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Positron–Lithium Inelastic Scattering with Polarisation Potentials

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Abstract

Positron–lithium inelastic scattering is studied at positron energies ranging from 0·005 to 20 eV using the coupled static model. Two channels are open namely the elastic and positronium formation. The polarisation potentials of the Li atom in the first channel and that of the positronium atom in the second channel are taken into consideration in calculating the corresponding cross sections. The partial cross sections in each channel are calculated for eight values of the total angular momentum ($0 \leq \ell \leq 7$). In the elastic channel the total cross section σ_{11} has its maximum value at the lowest energy, and decreases with an increase in positron energy K_1^2. The total positronium formation cross section has a small dip at 0·1 eV, and maximum value at $K_1^2 = 1{\cdot}4$ eV, and then decreases smoothly with e^+ energy. We compare our results with those of Ward *et al.* (1989) where positronium formation is ignored. The agreement in elastic cross sections improves with e^+ energy, while the total collisional cross sections have the closest agreement at 1·0 eV. From this comparison, we find that positronium formation is important in the very low energy region, and the role of the excitation cross section increases steadily with e^+ energy.

1. Introduction

Over the last few years the polarised orbital method (POM) has been applied to study the elastic scattering of positrons by large atoms (Horbatsch *et al.* 1983). McEachran *et al.* (1977, 1978, 1979, 1980) found that this method is extremely successful in the treatment of elastic scattering of positrons by noble gases. Drachman and Temkin (1972) noticed that the POM yields a considerable improvement in the static phase shifts which were always shifted towards the variational ones. The improvement was due to the effect of the polarisation potentials which play an important role in the real physical picture of the collision process considered.

In this work we investigate inelastic scattering of positrons by lithium atoms. We assume that the elastic and rearrangement (positronium formation) channels are open and that all excitation channels of the target are closed. In particular, our aim is to study the effect of adding the polarisation potentials of the lithium and positronium atoms to the static potentials of the first and second channels, respectively, on the elastic, positronium formation and total collisional cross sections calculated by the restricted coupled static approximation. Furthermore, we compare our resulting cross sections with the

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results of Ward *et al.* (1989) obtained using the close coupling approximation in which positronium formation is ignored.

2. Theoretical Formalism

The solution of the scattering problem under consideration is subject to the coupled integro-differential equations (Abdel-Raouf 1988*b*)

$$\left(\frac{d^2}{dx^2} - \frac{\ell(\ell+1)}{x^2} + K_1^2\right) f_\ell(x) = U_x f_\ell(x) + \int_0^\infty K_{12}(\sigma,x)\, g_\ell(\sigma)\, d\sigma, \tag{1}$$

$$\left(\frac{d^2}{d\sigma^2} - \frac{\ell(\ell+1)}{\sigma^2} + K_2^2\right) g_\ell(\sigma) = U_\sigma g_\ell(\sigma) + \int_0^\infty K_{21}(\sigma,x)\, f_\ell(x)\, dx, \tag{2}$$

where

$$U_x = U_{\rm st}(x) + V_{\rm pol}^{\rm Li}(x), \qquad U_\sigma = U_{\rm st}(\sigma) + V_{\rm pol}^{\rm ps}(\sigma), \tag{3,4}$$

and where x and σ are the position vectors of the positron and the centre of mass of the positronium atom respectively (see Fig. 1). The polarisation potentials in these equations were neglected previously (Abdel-Raouf 1988*a*). Here $U_{\rm st}(x)$ is the static potential of the first channel which is defined as

$$U_{\rm st}(x) = \langle \Phi_{\rm v}(r)\,|\, V_{\rm int}^{(1)}\,|\, \Phi_{\rm v}(r)\rangle, \tag{5}$$

where $\Phi_{\rm v}(r)$ is the wavefunction of the valence (2s) electron which has been chosen in the form

$$\Phi_{\rm v}(r) = a_1\, e^{-\alpha_1 r} + a_2\, e^{-\alpha_2 r}.$$

We can easily show that (Walters 1973)

$$\alpha_1 = 2\cdot 7, \quad \alpha_2 = 0\cdot 65, \quad a_1 = -0\cdot 422, \quad a_2 = 0\cdot 113.$$

In equation (5), $V_{\rm int}^{(1)}$ stands for the interaction between the incident positron and the one-valence electron atom, i.e.

