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Positronium Formation Cross Sections for Scattering of Positrons from Potassium and Rubidium

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Abstract

Total cross sections for positronium formation in positron–potassium and positron–rubidium scattering have been calculated in a distorted wave approximation for incident positrons in the energy range 1 to 50 eV. The present results are compared with other theoretical results and with measurement where available.

1. Introduction

The formation of the exotic atom positronium (Ps) as a result of collisions of positrons with atoms is a very important process in positron–atom scattering. The process is more significant in the case of positrons colliding with alkali atoms, because the Ps formation channel is always energetically available. Recent measurements (Stein *et al.* 1992*a*, 1992*b*; Parikh *et al.* 1993) of total cross sections (TCS) show that below an incident positron energy of 30 eV, the TCS for e^+–K and e^+–Rb scattering is larger than the corresponding TCS for e^-–K and e^-–Rb scattering. Since the Ps formation channel is always open for alkali atoms, it might be that Ps formation is responsible for the dominance of the positron TCS over electron TCS at low incident energies. Being aware of this possibility Stein *et al.* (1992*b*) measured the TCS for Ps formation in positron–potassium scattering for an energy range 1–20 eV of incident positrons. They could not measure directly the values of the TCS for Ps formation, but instead reported its upper and lower limits. On the theoretical side there exists only one calculation for Ps formation in e^+–K and e^+–Rb scattering, namely that of Guha and Mandal (1980) who studied the process in the range 0·5–20 eV by using the distorted wave approximation (DWA) and first Born approximation (FBA).

In the present work we compute the TCS Q_{Ps} for positronium formation in e^+–K and e^+–Rb scattering by using a distorted wave approximation that has been successfully applied to Ps formation in positron scattering from atomic hydrogen, helium, lithium and sodium (Khan and Ghosh 1983*a*, 1983*b*; Khan

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et al. 1984, 1985; Mazaumdar and Ghosh 1986; Singh *et al.* 1992). Our distorted wave model, unlike that of Guha and Mandal (1980), takes into account the effect of polarisation, i.e. the long-range correlation arising from the distortion of the atomic charge cloud by the incoming positron. This effect is more important for positron scattering from alkalis because of their large polarisabilities.

2. Theory

To a good approximation, an alkali atom can be considered to be a one-electron system where the active valence electron moves outside a core made up of the nucleus and remaining electrons (Ward *et al.* 1989; McEachran *et al.* 1990, 1991). We assume the core to be frozen. Since the valence electron lies well outside the core this approximation introduces only a small error. Under these conditions the scattering amplitude for Ps formation in the ground state for positrons scattering from alkali atoms can be written as

$$f(\boldsymbol{k}_\mathrm{i}, \boldsymbol{k}_\mathrm{Ps}) = -\frac{\mu_\mathrm{f}}{2\pi} \int \eta^*_{1\mathrm{s}}(|\boldsymbol{r} - \boldsymbol{x}|) \exp[-\tfrac{1}{2}\mathrm{i}\, \boldsymbol{k}_\mathrm{Ps}(\boldsymbol{r} + \boldsymbol{x})] \times V_\mathrm{f}(r, x)\, \phi_\mathrm{i}(\boldsymbol{r})\ F(\boldsymbol{x})\ \mathrm{d}\boldsymbol{r}\, \mathrm{d}\boldsymbol{x}\,, \tag{1}$$

where $\boldsymbol{r}$ and $\boldsymbol{x}$ are respectively the position vectors of the active valence electron and incident positron, $\boldsymbol{k}_\mathrm{i}$ and $\boldsymbol{k}_\mathrm{Ps}$ are the wavevectors of the incident positron and moving positronium, and $\phi_\mathrm{i}(\boldsymbol{r})$ is the active valence electron orbital taken from Szazs and McGinn (1967). The effect of the core electrons on the scattering process has been taken into account through the potential $V_\mathrm{c}(r)$, following Gien (1991), while V_f is the interaction potential in the final channel, given by

$$V_\mathrm{f}(r, x) = \left(\frac{1}{x} - \frac{1}{r}\right) + V_\mathrm{c}(x) - V_\mathrm{c}(r)\,. \tag{2}$$

This is so because in the final channel we have the residual alkali ion and the moving positronium. The electron–positron interaction is accounted for in the unperturbed Hamiltonian. The wavefunction $F(\boldsymbol{x})$ of the incident positron is decomposed into partial waves as

$$F(\boldsymbol{x}) = k_\mathrm{i}^{-\frac{1}{2}} \sum_{l_\mathrm{i}=0}^{\infty} (2l_\mathrm{i} + 1) \exp(\mathrm{i}\,\delta_{l_\mathrm{i}})\, \frac{u_{l_\mathrm{i}}(k_\mathrm{i}, x)}{x} \times P_{l_\mathrm{i}} \cos(\hat{\boldsymbol{k}}_\mathrm{i} \,.\, \hat{\boldsymbol{x}})\,, \tag{3}$$

where l_i is the orbital angular momentum quantum number of the incident positron, δ_{l_i} is the phase shift of the l_ith partial wave, while $u_{l_\mathrm{i}}(k_\mathrm{i}, x)$ is the radial part of the incident electron wavefunction obtained by solving the differential equation

