Total cross sections of positron–sodium scattering at low energies*

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A new calculation for the total cross section of positron–sodium scattering is performed in an energy range down to a few tenths of one electron volt using the coupled-channel optical method. The ionization continuum and the positronium formation channels are included via an equivalent-local complex potential. The role played by the break-up and rearrangement processes in the low energy positron–sodium scattering is also investigated. The total scattering cross section is reported and compared with the available theoretical and experimental data.

Keywords: positron, sodium, cross section

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1. Introduction

Positron scattering with atoms has long been an important subject in atomic and molecular physics. It is not only of special fundamental importance but is also necessary for the development of many other applications and scientific areas such as plasma physics and material physics.[1,2] In the past decades positron scattering from atomic sodium has aroused the considerable interest of both experimentalists and theoreticians due to its interesting characteristics. First of all, the atomic sodium has a relatively simple structure and can be viewed to a certain degree as an approximate one-electron atom. Secondly, the positronium (Ps) formation channels are expected to play an important role especially at low energies since positronium formation is possible in energy even at zero incident energy. In the past decades, a number of experimental measurements and theoretical calculations have been performed for positron–sodium scattering.

On the experimental side, the total cross sections and the upper and lower limits of the total Ps formation cross sections for e^+–Na scattering have been measured by Kwan *et al.*,[3] Kauppila *et al.*,[4] Zhou *et al.*,[5] and Surdutovich *et al.*[6] Those experimental measurements are consistent with each other in both shape and magnitude.

From a theoretical perspective, various calculations of the positron–sodium system have been carried out by using different methods. In the early close coupling calculations performed by Ward *et al.*,[7] the positronium channels were not included and they overestimated the total scattering cross sections significantly at low energies. The first calculation including the positronium channels was done by Abdel–Raouf[8] in 1988; however, only one atomic and one positronium channels were included. Hewitt *et al.*[9] reported on their studies using the CC(4, 3) model with atomic states (3s, 3p, 4s, 4p) coupled to Ps(n = 1) and Ps(n = 2) states. Mitroy and Ratnavelu[10] investigated the positron–sodium scattering with the CC(5, 3) model in which the atomic states (3s, 3p, 3d, 4s, 4p) and Ps(n = 1) and Ps(n = 2) states were included and the interactions between the positron and the inert core electrons were also taken into account via a core potential. An extension to this work was done by Ryzhikh and Mitroy[11] with the CC(5, 6) model where the Ps(n = 3) and Ps(n = 4) states were added into the coupling. However, the effect of the ionization continuum was omitted at all energies in these calculations. The CC(27, 6) calculation of Campbell *et al.*[12] is the biggest close-coupling calculation to date, in which the ionization continuum states were included by employing the pseudo-states. Recently, Natchimuthu and Ratnavelu[12] reported on their calculations with the close-coupling optical potential method (CCOM) where the ionization continuum states were taken into account via an optical po-

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tential. Both the CC(27, 6) calculation by Campbell *et al.*[12] and the CCOM calculation by Natchimuthu and Ratnavelu[13] produced similar qualitative total scattering cross sections to the CC(5, 6) calculation by Ryzhikh and Mitroy.[11]

The motivation of this paper is to study the low energy scattering of a positron–sodium system and investigate the role played by the ionization and positronium formation processes using the coupled-channel optical method (CCO).[14] The ionization continuum and the positronium formation channels are included via a complex equivalent-local optical potential. This method has been used in positron collisions with hydrogen and helium at all energies.[14,15] In the present work, the total scattering cross sections of the e^+–Na collision are calculated in the energy range from 0.1 eV to 10 eV and compared with available theoretical and experimental data.

2. Model and method

A detailed description of the CCO method for positron scattering has been reported in Ref. [16]. Here, we only outline the essential features of the method and show the present description of the positronium formation process.

