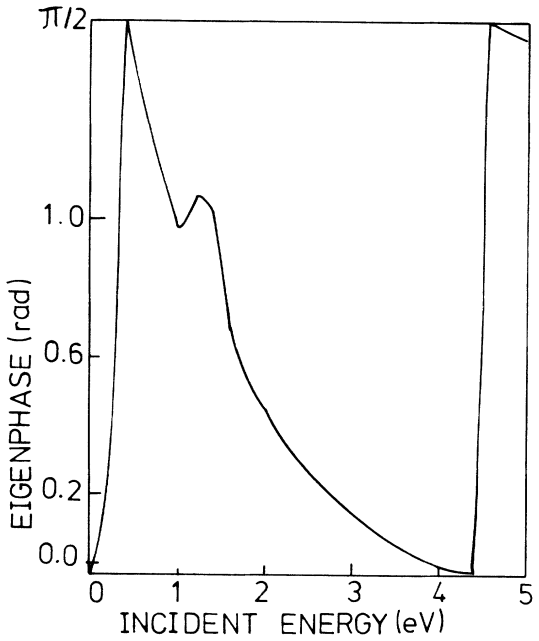

FIG. 4. Eigenphases of the second channel of e^+-Li scattering at $l=0$.

cate the existence of fundamental changes between 0.3 and 1.5 eV. The two P-wave cross sections exhibit similar behavior; they first increase steadily to maximum values and then decrease monotonically with the increase of k_1^2. However, the P-wave positronium-formation cross section is more sharply peaked than is the elastic cross section. The D- and F-wave elastic cross sections, as well as the F-wave Ps-formation cross sections, show similar behavior, but with peaks much flatter than their P-wave cross sections. The D-wave Ps-formation cross section possesses two maxima around 0.2 and 4.6 eV and a local minimum at 0.9 eV.

In Figs. 3 and 4 we plot the variation of the eigenphases of the two channels with the variation of the incident energy. The figures indicate the existence of $l=0$ resonance states around 0.5 and 4.5 eV. Thus, they suggest the possible formation of e^+-Li (or Ps-Li^+) bound states at these energies. The fact that each of the eigenphases diminishes at $k_1^2=0$ can be used as an indication of the existence of a real bound state composed of a positron and a lithium atom.

In Figs. 5 and 6 we plot the variation of the P-wave

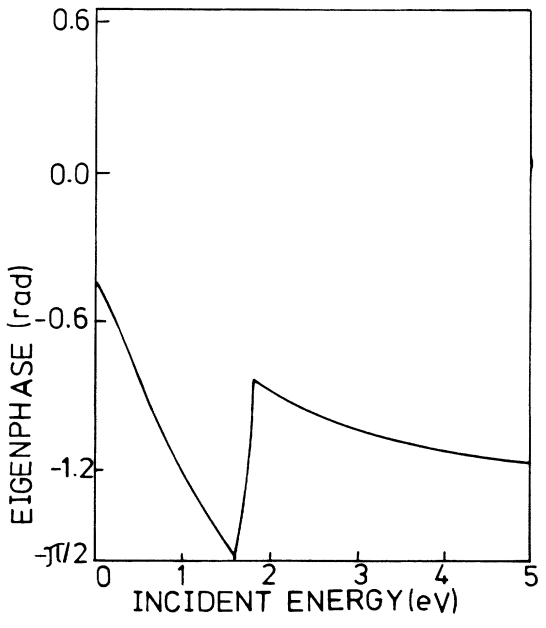

FIG. 5. Elastic eigenphases of e^+-Li scattering at $l=1$.

