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Positronium Formation in e^+–Na Scattering

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Abstract

The positronium formation cross section in positron–sodium scattering has been evaluated by employing a distorted wave approach in the low and intermediate energy region. The effect of the positronium formation cross section on the total cross section for positron–sodium scattering has also been discussed.

1. Introduction

Recently the total cross section (TCS) for e^+–Na scattering has been measured (Kwan *et al.* 1991). The elastic and excitation cross sections for e^+–Na scattering have been studied by Ward *et al.* (1989) in the framework of the five-state close coupling approximation (CCA). Gien (1991) calculated the TCS for e^+–Na scattering by using the modified Glauber approximation within the model potential approach.

Positronium (Ps) formation is one of the important inelastic processes in positron–atom scattering. This process assumes more importance in positron scattering from alkali atoms because the Ps formation channel is always open. Guha and Mandal (1980) studied Ps formation in e^+–Na scattering in the energy range 0·5–20 eV by employing the first Born approximation and the distorted wave approximation, but they did not take into account the effect of polarisation which has been found to be important in positron–atom scattering (Ghosh *et al.* 1982; Drachman and Temkin 1972). Moreover, they used a 1s type wavefunction for the valence electron which is actually a 3s electron. Abdel-Raouf (1988) used the coupled static and frozen core approximation in the incident positron energy range 0·1–1000 eV in order to study the process. In the present paper we compute the TCS for Ps formation in the ground state in e^+–Na scattering over the energy range 1–50 eV by using a distorted wave approximation, which unlike the distorted wave formalism of Guha and Mandal (1980), incorporates the effect of polarisation. This approach has been used successfully to study Ps formation in positron scattering from hydrogen, helium and lithium (Khan and Ghosh 1983*a*, 1983*b*; Khan *et al.* 1984, 1985; Mazumdar and Ghosh 1986).

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2. Theory

We use a one-electron model of the sodium atom where the valence electron orbital, either in the ground or an excited state, moves in the central potential of a fixed (frozen) core (Ward *et al.* 1989). Within this framework the scattering amplitude for positronium formation in the ground state in e^+–Na scattering is given by

$$f_{\mathrm{Ps}} = -\frac{\mu_{\mathrm{f}}}{2\pi}\int \mathrm{d}\boldsymbol{r}_1\,\mathrm{d}\boldsymbol{r}_2 \exp(-\mathrm{i}\,\boldsymbol{k}_{\mathrm{f}}\,.\,\boldsymbol{s})\,\Phi_{\mathrm{Ps}}(\boldsymbol{k})\,V_{\mathrm{int}}(r_1,\,r_2)$$
$$\times\,\Phi_{\mathrm{i}}(\boldsymbol{r}_2)\,F_{\boldsymbol{k}_{\mathrm{i}}}(\boldsymbol{r}_1)\,\mathrm{d}\boldsymbol{r}_1\,\mathrm{d}\boldsymbol{r}_2\,, \tag{1}$$

where $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ are the position vectors of the incident positron and the active valence electron, while $\boldsymbol{k}_{\mathrm{i}}$ and $\boldsymbol{k}_{\mathrm{f}}$ are the wave vectors of the incident positron and the moving positronium. Further, $\Phi_{\mathrm{Ps}}(\boldsymbol{k})$ is the ground state wavefunction of the positronium, $F_{\boldsymbol{k}_{\mathrm{i}}}(\boldsymbol{r}_1)$ is the wavefunction of the incident positron, while

$$\boldsymbol{s} = (\boldsymbol{r}_1 + \boldsymbol{r}_2)/2; \qquad \boldsymbol{R} = \boldsymbol{r}_1 - \boldsymbol{r}_2\,. \tag{2}$$

The interaction potential is given by

$$V_{\mathrm{int}}(r_1,\,r_2) = (1/r_1 - 1/r_2) + V_{\mathrm{c}}(r_1) - V_{\mathrm{c}}(r_2)\,. \tag{3}$$