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{l_\mathrm{i}(l_\mathrm{i}+1)}{x^2} - 2V_\mathrm{st}(x) - 2V_\mathrm{pol}(x) - 2V_\mathrm{e}(x)\right) u_{l_\mathrm{i}}(k_\mathrm{i}, x) = F_\mathrm{i}\, u_{l_\mathrm{i}}(k_\mathrm{i}, x)\,. \tag{4}$$

The static potential $V_{st}(x)$ and the polarisation potential $V_{pol}(x)$ have been calculated following McEachran *et al.* (1991). In the case of alkalis, because the polarisability is quite high, the use of the straightforward polarisation potential is inconvenient. As a result, a number of authors (Walters 1976; Bhatia *et al.* 1978) have noted that for the highly polarisable alkali systems, the orthodox formalism of Temkin and Lamkin (1961) should be modified. To overcome this difficulty McEachran *et al.* (1991) employed the method of Stone (1966) to calculate $V_{pol}(x)$ by minimising the adiabatic energy of the atom in the field of the stationary positron. The core potential has been computed by following Gien (1991). The total cross section Q_{Ps} for Ps formation has been obtained by using standard relations.

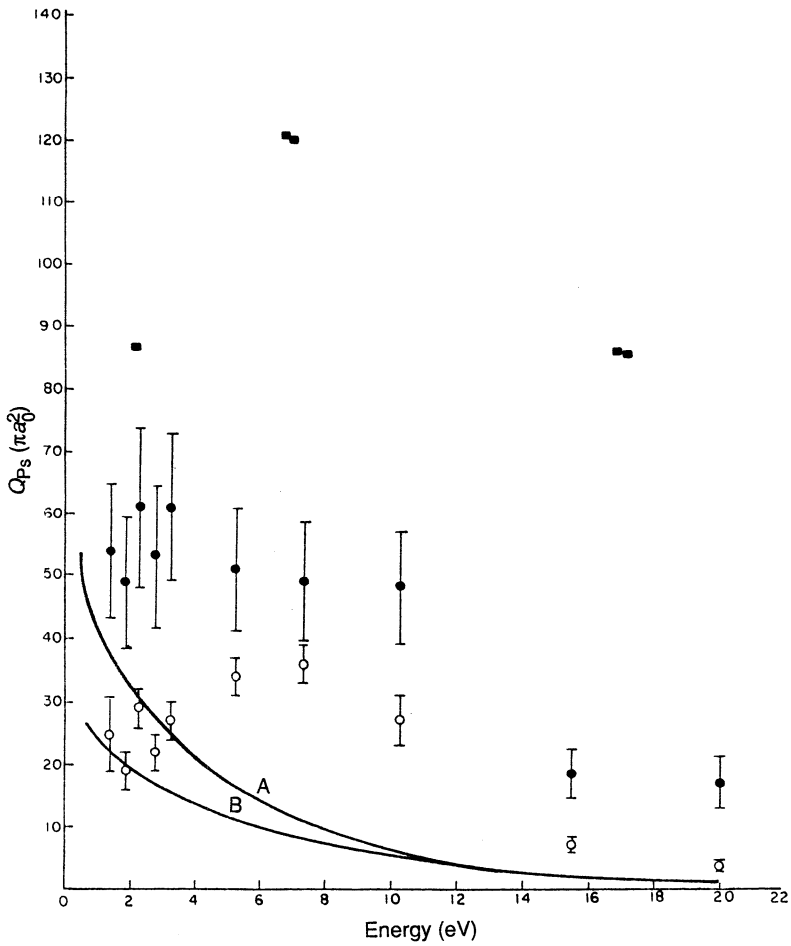

Fig. 1. Total cross section Q_{Ps} for positronium formation in e^+–K scattering: curve A, present distorted wave results; curve B, distorted wave results of Guha and Mandal (1980); solid circles, upper limit of experimental cross section (Stein *et al.* 1992*b*); open circles, lower limit of experimental cross section; and squares, experimental total cross section for e^+–K scattering (Stein *et al.* 1992*a*; Parikh *et al.* 1993).

