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Ground State Positronium Formation Cross Sections for Scattering of Positrons from Li

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Abstract

Total cross sections for positronium formation in e^+–Li scattering have been studied in the framework of the distorted wave approximation in the energy range 1–50 eV by taking consistent account of the effect of the target distortion. The results are compared with existing theoretical predictions.

1. Introduction

During recent years there has been an outburst of work on collisions of positrons with atoms and molecules. This is mainly due to progress on the experimental front where intense energy-resolved positron beams and improved detectors have made possible much more sophisticated experiments (Charlton 1985; Griffith 1986; Charlton and Laricchia 1990). Recently there has been considerable experimental interest in positron scattering from alkali atoms resulting in measurements of total positron scattering cross sections from Na, K and Rb (Stein *et al.* 1985, 1990), stimulating a series of theoretical work (Ward *et al.* 1988, 1989*a*, 1989*b*; McEachran *et al.* 1990*a*, 1990*b*; Horbatsch *et al.* 1990; Gien 1989*a*, 1989*b*, 1990). These measurements of the total cross section (TCS) from alkali atoms indicate that the inelastic processes might give significant contributions to the TCS at low incident energies (Stein *et al.* 1990). Apart from ionisation and excitation processes, positronium (Ps) formation is the only other important inelastic process in positron–atom scattering. The process of Ps formation, although important and interesting in any target, is especially intriguing in the alkalis because this channel is energetically open at the elastic scattering threshold. This possibility is expected to have a pronounced influence on the elastic and various excitation cross sections at low energies. So, for a profound understanding of the mechanism of positron scattering from alkalis, a detailed knowledge of Ps formation cross sections is essential.

There have been a few calculations of Ps formation in e^+–Li scattering. Guha and Saha (1980) calculated the TCS for electron capture by positrons

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in the energy range 0·1–500 eV by using the first Born approximation (FBA). Abdel-Raouf (1988) studied Ps formation in e^+–Li scattering using the coupled static and frozen core approximations over the energy range 0·1–1000 eV of the incident positron. Nahar and Wadhera (1987) considered Ps formation in the scattering of positrons from Li in the framework of the FBA and the distorted wave Born approximation (DWBA) in the range 100–300 eV.

In the present paper we plan to calculate the TCS for Ps formation in e^+–Li scattering in the range 1–50 eV taking into account the effects of both the distortion of the incident positron wave and the distortion of the atomic charge cloud due to the presence of the incident positron. The effect of target distortion has been found to be important in positron–atom scattering. In view of the fact that in alkali atoms (Li, Na, K, Rb) the energy of the first p state of the valence electron is only about 2 eV above its loosely bound state (Gien 1990), the inclusion of the matrix element arising from the distorted part of the target wavefunction becomes very important.

2. Theory

The alkali atoms to a good approximation can be considered to be one-electron systems where the valence electron moves outside a fixed or frozen core, consisting of the nucleus and the remaining electrons (McEachran *et al.* 1990). We have taken into account the effect of core electrons by a core potential (Saxena and Mathur 1985, 1986; Mathur 1989). The scattering amplitude for Ps formation in e^+–Li scattering can be written as

$$f(\boldsymbol{k}_i, \boldsymbol{k}_{Ps}) = \frac{\mu_f}{2\pi}\int \exp\{-i\,\boldsymbol{k}_{Ps}(\boldsymbol{r}+\boldsymbol{x})/2\}\, n_{1s}^*(|\,\boldsymbol{r}-\boldsymbol{x}\,|) \times V(r,x)\,\Phi_{2s}(\boldsymbol{r},\boldsymbol{x})\,F(\boldsymbol{x})\,d\boldsymbol{r}\,d\boldsymbol{x}, \tag{1}$$

where μ_f is the reduced mass in the final channel, $n_{1s}(|\,\boldsymbol{r}-\boldsymbol{x}\,|)$ is the ground state Ps wavefunction, and $\boldsymbol{r}$ and $\boldsymbol{x}$ are respectively the position vectors of the valence electron and incident positron. The interaction potential $V(r,x)$ is given by