The CCO method consists of the solution of a discrete set of coupled Lippmann–Schwinger integral equations for T-matrix elements as

$$\begin{aligned}&\langle \boldsymbol{k}, \Phi_i|T|\Phi_0, \boldsymbol{k}_0\rangle \\ &= \langle \boldsymbol{k}, \Phi_i|V^{(Q)}|\Phi_0, \boldsymbol{k}_0\rangle \\ &\quad + \sum_{j\in P}\int \mathrm{d}^3\boldsymbol{k}'\langle \boldsymbol{k}, \Phi_i|V^{(Q)}|\Phi_j, \boldsymbol{k}'\rangle \\ &\quad \times \frac{1}{E^{(+)} - \epsilon_j - \frac{1}{2}k'^2}\langle \boldsymbol{k}', \Phi_j|T|\Phi_0, \boldsymbol{k}_0\rangle. \end{aligned} \quad (1)$$

The optical potential $V^{(Q)}$ can be expressed as the sum of the channel-coupling potential V and the non-local complex polarization potentials $W_{\mathrm{I}}^{(Q)}$ and $W_{\mathrm{Ps}}^{(Q)}$ that account for the ionization continuum and positronium formation channels, respectively.

The matrix element of the polarization potential can be calculated in the weak-coupling approximation as

$$\begin{aligned}&\langle \boldsymbol{k}'i|W^{(Q)}|j\boldsymbol{k}\rangle \\ &= \sum_{n\in Q}\langle \boldsymbol{k}'i|V|X_n^{(-)}\rangle \frac{1}{E^{(+)} - E_n}\langle X_n^{(-)}|V|j\boldsymbol{k}\rangle, \end{aligned} \quad (2)$$

where $X_n^{(-)}$ represents the time reverse of the exact state vector for a reaction starting in channel n. The explicit form for the positronium formation process is

$$\begin{aligned}&\langle \boldsymbol{k}'i|W_{\mathrm{Ps}}^{(Q)}|j\boldsymbol{k}\rangle \\ &= \sum_n \langle \boldsymbol{k}'i|V|X_n^{(-)}\rangle \frac{1}{E^{(+)} - \varepsilon_n - \boldsymbol{K}_{\mathrm{Ps}}^2}\langle X_n^{(-)}|V|j\boldsymbol{k}\rangle. \end{aligned} \quad (3)$$

The $X_n^{(-)}$ is orthogonalized to ψ_i from which the electron is captured, and

$$|X_n^{(-)}\rangle = (1 - |\psi_i\rangle\langle\psi_i|)|\Psi_n^{(-)}\rangle, \quad (4)$$

with

$$\Psi_n^{(-)} = \Phi_\mu(\boldsymbol{k}_{\mathrm{Ps}}, \boldsymbol{R}, \boldsymbol{r}) = \varphi_\mu\, \mathrm{e}^{\mathrm{i}\,\boldsymbol{k}_{\mathrm{Ps}}\cdot\boldsymbol{R}}. \quad (5)$$

Here, $\boldsymbol{k}_{\mathrm{Ps}}$ is the momentum of the positronium centre of mass and φ_μ is the wavefunction of the positronium bound state. The plane-wave $\mathrm{e}^{\mathrm{i}\,\boldsymbol{k}_{\mathrm{Ps}}\cdot\boldsymbol{R}}$ represents the motion of the positronium centre of mass since only the short-range terms survive in the interactions between the positronium and the ionic core of the target. $\boldsymbol{r} = \boldsymbol{r}_{\mathrm{p}} - \boldsymbol{r}_{\mathrm{e}}$ and $\boldsymbol{R} = \frac{1}{2}(\boldsymbol{r}_{\mathrm{p}} + \boldsymbol{r}_{\mathrm{e}})$, where $\boldsymbol{r}_{\mathrm{p}}$ and $\boldsymbol{r}_{\mathrm{e}}$ are the coordinates of the positron and the electron.

In the present case, for positron collision with atomic sodium of ground 3s state, the matrix element $\langle \boldsymbol{k}'i|V|X_n^{(-)}\rangle$ can be calculated as follows:

$$\begin{aligned}&\langle \boldsymbol{k}'i|V|X_n^{(-)}\rangle \\ &= \frac{1}{(2\pi)^3}\int\int \mathrm{d}^3\boldsymbol{r}_{\mathrm{p}}\mathrm{d}^3r_{\mathrm{e}}\varphi_\mu^*\,\mathrm{e}^{-\mathrm{i}\,\boldsymbol{k}_{\mathrm{Ps}}\cdot\boldsymbol{R}} \\ &\quad \times\left(-\frac{1}{r} - V_{3\mathrm{s}}(r_{\mathrm{p}})\right)\psi_{3\mathrm{s}}(\boldsymbol{r}_{\mathrm{e}})\,\mathrm{e}^{\mathrm{i}\,\boldsymbol{k}\cdot\boldsymbol{r}_{\mathrm{p}}}. \end{aligned} \quad (6)$$