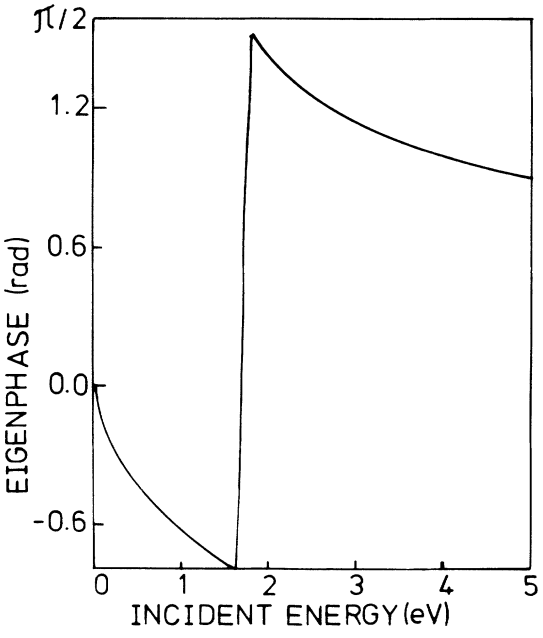

FIG. 6. Eigenphases of the second channel of e^+-Li scattering at $l=1$.

TABLE II. Comparison between present total cross sections (in units of πa_0^2) obtained via the Clementi-Roetti basis set, and those of other authors calculated using five-state close coupling method. σ_t stands for the total elastic and excitation cross section.

	Present work		Ward *et al.*[a]		Khan, Dutta, and Ghosh[b]	
k_1^2 (eV)	σ_{11}	$\sigma_{11}+\sigma_{12}$	σ_{11}	σ_t	σ_{11}	σ_t
0.005	386.84	518.61				
0.01	378.04	475.60				
0.05	332.87	389.23				
0.1	299.99	347.07				
0.5	234.82	258.99	351.95	351.95		
1.0	201.71	224.82	212.15	212.15		
2.0	151.35	176.81	169.49	190.72		
3.0	117.46	141.15	106.87	179.16		
4.0	92.62	113.81	71.86	160.36	67.79	151.11
5.0	73.20	92.00	52.11	145.11	48.46	135.29
7.0	48.37	63.70	31.19	121.04	29.14	109.08
10.0	26.69	34.75	18.13	97.27	17.68	94.70
20.0	8.59	9.73	7.51	61.00		

elastic and Ps-formation eigenphases with k_1^2. There is a sharp resonance occurring at 1.5 eV, indicating the existence of e^+-Li (or Ps-Li^+) bound states at this energy.

Finally, in Table II we present a comparison between the present total elastic and collisional (elastic plus Ps formation) sections and the total elastic and collisional (elastic plus excitation) cross sections determined by Khan, Dutta, and Ghosh[9] and Ward *et al.*,[10] using the five-state close-coupling approximation. The last two sets of cross sections are distinguished from each other by the form of the target wave functions. While the former authors employed analytical Hartree-Fock wave functions, the latter used wave functions derived from the model potential of Peach.[7] (Both groups of authors have employed the lithium polarization potential defined in Ref. 7.) From the table we conclude the following points

(i) The five-state close-coupling elastic cross sections of Ward *et al.* are higher than our elastic cross sections determined at $k_1^2=0.5$, 1.0 and 2.0 eV.

(ii) All five-state elastic cross sections calculated at $k_1^2 \geq 3.0$ eV are smaller than our corresponding cross sections.

(iii) Apart from $k_1^2=1.0$ eV, all total collisional cross sections determined by Ward *et al.* and Khan, Dutta, and Ghosh are larger than the sum of the total elastic and Ps-formation cross sections obtained from our technique.

Since the appearance of a false resonance is the main defect of most mathematical approaches (including RCSA and the close-coupling approximation) applied to scattering problems,[11] we would like to emphasize the need to further investigation of the resonance problem in e^+-Li scattering using other techniques. We suggest the use of the method of complex coordinates, in the same manner as that employed by Ho.[12] It is commonly agreed that the confirmation of resonance at a certain energy by various mathematical approaches supports the existence of a true resonance at that energy.

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[1]See, e.g., S. Guha and A. S. Ghosh, Phys. Rev. A **23**, 743 (1981); P. S. Mazumdar and A. S. Ghosh, *ibid.* **34**, 4433 (1987); S. Nahar and J. M. Wadhera, Phys. Rev. A **35**, 4533 (1987).

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