Positronium formation for $e^+$-Na scattering at low and intermediate energies

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Abstract. There have been various theoretical calculations for positron-sodium scattering that attempt to calculate accurate positronium(Ps) formation cross sections at low and intermediate energies. The recent hyperspherical close-coupling (HSCC) calculations (Le et al. 2005 Phys. Rev. A 71, 032713) has handled the contribution from the positronic bound states to a great extent. Their calculations have further strengthened the argument that the theoretical Ps cross sections at low energies deviate from the predictions of the experimental measurements (Surdutovich et al. 2002 Phys. Rev. A 65, 032713). Here we examine whether the inclusion or the neglect of the positronic bound states in the calculation have any significant effects on the low energy Ps formation cross sections. Thus, we attempt to investigate if large-scale CC calculations are deficient in this respect.

1. Introduction
There is no question that the positronium(Ps) channel gives a very significant effect on the positron-sodium(Na) scattering system [1-4] at low and intermediate energies. In the earlier calculations [5-8], the close-coupling equations have been used to treat this system by excluding the possibility of Ps formation. Abdel Raouf [9], performed the first close coupling calculation which included only one atomic state as well as one Ps channel. This motivated the realistic close-coupling calculations which explicitly included the Ps channels [10-12]. Walters and co-workers [4,13] as well as Ryzhikh and Mitroy [3], working independently, predicted that the Ps formation cross section will rapidly diminish as the incident energy decreases. The prediction was experimentally [2] verified for Li but not for Na. At incident energies about or less than 1 eV, the Ps formation cross section for $e^+$-Na seems to increase tremendously. Questions have been raised about the inadequacy of CC calculations for Li and Na as these atoms can form positronic states [14-17]. The recent theoretical work by Bromley’s group[1], tries to incorporate the positronic bound state in the HSCC calculations by implementing two model potentials which are the FCLX$_{pol}$ (frozen core+local exchange+polarization) and the SFG (Schweizer-Faßbinder-Gonzalez-Ferez). The present work has been largely motivated by the disagreement between the theoretical and experimental measurements especially at these low incident energies (<= 1eV). In this paper, the CC calculations [18] are extended to 15 (CC(9,6)) and 12 states (CC(9,3)). The atomic states used are taken from Zhou’s private communication [19]. Our aim is to investigate the effects of including the larger n-states in Ps formation cross sections.
2. Theory

The present close-coupling method is based on the work of Mitroy and Ratnavelu [11]. Briefly, we present the pertinent details. The Schrödinger equation, for a (N+1)-body system is given by:

\[
(H - E) \Psi(r_i, r_0) = 0
\]  

(1)

where \( E \) is the total energy of the \((N+1)\) body system. The \( H \) can be divided into \( H_e \) and \( H_{\text{atom}} \) where \( H_e \), is the Hamiltonian of the incident particle with respect to the target atom and \( H_{\text{atom}} \) represents the \( N \)-electron Hamiltonian of the target atom,

\[
H_e = -\frac{1}{2} \nabla^2_0 + \frac{Z}{r_0} - \sum_i \frac{1}{r_{i0}}
\]

(2)

\[
H_{\text{atom}} = \sum_i \left( -\frac{1}{2} \nabla^2_i - \frac{Z}{r_i} \right) + \frac{1}{2} \sum_{ij} \frac{1}{r_{ij}}
\]

(3)

Thus, incorporating the Ps channels, an alternative partitioning of the Hamiltonian can be used:

\[
H = H_{ps}(m) + H_{ion}(m) + H_{\text{int}}(m), \quad \forall m \in \{1, \ldots, N\}
\]

(4)

where

\[
H_{ps}(m) = -\frac{1}{4} \nabla^2_R + \frac{Z}{r_m} - \sum_{i \neq m} \left( \frac{1}{2} \nabla^2_i - \frac{1}{r_i} \right)
\]

(4a)

\[
H_{ion}(m) = \sum_{i, i \neq m} \left( -\frac{1}{2} \nabla^2_i - \frac{Z}{r_i} \right) + \frac{1}{2} \sum_{i \neq j, i \neq m, j \neq m} \frac{1}{r_{ij}}
\]

(4b)

\[
H_{\text{int}}(m) = -\nabla^2_{\rho m} - \frac{1}{r_{m0}}
\]

(4c)