The core potential $V_{\mathrm{c}}(r)$ and the valence electron wavefunction $\Phi_{\mathrm{i}}(\boldsymbol{r})$ are taken from Daniele (1980). The wavefunction $F_{\boldsymbol{k}_{\mathrm{i}}}(\boldsymbol{r}_1)$ of the incident positron is decomposed into partial waves as

$$F_{\boldsymbol{k}_{\mathrm{i}}}(\boldsymbol{r}_1) \;=\; k_{\mathrm{i}}^{-1/2}\sum_{l_{\mathrm{i}}=0}^{\infty}(2l_{\mathrm{i}}+1)\exp(\mathrm{i}\,\delta_{l_{\mathrm{i}}})\,\frac{\mu_{l_{\mathrm{i}}}(k_{\mathrm{i}},\,r_1)}{r_1}$$
$$\times\,P_{l_{\mathrm{i}}}(\cos(\hat{\boldsymbol{k}}_{\mathrm{i}}\,.\,\hat{\boldsymbol{r}}_1))\,, \tag{4}$$

where $P_{l_{\mathrm{i}}}$ is a Legendre polynomial, $\delta_{l_{\mathrm{i}}}$ the phase shift and l_{i} the orbital angular momentum quantum number of the incident positron. The radial part $u_{l_{\mathrm{i}}}(k_{\mathrm{i}}, r_1)$ of the incident positron wavefunction satisfies the differential equation

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r_1^2} - \frac{l_{\mathrm{i}}(l_{\mathrm{i}}+1)}{r_1^2} - 2V_{\mathrm{st}}(r_1) - 2V_{\mathrm{pol}}(r_1)\right.$$
$$\left. -2V_{\mathrm{c}}(r_1)\right)\mu_{l_{\mathrm{i}}}(k_{\mathrm{i}},\,r_1) = 0\,, \tag{5}$$

where $V_{\mathrm{st}}(r_1)$ and $V_{\mathrm{pol}}(r_1)$ are respectively the static and polarisation potentials, and where

$$V_{\mathrm{st}}(r_1) = \langle\Phi_{\mathrm{i}}(\boldsymbol{r}_2)\,|-1/r_{12}\,+1/r_1\,|\,\Phi_{\mathrm{i}}(\boldsymbol{r}_2)\rangle\,, \tag{6}$$

while V_{pol} is taken from Wadehra (1982). The differential equation (5) satisfied by the radial part of the incident positron wavefunction has been solved corresponding to the boundary conditions

$$\mu_{l_{\mathrm{i}}}(k_{\mathrm{i}},\,r_1) \;\to\; 0, \quad r_1 \to 0\,; \tag{7}$$

$$\mu_{l_{\mathrm{i}}}(k_{\mathrm{i}},\,r_1) \;\to\; k_{\mathrm{i}}^{-1/2}\sin(k_{\mathrm{i}}\,r_1\;-l_{\mathrm{i}}\pi/2\,+\delta_{l_{\mathrm{i}}}), \quad r_1 \to \infty\,. \tag{8}$$

We carried out the partial wave analysis for f_{Ps} by using standard angular momentum algebra (Rose 1957). The TCS Q_{Ps} for Ps formation in e$^+$–Na scattering can be calculated from the relation

$$Q_{\mathrm{Ps}} = 2\pi \frac{\mu_{\mathrm{i}}}{\mu_{\mathrm{f}}} \frac{k_{\mathrm{f}}}{k_{\mathrm{i}}} \int_0^{\pi} |\, f_{\mathrm{Ps}} \,|^2 \sin\theta \, \mathrm{d}\theta \,, \tag{9}$$

where μ_{i} and μ_{f} are the reduced masses in the initial and final channels respectively.

3. Results and Discussions

The differential equation (5) satisfied by $u_{l_{\mathrm{i}}}(k_{\mathrm{i}}, r_1)$ has been solved by using a non-iterative method (Sloan 1964) up to a radial distance of 30 a.u. with a step size of 0·01 a.u. For higher values of the radial distance we replace $u_{l_{\mathrm{i}}}(k_{\mathrm{i}}, r_1)$ by its asymptotic form (8). The final expression for f_{Ps} was reduced to a two-dimensional radial integral which was solved numerically by using suitable Gauss–Legendre quadrature. The sum over l_{i} was carried up to $l_{\mathrm{i}} = 8$ for $E_{\mathrm{i}} = 1$ eV (E_{i} is the energy of the incident positron) and to $l_{\mathrm{i}} = 20$ for $E_{\mathrm{i}} = 50$ eV.