$$V_{\rm int}^{(1)} = \frac{2}{x} - \frac{2}{\rho} + V_{\rm c}^{\rm D}(x),$$

where $V_{\rm c}^{\rm D}(x)$ is the direct part of the core potential given by

$$V_{\rm c}^{\rm D}(x) = \sum_{i=1}^{2}{}' \,\langle \Phi_{1s}(r_i) \left| \frac{2}{|x - r_i|} - \frac{2}{x} \right| \Phi_{1s}(r_i)\rangle,$$

and $\rho = x - r$, where r is the position of the valence electron and r_i that of the ith electron in the core. Taking the wavefunction $\Phi_{1s}(r_i) = b e^{-\beta_1 r_i}$, where $\beta_1 = 2\cdot 7$ and $b = (\beta_1^3/\pi)^{\frac{1}{2}}$, we get

$$V_{\rm c}^{\rm D}(x) = -4\left(\frac{1}{x} + \beta_1\right) e^{-2\beta_1 x}.$$

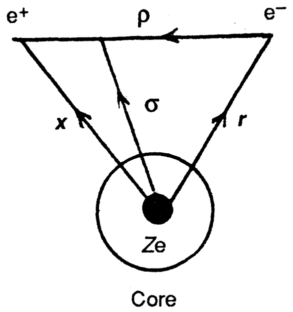

Fig. 1. Configuration space of e^+–Li scattering.

Substituting into (5) we obtain

$$U_{st}(x) = 4\pi\Big\{(a_1^2/2\alpha_1^3)e^{-2\alpha_1 x}\Big(\frac{1}{x}+\alpha_1\Big)$$

$$+\{4a_1\,a_2/(\alpha_1+\alpha_2)^4\}e^{-(\alpha_1+\alpha_2)x}\Big(\frac{1}{x}+\tfrac{2}{3}(\alpha_1+\alpha_2)+\frac{x}{6}(\alpha_1+\alpha_2)^2\Big)$$

$$+(3a_2^2/2\alpha_2^5)e^{-2\alpha_2 x}\Big(\frac{1}{x}+\tfrac{3}{2}\alpha_2+x\alpha_2^2+\tfrac{1}{3}\alpha_2^2x^2\Big)\Big\}+V_c^D(x),$$

where we have used the fact that $\langle\Phi_v\,|\,\Phi_v\rangle=1$.

The static potential $U_{st}(\sigma)$ of the second channel is defined by

$$U_{st}(\sigma)=\langle\Phi_{ps}\,|\,V_{int}^{(2)}\,|\,\Phi_{ps}\rangle$$

$$=\langle\Phi_{ps}(\rho)\Big|\frac{2}{|\,\sigma+\frac{1}{2}\rho\,|}-\frac{2}{|\,\sigma-\frac{1}{2}\rho\,|}\Big|\Phi_{ps}(\rho)\rangle+\langle\Phi_{ps}(\rho)\,|\,V_c^{ex}(|\,\sigma-\tfrac{1}{2}\rho\,|)\,|\,\Phi_{ps}(\rho)\rangle.$$

The first term on the right-hand side of this equation vanishes because it consists of two parts which have the same magnitude but different signs. Thus, the static potential is given by

$$U_{st}(\sigma)=\tfrac{1}{2}\int_0^\infty e^{-\rho}\Big(\int_{-1}^{+1}V_c^{ex}(|\,\sigma-\tfrac{1}{2}\rho\,|)\,dz\Big)\rho^2\,d\rho, \tag{6}$$

where

$$V_c^{ex}(r)=16\pi b\{a_1\,e^{-(\alpha_1+\beta_1)r}[2+r(\alpha_1+\beta_1)]/r(\alpha_1+\beta_1)^3$$

$$+a_2\,e^{-(\alpha_2+\beta_1)r}[r^2(\alpha_2+\beta_1)^2+4r(\alpha_2+\beta_1)+6]/(\alpha_2+\beta_1)^4\}.$$

Setting $r=|\,\sigma-\frac{1}{2}\rho\,|$, we obtain $V_c^{ex}(|\,\sigma-\frac{1}{2}\rho\,|)$ and $z=\cos\theta$, θ being the angle between $\boldsymbol{\rho}$ and $\boldsymbol{\sigma}$. The integral in the large parentheses in (6) can be calculated using a Gauss quadrature formula and the integration with respect to $d\rho$ can be evaluated using a Gauss–Laguerre expansion.

