Two-center convergent-close-coupling calculations for positron-sodium collisions

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Positron scattering from sodium atoms has been studied theoretically with the use of the two-center convergent-close-coupling method. The target has been treated in the framework of a one-active-electron approach. The positronium formation channels are taken into account explicitly utilizing Laguerre-based states. Our calculations are overall in good agreement with the previous theoretical results, and so the discrepancy with experiment at low energies remains unresolved.

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I. INTRODUCTION

Interactions of positrons with matter have been the subject of considerable interest starting with the discovery of positrons in 1933 [1]. Many applications utilizing these esoteric particles have been developed since then. Today positrons are used routinely for structural and elemental analysis of surfaces, films, and solids [2]. Positron emission tomography (PET) revolutionized many fields of medical diagnosis. Metallurgical, food, and chemical industries benefit from the use of the positron emission particle tracking technique (PEPT) [3].

A deep understanding of the underlying positron-atom interactions is a prerequisite for further development of the high-tech positron-based applications. The theoretical approach that we use in this paper for numerical solution of the positron–sodium-atom scattering problem originates from the close-coupling method of Massey and Mohr [4]. Studying electron-atom collisions, they suggested expanding the system wave function over the eigenstates of the unperturbed target Hamiltonian, and they derived the set of close-coupling equations in the momentum space to get the expansion weight functions. This approach culminated in the development of the convergent-close-coupling (CCC) method for electron scattering from quasi-one-electron and two-electron targets [5]. The CCC method additionally incorporates the target continuum systematically utilizing the complete Laguerre basis, and it has been shown to yield accurate excitation and ionization differential cross sections [6–8].

The one-center expansion method of Massey and Mohr [4] can also be applied for analysis of the positron-atom scattering problem [9]. However, it yields cross sections for direct transitions only. The rearrangement transition cross sections cannot be calculated within this approach. To overcome this limitation, a two-center expansion with both atomic and positronium (Ps) states taken into account explicitly can be used [10].

The first calculations utilizing the two-center approach were conducted with just a few target and Ps states [11–14]. Though some unusual pseudoresonances were identified, generally good agreement of the calculated Ps formation cross sections with available experimental data was found. Subsequently, more complex studies supported the results of the earlier two-center works with one notable exception. The first calculations for positron scattering from sodium atoms predicted that the Ps formation cross section decreased gradually with the impact energy for the region above 0.1 eV [15,16]. These predictions were later confirmed experimentally [17,18]. However, the calculations with larger numbers of basis states, presumably more accurate, showed that the cross section increased with energy in the range from 0.1 to 1 eV [19–21]. This discrepancy has not been resolved.

In this paper, we study positron scattering from sodium atoms with the use of the two-center CCC method. Together with the target and Ps bound states, our approach allows systematic accounting of the target and Ps continuum states in the wave-function expansion. The CCC method is sufficiently flexible to let us use any arrangement of the basis sets. This flexibility ensures obtaining convergent parameter-independent results, though inclusion of both the atomic and Ps centers makes our calculations computationally expensive.

II. THEORY

Consider a positron scattering from a sodium atom being initially in the ground state. Our interest is in collision processes involving primarily just the valence electron where core electron excitation may be neglected. So, we describe the target as an inert Hartree-Fock core together with a single valence electron (frozen-core approximation) [22]. Thus, our system consists of the impinging positron, the ion core Na^+, and the valence electron. The wave function Ψ of this system is sought as an expansion,

$$\Psi = \sum_{\alpha}^{N_\alpha} F_\alpha(\boldsymbol{\rho}_\alpha)\psi_\alpha^{N_\alpha}(\boldsymbol{r}_\alpha) + \sum_{\beta}^{N_\beta} F_\beta(\boldsymbol{\rho}_\beta)\psi_\beta^{N_\beta}(\boldsymbol{r}_\beta), \qquad (1)$$

where $\psi_\alpha^{N_\alpha}$ and $\psi_\beta^{N_\beta}$ are atomic and positronium pseudostates, respectively, and F_α and F_β are their associated weight functions. In expansion (1) we use two different sets of Jacobi coordinates $\{\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha\}$ and $\{\boldsymbol{r}_\beta, \boldsymbol{\rho}_\beta\}$, where $\boldsymbol{r}_{\alpha(\beta)}$ corresponds to the electron position with respect to the ion core (positron) and $\boldsymbol{\rho}_{\alpha(\beta)}$ is the positron (ion core) position with respect to the sodium atom (electron-positron pair) center of mass. The pseudostates, $\psi_\alpha^{N_\alpha}$ and $\psi_\beta^{N_\beta}$, are generated by diagonalizing the one-particle Hamiltonians,

$$H_\alpha = -\tfrac{1}{2}\nabla_{\boldsymbol{r}} + V_\alpha(r) \quad \text{and} \quad H_\beta = -\tfrac{1}{4}\nabla_{\boldsymbol{r}} + V_\beta(r). \qquad (2)$$

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The potentials V_α and V_β in Eqs. (2) are, respectively, the electron-ion core and electron-positron potentials. For V_α, we use

$$V_\alpha = V_{\rm st} + V_{\rm ex} + V_{\rm pol}, \tag{3}$$

where $V_{\rm st}$ and $V_{\rm ex}$ are the static and exchange terms of the Hartree-Fock potential. The exchange part $V_{\rm ex}$ of the electron-ion core potential V_α is taken into account in the framework of the equivalent local-exchange approximation, which was successfully applied previously for treating the electron–sodium-atom collision by Bartschat and Bray [23]. Finally, the positron-ion potential V_e was taken to be

$$V_e(r) = -V_{\rm st}(r) + V_{\rm pol}(r). \tag{4}$$

Each complete set of generated pseudostates contains both negative-energy and positive-energy states. The lower ones correspond to the bound states. The higher ones provide a discrete representation of the continuum. The number of negative-energy states depends on the basis size N_l and the exponential fall-off parameter λ_l specific for every given orbital momentum number l. These parameters were chosen so that the pseudoenergies of the low-energy states reproduced the corresponding experimental energies with accuracy comparable to that of the self-consistent-field Hartree-Fock calculations.