The potential

$$V_{3\mathrm{s}}(r_{\mathrm{p}}) = -\int \mathrm{d}^3r_{\mathrm{e}}\frac{|\psi_{3\mathrm{s}}(\boldsymbol{r}_{\mathrm{e}})|^2}{\boldsymbol{r}_{\mathrm{p}} - \boldsymbol{r}_{\mathrm{e}}}$$

is the electrostatic potential of the valence electron in atomic sodium. The target bound state $\psi(\boldsymbol{r}_{\mathrm{e}})$ is represented by a Hartree–Fock wavefunction using the Slater basis. The potential matrix elements for positronium formation can be calculated by using Cheshire's numerical method.[17]

3. Results and discussion

In the present calculation, the atomic sodium state is represented by a modified Roothan Hartree–Fock wavefunction,[11] in which the core polarization effect is included by an semi-empirical potential. There are eight physical discrete channels (3, 4, 5s; 3, 4, 5p; 3, 4d) included in the present calculation. The total scattering cross sections are reported and

compared with available experimental and theoretical data at the impact energy range from 0.1 to 10 eV in Figs. 1 and 2.

In order to demonstrate the role of the ionization and the positronium formation channels, the present calculations are performed with different models: the CCO model including both the ionization continuum and positronium formation channels, the CCI model including only the ionization continuum states, and the pure close-coupling calculation (CC). The comparison among our calculation results with different models (CC, CCI, CCO) are displayed in Fig. 1. Compared with the present CCO results, the present CC and CCI calculations produce similar qualitative cross sections, which are much higher at the energies below 4 eV. This indicates that the ionization continuum states have little influence on the total cross section, while the inclusion of positronium formation channels reduces the cross sections significantly below 4 eV and this effect decreases rapidly as the incident energy increases.

The present CCO results are also compared with the experimental data given by Kwan *et al.*[3] and Kauppila *et al.*[4] in Fig. 1. The present calculation overestimates the experimental measurements at the energies between 2.5 and 8 eV. However, both measurements are attenuation experiments and cannot discriminate the forward-direction elastically scattered positrons. Consequently, the experimentally reported cross section underestimates the actual total cross sections. At energies below 10 eV, this contribution can make a difference of 10% or more from the empirical cross sections.[11] For instance, the present CCO model predicts an elastic cross section of $37\pi a_0^2$ from 0° to 21° at 2.7 eV, which is about 30% of the total cross sections ($125\pi a_0^2$). In order to make a direct comparison with experimental data, we also present the modified CCO results (MCCO), which are calculated from

$$\sigma_{\mathrm{MCCO}} = \sigma_{\mathrm{CCO}} - 2\pi \int_0^{\theta_{\mathrm{R}}} \sigma_{\mathrm{el}}(\theta)\,\mathrm{d}\theta, \qquad (7)$$

where σ_{el} is the present differential elastic cross section computed using the CCO model; θ_{R} is the cut-off angle in the present calculation, which is about 26° below 1 eV, 23° near 2 eV, 20° near 5 eV, 13° near 8 eV, and 11° near 10 eV separately. The present MCCO results are in good agreement with the measurement results given by Kwan *et al.*[3] and Kauppila *et al.*[4] The apparent discrepancies between the CCO and MCCO results are due to the large contribution from elastic cross sections below the cut-off angle θ_{R} in our calculations.

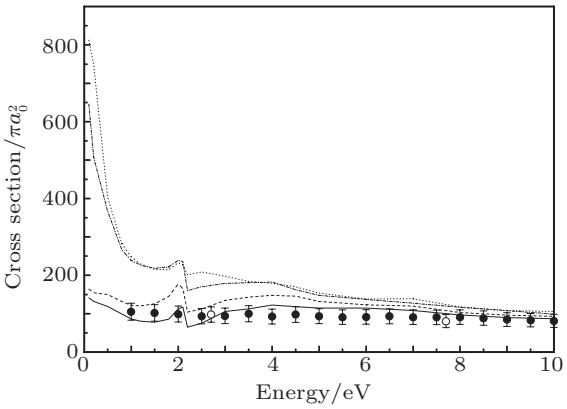


Fig. 1. Total cross sections for positron–sodium scattering. Solid line represents the results obtained by the present MCCO; dashed line by the present CCO calculation, dotted line by the present CC calculation, dash–dotted line by the present CCI calculation, ○ is for measurement results given by Kwan *et al.*,[3] and •, by Kauppila *et al.*[4]