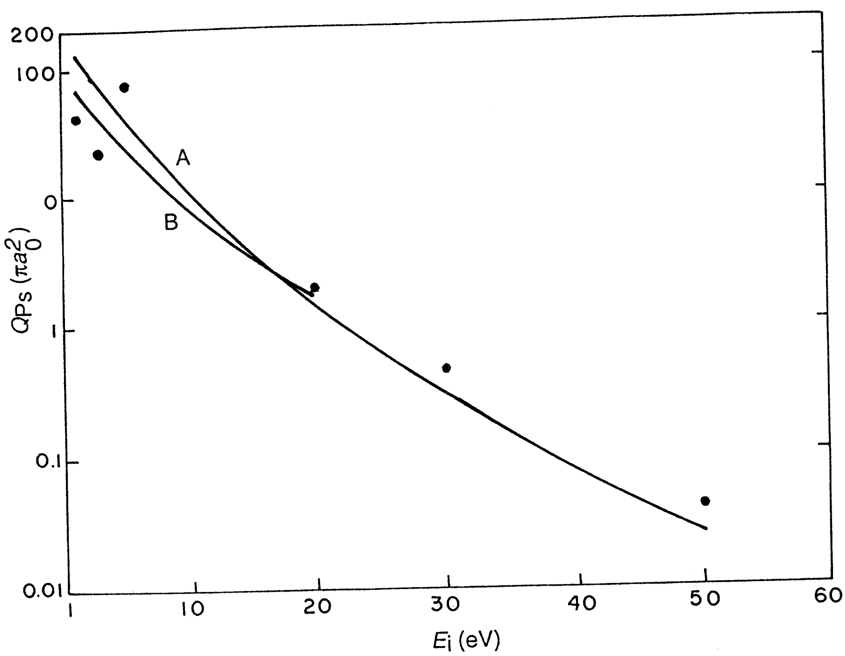

Fig. 1. Total cross section positronium formation in e$^+$–Na scattering: curve A, present distorted wave results; curve B, distorted wave results of Guha and Mandal (1980); while the points are the coupled static results of Abdel-Raouf (1988).

In Fig. 1 we show the present TCS results together with the distorted wave results of Guha and Mandal (1980) and the coupled static results of Abdel-Raouf (1988) which exhibit a sudden increase at $E_{\mathrm{i}} = 5$ eV. Our results, however, show a smooth decrease with increasing E_{i}. The present TCS is larger than that of

Guha and Mandal (1980) and Abdel-Raouf (1988) for $E_i < 20$ eV, but above 20 eV the present distorted wave results fall below the results of Abdel-Raouf (1988).

Table 1. Present total cross section Q_{Ps} for positronium formation in e$^+$–Na scattering, together with the elastic Q_{el} and the total Q_{exc} excitation cross sections for e$^+$–Na scattering as calculated by Ward *et al.* (1989) using the five-state close coupling approximation

E_i (eV)	Q_{Ps} (πa_0^2)	Q_{el} (πa_0^2)	Q_{exc} (πa_0^2)
1	136·21	205·18	—
2	92·83	189·47	—
5	35·83	54·13	90·58
10	10·66	19·84	78·97
20	1·52	8·98	54·80
30	0·299	6·49	42·03
50	0·0233	4·67	28·94

In Table 1 we give the present Q_{Ps} values together with the CCA results of Ward *et al.* (1989) for elastic and total excitation cross sections in e$^+$–Na scattering. It is to be noted that the CCA total cross sections of Ward *et al.* are in good agreement with the experimental results (Kwan *et al.* 1991) for the total cross section. We observe from Table 1 that the values of Q_{Ps} are almost the same order of magnitude as the elastic scattering cross section Q_{el}. We find that, as predicted by Kwan *et al.*, Q_{Ps} plays a relatively unimportant role in e$^+$–Na scattering for $E_i > 10$ eV.

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