\( H_{ps}(m) \) is the interaction of the positronium atom containing the \( m \)th electron with the residual ion,

\( H_{ion}(m) \) is the Hamiltonian of the residual ion with the \( m \)th electron removed

and \( H_{\text{int}}(m) \) is the internal Hamiltonian for a positronium atom containing the \( m \)th electron. Thus, the Schrodinger equation can be written as

\[
(E - H) \left[ \sum \Psi_a^* (r_i) F_a (r_0) + \sum \phi_{\beta}(\rho) \Omega(r_i) G_{\beta}(R) \right] = 0
\]

(5)

By using standard procedures, the Schrodinger equation can be reduced to the momentum-space Lippmann-Schwinger equations for a positron with momentum \( k \) on a sodium atom which can be written as

\[
\langle k' \Psi_a' | T | k \Psi_a \rangle = \langle k' \Psi_a' | V | k \Psi_a \rangle + \sum_{a'} \int d^3 k^* \frac{\langle k' \Psi_a' | V | k' \Psi_a' \rangle \langle k \Psi_a' | T | k' \Psi_a \rangle}{E^{(\ast)} - E_{a'} - E_{\text{core}} - \frac{1}{2} k^*^2}
\]

\[
+ \sum_{\beta'} \int d^3 k^* \frac{\langle k' \Psi_a' | V | k' \Psi_{\beta'} \rangle \langle k' \Psi_{\beta'} | T | k \Psi_a \rangle}{E^{(\ast)} - E_{\beta'} - E_{\text{core}} - \frac{1}{4} k^*^2}
\]

(6a)

\[
\langle k' \Omega \phi_{\beta'} | T | k \Psi_a \rangle = \langle k' \Omega \phi_{\beta'} | V | k \Psi_a \rangle + \sum_{a'} \int d^3 k^* \frac{\langle k' \Omega \phi_{\beta'} | V | k' \Psi_a \rangle \langle k \Psi_a | T | k' \Omega \phi_{\beta'} \rangle}{E^{(\ast)} - E_{a'} - E_{\text{core}} - \frac{1}{2} k^*^2}
\]

\[
+ \sum_{\beta''} \int d^3 k^* \frac{\langle k' \Omega \phi_{\beta'} | V | k' \Omega \phi_{\beta''} \rangle \langle k' \Omega \phi_{\beta''} | T | k \Psi_a \rangle}{E^{(\ast)} - E_{\beta''} - E_{\text{core}} - \frac{1}{4} k^*^2}
\]

(6b)
3. Results and Discussion
The present work uses two sets of calculations:
(a) CC(9,6): consists of nine atomic states (Na(3s, 3p, 4s, 3d, 4p, 5s, 4d, 5p, 5d)) + six Ps (Ps(1s, 2s, 2p, 3s, 3p, 3d)).
(b) CC(9,3): similar to the CC(9,6) except for the Ps states we reduced it to only three Ps states (Ps(1s, 2s, 2p)).

The present results (CC(9,6) and CC(9,3)) for the total Ps formation cross section are displayed in Figure 1. The present cross sections are shown with the HSCC cross section [1] and the experimental measurements [2]. The previous CC calculations [3, 4] are also shown. The present results seems to be in good agreement with the measured data at energy above 1 eV. At energies ranging from 3 to 5 eV, a structure is seen except in the HSCC data. At energies <= 1 eV, the present results seems to support previous theoretical works. Further, the present results displays some structures in this low energy region. This could plausibly be due to the limitation of the present CC calculations.

In Figure 2, the total Ps(1s) formation cross section at energies within 0.01-2 eV are studied. The inclusion of (n = 3) Ps states in the CC(9,6) calculations reduces the cross sections nearer to the CC(5,6) and the HSCC (SFG pot) cross sections for energies up to 0.2 eV. The present CC(9,6) calculations shows obvious numerical artefacts at 0.4 and 0.5 eV. Our various convergence studies do not improve the cross section at these two energies.

4. Conclusion
The present calculations show similar trends with the HSCC and CC(5,6) in the low energy region. However, at energies below 1 eV, the present CC(9,6) and CC(9,3) calculations are in reasonable agreement with the qualitative trends of the HSCC except at 0.4 and 0.5 eV.

Figure 1. Total Ps formation cross section for e^-Na scattering

![Graph showing total Ps formation cross section vs energy](image-url)
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