Table 1. Partial and total elastic cross sections (in a_0^2) for e$^+$–Li scattering

K_1^2 (eV)	Partial cross section $\ell = 0$	1	2	3	4	5	6	7	Total σ_{11}
0·005	641·34	0·08							641·42
0·01	634·77	0·31							635·08
0·05	591·55	3·21							597·76
0·10	544·18	19·40	0·06						563·64
0·20	461·61	50·83	0·71						513·15
0·30	392·30	79·81	2·51	0·01					475·02
0·40	335·38	103·40	5·55	0·03					444·36
0·50	287·68	121·54	9·63	0·09					418·93
0·60	247·86	134·94	14·40	0·20					397·39
0·70	214·30	144·42	19·53	0·38					378·64
0·80	186·34	150·74	24·78	0·64	0·01				362·52
0·90	132·52	154·56	29·94	1·00	0·01				348·03
1·00	142·25	156·42	34·88	1·43	0·02				335·01
1·20	110·06	155·87	43·79	2·55	0·06				312·32
1·40	86·18	151·62	51·18	3·91	0·12				293·01
1·60	68·23	145·28	57·03	5·43	0·21				276·18
1·80	54·58	137·87	61·45	7·01	0·34	0·01			261·26
2·00	44·09	130·03	64·63	8·57	0·50	0·02			247·83
2·20	35·97	122·14	66·74	10·06	0·69	0·03			235·63
2·40	29·63	114·45	67·96	11·44	0·91	0·04			224·44
2·60	24·65	107·09	68·44	12·69	1·15	0·06			214·09
2·80	20·72	100·15	68·32	13·79	1·40	0·09			204·47
3·00	17·61	93·65	67·71	14·74	1·66	0·12	0·01		195·40
3·20	15·14	87·60	66·70	15·54	1·92	0·15	0·01		187·05
3·40	13·16	81·99	65·39	16·20	2·17	0·18	0·01		179·11
3·60	11·59	76·81	63·83	16·72	2·42	0·22	0·02		171·61
3·80	10·34	72·03	62·09	17·12	2·65	0·27	0·02		164·52
4·00	9·34	67·62	60·20	17·40	2·87	0·31	0·02		157·79
4·20	8·56	63·57	58·23	17·58	3·08	0·36	0·03		151·40
4·40	7·94	59·84	56·18	17·67	3·26	0·40	0·04		145·33
4·60	7·46	56·10	54·11	17·68	3·43	0·45	0·04		139·57
4·80	7·10	53·23	52·02	17·61	3·58	0·51	0·05		134·08
5·00	6·83	50·31	49·94	17·48	3·71	0·54	0·06	0·01	128·87
6·00	6·39	38·75	40·09	16·18	4·12	0·75	0·10	0·01	106·38
7·00	6·71	30·88	31·82	14·31	4·18	0·89	0·15	0·02	88·97
8·00	7·24	25·38	25·32	12·36	4·03	0·98	0·19	0·03	75·51
9·00	7·71	21·42	20·38	10·51	3·75	1·02	0·22	0·04	65·11
10·00	8·01	18·50	16·69	9·01	3·44	1·01	0·24	0·05	56·95
11·785	8·15	14·88	12·26	6·86	2·87	0·95	0·26	0·06	46·30
15·00	7·62	11·11	8·09	4·54	2·07	0·79	0·26	0·07	34·55
20·00	6·36	8·09	5·39	2·95	1·41	0·59	0·22	0·08	25·08

In the present work, we switch on the polarisation potentials of the lithium $V_{\rm pol}^{\rm Li}(x)$ and positronium $V_{\rm pol}^{\rm ps}(\sigma)$ (i.e. the polarisation potentials of the first and second channels respectively). We choose $V_{\rm pol}^{\rm Li}(x)$ in the Peach (1982) form

$$V_{\rm pol}^{\rm Li}(x) = -\frac{\alpha}{x^4}\left\{1\cdot 0 - \left(1\cdot 0 + \gamma x + \frac{(\gamma x)^2}{2}\right)e^{-\gamma x}\right\}, \qquad (7)$$

where $\alpha = 0\cdot 19$ and $\gamma = 3\cdot 91$. The ps polarisation potential is defined by

$$V_{\rm pol}^{\rm ps}(\sigma) = 2\beta(\sigma)\, V(\sigma),$$

Table 2. Partial and total positronium formation cross sections (in a_0^2) for e^+–Li scattering