$$V(r,x) = \frac{1}{x} - \frac{1}{r} - V_c(x) + V_c(r), \tag{2}$$

where $V_c(x)$ is the core potential. Further, $\boldsymbol{k}_{Ps}$ is the wave vector of the moving positronium and $\Phi_{2s}(\boldsymbol{r},\boldsymbol{x})$ is the wavefunction of the valence electron perturbed by the incident positron. Following Bhatia *et al.* (1978) we can write

$$\Phi_{2s}(\boldsymbol{r},\boldsymbol{x}) = \Phi_{2s}(\boldsymbol{r}) + \Phi_{2s\to p}(\boldsymbol{r},\boldsymbol{x}), \tag{3}$$

with

$$\Phi_{2s}(\boldsymbol{r}) = \frac{P_{2s}(r)}{r}\,Y_{00}(\hat{\boldsymbol{r}}), \tag{4}$$

$$\Phi_{2s\to p}(\boldsymbol{r},\boldsymbol{x}) = -\frac{\epsilon(x,r)}{x^2}\,\frac{P_{2s\to p}(r)}{r}\,\frac{1}{\pi}\sqrt{\tfrac{1}{4}}\cos(\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{x}}), \tag{5}$$

where ϵ is a step function

$$\epsilon(x, y) = \begin{cases} 1, & x > y \\ 0, & x < y, \end{cases} \tag{6}$$

and where

$$V_c(x) = -2\left(\frac{1}{x} + 2\cdot 7\right)\exp(-5\cdot 4x). \tag{7}$$

$P_{2s\to p}(r)$ satisfies the differential equation (Bhatia *et al.* 1978)

$$\left(\frac{d^2}{dr^2} - \frac{2}{r^2} + E_{2s} + \frac{2z}{r} - 4\Gamma_0(1s, 1s : r)\right)P_{2s\to p}(r)$$

$$+\tfrac{2}{3}P_{1s}(r)\Gamma_1(1s, 2s\to p : r) = -2rP_{2s}(r). \tag{8}$$

For P_{1s} and P_{2s} we take the frozen core Hartree–Fock (HF) orbitals of Cohen and Kelly (1967). In equation (8), E_{2s} is the energy of the 2s orbital. Again we have

$$\Gamma_\lambda(nl, n'l' : r) = \int_0^\infty P_{nl}(x)\, g_\lambda(x, r) P_{n'l'}(x)\, dx, \tag{9}$$

where

$$g(x, y) = \begin{cases} x/y^{\lambda+1}, & x < y \\ y/x^{\lambda+1}, & x > y. \end{cases} \tag{10}$$

The wavefunction $F(\boldsymbol{x})$ of the incident positron is decomposed into partial waves as

$$F(\boldsymbol{x}) = k_i^{-\frac{1}{2}}(4\pi)^{\frac{1}{2}} \sum_{l_i=0}^{\infty}(2l_i + 1)^{\frac{1}{2}} i^{l_i} \exp(i\,\delta_{l_i})$$

$$\times \frac{u_{l_i}(k_i, x)}{x} Y_{l_i 0}(\hat{\boldsymbol{k}}_i \cdot \hat{\boldsymbol{x}}), \tag{11}$$

where l_i is the orbital angular momentum quantum number and k_i the momentum of the incident positron, while δ_{l_i} is the phase shift. The radial part $u_{l_i}(k_i, x)$ of the incident positron wavefunction is obtained by solving the differential equation

$$\left(\frac{d^2}{dx^2} - l_i\frac{l_i + 1}{r^2} - 2V_i(x)\right)u_{l_i}(k_i, x) = E_i\, u_{l_i}(k_i, x), \tag{12}$$

where E_i is the energy of the incident positron.