In Fig. 2, the present CCO results are compared with the close-coupling calculations given by Ward *et al.* (CC(5, 0)),[7] Hewitt *et al.* (CC(4, 3)),[9] and Ryzhikh and Mitroy (CC(5, 6))[11] along with the experimental data.[3,4] A noticeable point is that the contribution from elastic scattering in the forward direction that has been omitted in both experimental measurements is included in all these calculations. In the CC(5, 0) calculation given by Ward *et al.*,[7] the positronium formation channels were not taken into account, and this is responsible mainly for the remarkable difference of the CC(5, 0) from other theoretical calculations and experimental measurements below 4 eV. The CC(4, 3) calculation given by Hewitt *et al.*[9] accords well with the experimental data above 4 eV and overestimates the cross sections at lower energies. The CC(5, 6) calculation results given by Ryzhikh and Mitroy[11] are consistent with the measurements above 2 eV. The present CCO calculation predicts much larger cross sections above 3 eV than the CC(4, 3) and CC(5, 6) calculations and the experimental measurements. At energies below 1 eV, where there have been no experimental measurements reported, the present CCO results disaccord strongly with the CC(5, 6) calculation. The present calculation suggests that the total cross section increases as the incident energy decreases while there is a peak value at about 0.5 eV in the CC(5, 6) results. The dominant cause of the difference between the calculations from the present

optical potential model and the CC(N, N') calculations may be the different treatment of the positronium formation process, which plays a prominent role in the low energy positron–alkali scattering. In the present model, the positronium formation channels are described via an equivalent-local complex potential while this rearrangement process is included in the CC(N, N') calculations by adding the positronium bound states into coupling. Since there exist significant discrepancies, more detailed and accurate measurements are needed.

Another noticeable feature in the present calculations is the cusp-like behaviour around 2 eV, which is exhibited in the CC calculation and enlarged by the inclusion of ionization and positronium formation channels in the CCI, CCO, and MCCO calculations. This position is close to the first excitation threshold of atomic sodium (2.104 eV) and a significant resonance at this energy has been confirmed by Ward *et al.*[18] (1.985 eV), Han *et al.*[19] (2.122 eV), and Kar and Ho[20] (2.219 eV). A detailed study of the resonance phenomenon and threshold behaviour in positron–sodium collision will be presented in another paper.

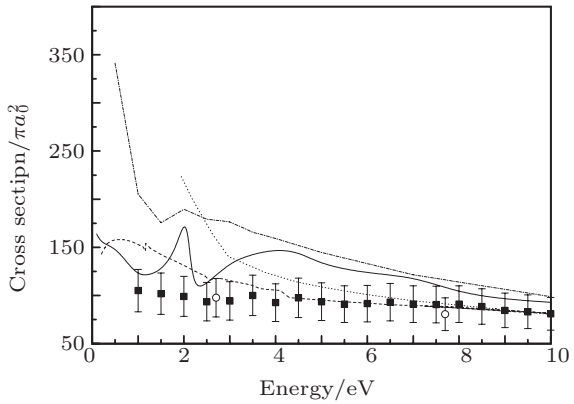


Fig. 2. Total cross sections for positron–sodium scattering. The solid line represents the results obtained by the present CCO calculation, the dashed line by the CC(5, 6) calculation of Ryzhikh and Mitroy,[11] dotted line by the CC(4, 3) calculation of Hewitt *et al.*,[9] the dash-dotted line by the CC(5, 0) calculation of Ward *et al.*,[7] ∘ represents measurements by Kwan *et al.*,[3] and ■ by Kauppila *et al.*[4]

4. Conclusion

The total scattering cross sections of low energy positron–sodium collisions are reported from 0.1 eV to 10 eV using the coupled-channel optical method. The ionization continuum and the positronium formation channels are included via an equivalent-local complex polarization potential. The present calculation shows that the inclusion of ionization continuum states has little influence on total cross sections while the inclusion of positronium channels significantly reduces the cross sections at low energies. A cusp-like behaviour around 2 eV, which is close to the excitation threshold of the Na (3p) state, is also found in the present calculations. The present predicted cross sections accord well with the experimental data given by Kwan *et al.*[3] and Kauppila *et al.*[4] However, the present calculation also shows an apparent difference from other theoretical results. Both further experimental measurements and theoretical studies are highly desired.

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