K_1^2	Partial cross section								Total
(eV)	$\ell=0$	1	2	3	4	5	6	7	σ_{12}
0·005	150·47	0·52	0·19						151·19
0·01	106·67	0·70	0·53						107·90
0·05	49·01	0·96	5·32	0·08					55·37
0·10	35·62	0·70	13·16	0·41	0·01				49·86
0·20	26·00	0·18	28·05	1·94	0·06				56·23
0·30	21·51	0·00	38·93	4·45	0·21	0·01			65·12
0·40	18·70	0·13	45·59	7·60	0·49	0·02			72·54
0·50	16·71	0·49	48·98	11·06	0·90	0·05	0·05		78·19
0·60	15·22	0·98	50·10	14·53	1·45	0·10	0·006		82·38
0·70	14·13	1·56	49·75	17·81	2·12	0·18	0·01		85·56
0·80	13·11	2·18	48·43	20·78	2·89	0·28	0·02		87·84
0·90	12·34	2·82	46·67	23·36	3·73	0·40	0·036		89·37
1·00	11·71	3·467	44·56	25·53	4·62	0·55	0·06		90·50
1·20	10·73	4·707	40·02	28·67	6·46	0·93	0·11	0·01	91·64
1·40	10·01	5·83	35·56	30·43	8·23	1·39	0·19	0·02	91·68
1·60	9·48	6·82	31·44	31·13	9·84	1·91	0·30	0·05	90·96
1·80	9·07	7·67	27·73	31·06	11·22	2·46	0·43	0·07	89·69
2·00	8·76	8·36	24·43	30·45	12·34	3·01	0·58	0·14	88·03
2·20	8·51	8·93	21·51	29·50	13·21	3·54	0·74	0·13	86·09
2·40	8·38	9·37	18·93	28·32	13·85	4·0	0·92	0·18	83·94
2·60	8·16	9·70	16·66	27·01	14·27	4·51	1·10	0·23	81·65
2·80	8·04	9·02	14·66	25·64	14·52	4·98	1·28	0·29	79·27
3·00	7·93	10·07	12·88	24·25	14·60	5·29	1·46	0·34	76·82
3·20	7·84	10·13	11·32	22·86	14·56	5·59	1·63	0·41	74·34
3·40	7·77	10·13	9·93	21·50	14·41	5·84	1·79	0·47	71·85
3·60	7·70	10·07	8·70	20·19	14·18	6·04	1·93	0·53	69·36
3·80	7·64	9·95	7·61	18·93	13·89	6·19	2·09	0·60	66·88
4·00	7·57	9·80	6·65	17·72	13·54	6·30	2·22	0·66	64·45
4·20	7·51	9·67	5·80	16·57	13·15	6·37	2·33	0·72	62·05
4·40	7·45	9·37	5·04	15·48	12·73	6·40	2·43	0·78	59·69
4·60	7·38	9·16	4·36	14·45	12·30	6·40	2·51	0·83	57·39
4·80	7·31	8·89	3·79	13·47	11·86	6·32	2·58	0·88	55·15
5·00	7·23	8·61	3·27	12·55	11·39	6·31	2·64	0·93	52·95
6·00	6·72	7·16	1·50	8·73	9·15	5·77	2·77	1·11	42·95
7·00	6·02	5·76	0·62	5·98	7·16	5·04	2·68	1·19	34·47
8·00	5·20	4·60	0·21	4·05	5·51	4·26	2·47	1·19	27·50
9·00	4·36	3·65	0·06	2·72	4·20	3·53	2·20	1·15	21·83
10·00	3·58	2·90	0·01	1·81	3·17	2·88	1·92	1·06	17·34
11·785	2·47	1·97	0·01	0·86	1·90	1·96	1·45	0·88	11·52
15·00	1·29	1·06	0·06	0·21	0·74	0·95	0·82	0·57	2·73
20·00	0·55	0·50	0·09	0·01	0·17	0·30	0·32	0·26	2·20

where $V(\sigma)$ is a potential of the form (see Abdel-Raouf 1988)

$$V(\sigma)=\left(\frac{32}{43}\right)^{\frac{1}{2}}\left[\left(\sigma^2+5\sigma+9+\frac{9}{\sigma}\right)\exp(-2\sigma)-\frac{9[1-\exp(-2\sigma)]}{2\sigma^2}\right]. \tag{8}$$