We solved equation (12) for $u_{l_i}(k_i, x)$ subject to the boundary conditions

$$u_{l_i}(k_i, 0) = 0, \tag{13}$$

$$u_{l_i}(k_i, x) \underset{x\to\infty}{\sim} k_i^{-\frac{1}{2}} \sin(k_i x - \tfrac{1}{2}l_i\pi + \delta_{l_i}). \tag{14}$$

We write

$$V_i(x) = V_{st}(x) + V_{pol}(x), \tag{15}$$

where $V_{st}(x)$ and $V_{pol}(x)$ are the static and polarisation potentials (Bhatia *et al.* 1978)

$$V_{st}(x) = 4\Gamma_0(1s, 1s : x) + 2\Gamma_0(2s, 2s : x) - \frac{2z}{x}, \tag{16}$$

$$V_{pol}(x) = -\frac{2}{3x^4}\int_0^x P_{2s}(r) r P_{2s\to p}(r)\, dr. \tag{17}$$

Now by substituting equation (3) into (1) the scattering amplitude can be written as

$$f(\boldsymbol{k}_i, \boldsymbol{k}_{Ps}) = f_1(\boldsymbol{k}_i, \boldsymbol{k}_{Ps}) + f_2(\boldsymbol{k}_i, \boldsymbol{k}_{Ps}), \tag{18}$$

with

$$f_1(\boldsymbol{k}_i, \boldsymbol{k}_{Ps}) = -\frac{\mu_f}{2\pi}\int \exp\{-i\,\boldsymbol{k}_{Ps}\cdot(\boldsymbol{r}+\boldsymbol{x})/2\} n_{1s}(|\,\boldsymbol{r}-\boldsymbol{x}\,|) \times V(r, x)\Phi_{2s}(\boldsymbol{r}) F(\boldsymbol{x})\, d\boldsymbol{r}\, d\boldsymbol{x}, \tag{19}$$

$$f_2(\boldsymbol{k}_i, \boldsymbol{k}_{Ps}) = -\frac{\mu_f}{2\pi}\int \exp\{-i\,\boldsymbol{k}_{Ps}\cdot(\boldsymbol{r}+\boldsymbol{x})/2\} n_{1s}(|\,\boldsymbol{r}-\boldsymbol{x}\,|) \times V(r, x)\Phi_{2s\to p}(\boldsymbol{r}, \boldsymbol{x}) F(\boldsymbol{x})\, d\boldsymbol{r}\, d\boldsymbol{x}. \tag{20}$$

It is to be noted that the term $f_2(\boldsymbol{k}_i, \boldsymbol{k}_{Ps})$ arises from the distorted part of the target wavefunction. We carried out the partial wave analysis of $f_1(\boldsymbol{k}_i, \boldsymbol{k}_{Ps})$ and $f_2(\boldsymbol{k}_i, \boldsymbol{k}_{Ps})$ following standard angular momentum algebra (Rose 1957).

3. Results and Discussion

As a check of our computer program we reproduced the FBA results of Guha and Saha (1980). In evaluating the scattering amplitudes in partial wave form we have to perform two-dimensional radial integrals, evaluated by suitable Gaussian quadratures. The effect of the matrix element $f_2(\boldsymbol{k}_i, \boldsymbol{k}_{Ps})$ arising from the distorted part of the target wavefunction was found to be negligible for $l_i > 7$ and so neglected. For a particular value of the incident energy we ran our program up to a value of l_i such that the difference between the distorted wave partial cross section and the FBA partial cross section is less than 1%. Higher partial wave cross sections were supplemented by the FBA results of Guha and Saha (1980).

In Fig. 1 we display the present results for the TCS together with the FBA results of Guha and Saha (1980). Our results are always lower than the FBA results. Up to an incident energy of 5 eV, the FBA results are about 50% higher than the present results. On the other hand, we observe that for $E_i < 20$ eV, the present distorted wave results are higher than these of the coupled static calculation by Abdel-Raouf (1988), but for $E_i > 30$ eV the results of Abdel Raouf are higher than ours. We note that in an earlier publication (Mazumdar and