Table 1. Present total cross section Q_{Ps} for positronium formation in positron scattering from potassium and rubidium

E_i (eV)	Q_{Ps} (πa_0^2) e^+–K	e^+–Rb
1	54·29	44·22
5	17·40	15·33
10	6·26	6·20
20	1·13	1·30
30	0·277	0·330
50	0·028	0·030

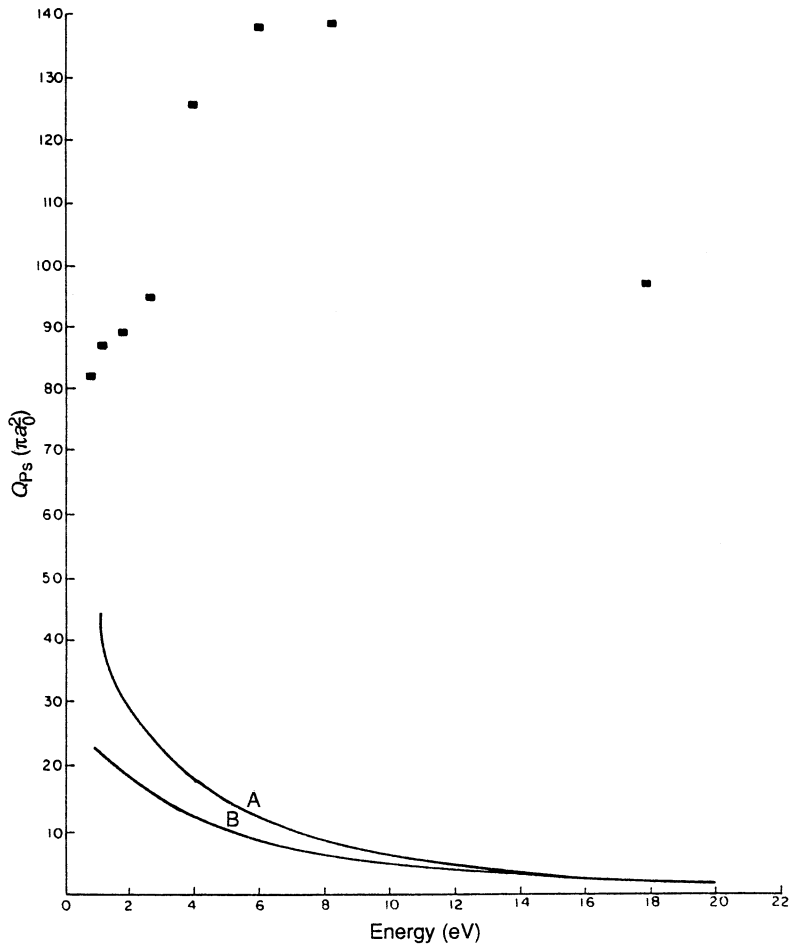

Fig. 2. Same as Fig. 1, except for e^+–Rb scattering and that no experimental results are available for the positronium formation cross section.

3. Results and Discussion

The differential equation satisfied by $u_{l_i}(k_i, x)$ has been solved by employing a noniterative procedure (Sloan 1964) out to a radial distance of 30 a.u. and with a stepsize of 0·01 a.u. For $x > 30$ a.u. we use the well known asymptotic form

(McDowell *et al.* 1973) of $u_{l_i}(k_i, x)$. For the evaluation of $f(k_i, k_{Ps})$ two-dimensional radial integrals have to be computed (Khan *et al.* 1985). These integrals have been evaluated by using suitable Gauss–Legendre quadratures. For a particular value of the incident positron energy E_i, the sum over l_i has been carried up to $l_i = l_{imax}$ such that the contribution of the partial wave l_{imax} to Q_{Ps} is of the order of 1% of the maximum contribution to Q_{Ps}.

In Fig. 1 we present a comparison between the present distorted wave results for the total cross section (TCS) for Ps formation in e^+–K scattering and that of Guha and Mandal (1980), together with the experimental results of Stein *et al.* (1992*b*) who reported the upper and lower limits of the TCS. Below an incident positron energy of 4 eV both the present results and the distorted wave results of Guha and Mandal (1980) lie within the predicted experimental upper and lower limits, although the present results are in marginally better agreement with experiment than those of Guha and Mandal. Between the incident energies of 4 and 20 eV, the present results as well as those of Guha and Mandal are lower than the measurements and lie outside the experimental limits. We note that below an incident energy of 10 eV the present results are higher than those of Guha and Mandal, but for $E_i > 10$ eV the present results do not differ too much.

In Table 1 we give the TCS for Ps formation in e^+–K and e^+–Rb scattering for the positron energy range 1–50 eV. It is to be noted that the distorted wave results of Guha and Mandal (1980) are not available for $E_i > 20$ eV. In Fig. 2 we display Q_{Ps} for e^+–Rb scattering over the energy range 1–20 eV, together with corresponding distorted wave results of Guha and Mandal. In this case the trends are similar to those for e^+–K scattering, except that no experimental results for positronium formation are available. In Figs 1 and 2 we have also shown experimental results for the total cross section Q_T of e^+–K and e^+–Rb scattering in order to assess the relative contribution of Q_{Ps}. For Fig. 1 it is evident both from the theoretical and experimental results that the contribution of Q_{Ps} to Q_T is not appreciable for $E_i > 5$ eV in e^+–K scattering. From Fig. 2 we can draw a similar inference for e^+–Rb scattering by comparing the experimental results for Q_T with the present results and those of Guha and Mandal (1980), because, unlike e^+–K scattering, in this case the experimental results for Q_{Ps} are not available.

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