The function $\beta(\sigma)$ is calculated as follows: let $\Delta E=E_{\rm ps}-E^*_{\rm ps}$ (where $E_{\rm ps}=-0\cdot5$ Ry is the ground state energy of the ps and $E^*_{\rm ps}=-21/258$ Ry is the binding energy of the polarised positronium), and $w = \Delta E/V(\sigma)$. Also, we consider the two functions $\beta^{\pm}$ such that

$$\beta^{\pm}(\sigma) = \tfrac{1}{2}\{-W \pm (W^2+4)^{\frac{1}{2}}\}.$$

The adiabatic energy of the positronium within the field of a unit positive charge is found to be

$$E_{\rm ad}^{\rm ps} = \{E_{\rm ps} + 2\beta^{\pm}V + E_{\rm ps}^{*2}(\beta^{\pm})\}/\{1+(\beta^{\pm})^2\}. \tag{9}$$

The proper $\beta(\sigma)$ for calculating $V_{\rm pol}^{\rm ps}(\sigma)$ is that one of β^{+} and β^{-} which yields a minimum value for $E_{\rm ad}^{\rm ps}$.

3. Results and Discussion

On considering the variation of the total elastic cross section σ_{11} (see Table 1) with respect to the incident energy of the positron K_1^2, we notice that it has its maximum value at $K_1^2 = 0\cdot005$ eV and decreases smoothly thereafter. While the S-wave partial σ_{11} decreases with e^+ energy until $K_1^2 = 6\cdot0$ eV where it has a dip at $6\cdot39a_0^2$, it increases to $8\cdot15a_0^2$ at $11\cdot785$ eV and then decreases again with e^+ energy. The higher partial elastic cross sections ($\ell \geq 1$) each have a feature in common in that they increase first with e^+ energy to maximum values and decrease thereafter. The value of K_1^2 at which each maximum occurs increases with the value of ℓ, while the maximum value itself decreases with ℓ.

On the other hand, the variation of the total positronium formation cross section σ_{12} with K_1^2 (see Table 2) shows that σ_{12} has a small dip at $0\cdot1$ eV, then increases to reach a maximum value at $1\cdot4$ eV and decreases smoothly with an increase in e^+ energy. For $\ell = 0$, σ_{12} starts with a maximum value and decreases with e^+ energy. The higher σ_{12} ($\ell \geq 1$) show oscillatory behaviour. The first maximum value shifts towards higher e^+ energy with an increase in ℓ. From the previously described features of partial and total elastic and positronium formation cross sections we conclude that various resonant states should show up in any positron–lithium inelastic collisions.

Table 3. Comparison between various total cross sections (in πa_0^2) for e^+–Li inelastic scattering

σ_t is the sum of total elastic and excitation cross sections obtained using the two-state approximation

K_1^2 (eV)	Present total cross section σ_{11}	σ_{12}	$\sigma_{11}+\sigma_{12}$	Ward et al. (1989) σ_{11}	σ_t
0·5	133·419	24·9	158·32	229·18	229·18
1·0	106·69	28·822	135·51	139·3	139·3
2·0	78·93	28·035	106·96	112·26	120·61
3·0	62·26	24·47	86·725	79·1	127·14
4·0	50·25	20·53	70·78	56·92	124·0
5·0	41·04	16·86	57·90	42·81	117·92
10·0	18·14	5·52	23·66	16·68	88·59
20·0	7·99	0·70	8·69	7·52	58·35

In Table 3 we compare our results with those of Ward *et al.* (1989) where positronium formation was ignored and the two-state approximation (2s–2s and 2s–2p) was employed. It is clear that the agreement in σ_{11} values improves with an increase in e^+ energy. In both cases the total elastic cross section shows the same behaviour, decreasing with an increase in e^+ energy. The best agreement between our total collisional cross section $\sigma_{11}+\sigma_{12}$ and the total collisional cross section of Ward *et al.* (1989) (i.e. the elastic plus the 2s–2p excitation cross sections) occurs at $K_1^2 = 1\cdot0$ eV. From both sets of results, it is clear that while positronium formation is rather important in the very low energy region (see Tables 2 and 3), the role of the excitation cross section increases steadily with K_1^2. Thus, we conclude that the ps channel is essential in any theoretical treatment of e^+–Li scattering below $K_1^2 = 5$ eV. Therefore, on the basis of our improved coupled static approximation and the two-state close coupling approximation of Ward *et al.* (1989), it is advisable to consider both rearrangement and excitation channels in future.

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