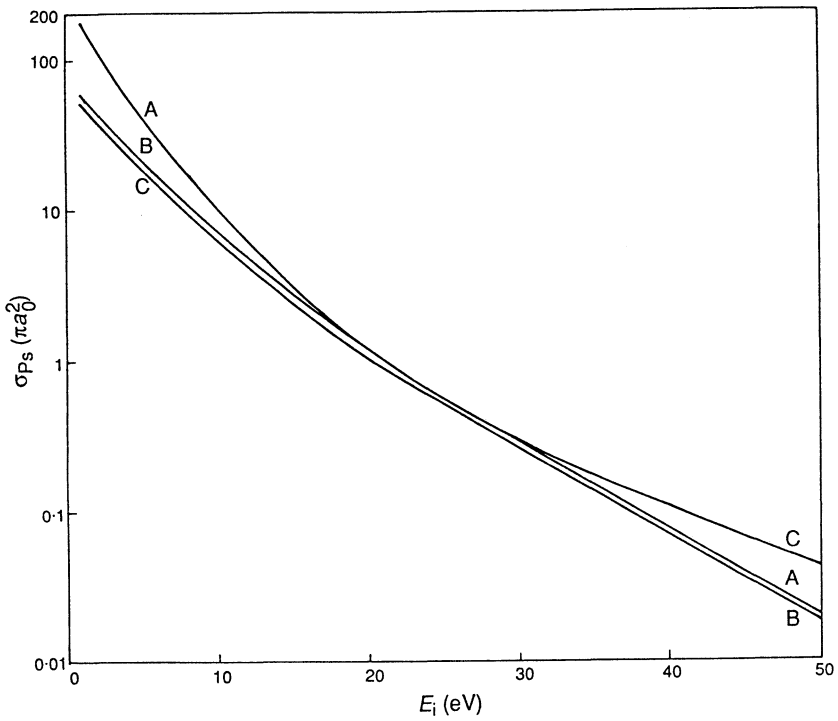

Fig. 1. Total cross section σ_{Ps} in units of πa_0^2 for Ps formation in e^+–Li scattering: curve A, FBA results of Guha and Saha (1980); curve B, present results; curve C, coupled static results of Abdel-Raouf (1988).

Ghosh 1986) one of us presented Ps formation cross sections in e^+–Li scattering in a distorted wave model. The difference between that calculation and the present one is the absence of the term $f_2(\boldsymbol{k}_i, \boldsymbol{k}_{Ps})$ in the former calculation. We have already noted that this term arises from the distorted part of the target wavefunction. The omission was done for the sake of simplicity. But we find that up to $E_i = 5$ eV the two sets of results differ by about 40%, the present results being lower. The considerable difference between the two results indicates the importance of this matrix arising from the distorted part

Table 1. Present results for the total cross section for Ps formation in e^+–Li scattering together with those for elastic scattering and excitations calculated in the five-state close coupling approximation by Ward *et al.* (1989)

E_i (eV)	σ_{Ps} (πa_0^2)	Five-state close coupling results	
		Total excitation	Total elastic scattering
1	58·17	—	212·15
2	44·23	21·24	169·49
5	20·31	93·01	52·11
10	7·16	79·14	18·13
20	1·04	53·50	7·51
30	0·27	40·42	5·14
50	0·019	27·34	3·44

of the target wavefunction, as in the case of electron scattering (Bransden and McDowell 1977), and demonstrates that its omission is not justified. Again we find that although the results of Abdel-Raouf for TCS are smooth and reasonable in appearance, his partial wave cross sections have remarkable oscillations in energy. There is no such trend in the present partial wave cross sections.

Finally, in Table 1, we compare the present Ps formation cross sections with the TCS for elastic scattering and discrete excitations in e^+–Li scattering calculated in the five-state close coupling approximation by Ward *et al.* (1989). We have not included total ionisation cross sections for e^+–Li scattering since it is evident from the calculations of Mukherjee and Mazumdar (1988) that ionisation is negligible in comparison with Ps formation and excitation cross sections. Keeping in mind that the predictions of the close coupling approximation are in good agreement with measured values for e^+–Na and e^+–K scattering (Stein *et al.* 1990), we find that as in e^+–Na and e^+–K scattering over the range 5–50 eV inelastic processes dominate e^+–Li scattering.

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