Momentum-space coupled-channel equations for transition matrix elements are [24]

$$T_{\gamma',\gamma}(\boldsymbol{q}_{\gamma'},\boldsymbol{q}_\gamma) = V_{\gamma',\gamma}(\boldsymbol{q}_{\gamma'},\boldsymbol{q}_\gamma) + \sum_{\gamma''}^{N_\alpha+N_\beta} \int \frac{d\boldsymbol{q}_{\gamma''}}{(2\pi)^3} \times \frac{V_{\gamma',\gamma}(\boldsymbol{q}'_\gamma,\boldsymbol{q}_{\gamma''})T_{\gamma',\gamma}(\boldsymbol{q}_{\gamma''},\boldsymbol{q}_\gamma)}{\left[E + i0 - \epsilon_{\gamma''} - q^2_{\gamma''}/(2M_{\gamma''})\right]}, \tag{5}$$

where $\boldsymbol{q}_\gamma$ is the momentum of the free particle γ relative to the center of mass (c.m.) of the bound pair in channel γ ($\gamma = \alpha$ or β), M_γ is the reduced mass of these two fragments, ϵ_γ is the energy of the bound pair, and E is the total energy.

Calculation of the effective potential $V_{\gamma',\gamma}$ is done as described in Refs. [24] and [22]. To obtain $T_{\gamma',\gamma}(\boldsymbol{q}_{\gamma'},\boldsymbol{q}_\gamma)$, we first perform partial-wave expansion of Eqs. (5) in the total orbital angular momentum J. Finally, the derived set is converted into equations for the K matrix and solved numerically with the use of real arithmetic [24].

III. RESULTS

Calculation of transition matrix elements $T_{\gamma',\gamma}(\boldsymbol{q}_{\gamma'},\boldsymbol{q}_\gamma)$ was done for a limited number of partial waves J. We found that the first ten partial waves were enough to get reliable results for the Ps formation cross sections at all energies. Direct scattering channels required at least ten partial waves more at the higher energies.

With our CCC approach, we are able to use any number of pseudostates from both centers. We conducted calculations with different numbers of states using both one-center and two-center expansions to check convergence with increasing bases sizes. In what follows, we present our most accurate one- and two-center calculations.

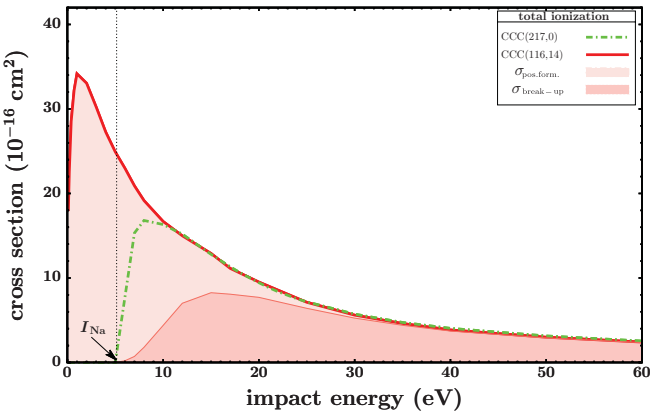

FIG. 1. (Color online) The cross section of a sodium atom ionized by positron impact calculated with the use of two CCC models described in the text. Shown with the thick solid line is the sum of the Ps formation cross section $\sigma_{\rm pos.form.}$ and the breakup cross section $\sigma_{\rm breakup}$. The position of the ionization threshold is labeled with $I_{\rm Na}$.

The one-center set arrangement, which we will label CCC(217,0), has 217 sodium pseudostates and no Ps states. The atomic states were obtained by diagonalizing H_α with the use of the Laguerre basis of the size $N_{\rm max} = 25 - l$ for each orbital quantum number l from 0 to $l_{\rm max} = 10$, with the fall-off parameter $\lambda = 1$. The two-center set, CCC(116,14), had 116 sodium pseudostates ($N_{\rm max} = 20 - l$, $l_{\rm max} = 6$, and $\lambda = 2$) and 14 negative-energy Ps $n \leqslant 5$ eigenstates with $l \leqslant 3$. Calculations with larger numbers of Ps states yielded results quite similar to CCC(116,14), but due to greater ill-conditioning of the underlying numerical system they were less stable.

Figure 1 shows the cross section $\sigma_{\rm ion}$ for the sodium atom to lose its electron occupying the $3s$ state due to positron impact. Within the one-center approach, this quantity can be estimated as

$$\sigma_{\rm ion} = \sum_{n:\epsilon_n^{\rm Na}>0} \sigma_n^{\rm (one\ center)}, \tag{6}$$

where $\sigma_n^{\rm (one\ center)}$ is the cross section for electron excitation of the nth pseudostate of a sodium atom. Summation in Eq. (6) is carried out over all positive-energy sodium states. We compare this quantity with the Ps formation cross section

$$\sigma_{\rm pos.form.} = \sum_{n:\epsilon_n^{\rm Ps}<0} \sigma_n^{\rm (two\ center)}, \tag{7}$$

plus the breakup cross section

$$\sigma_{\rm breakup} = \sum_{n:\epsilon_n^{\rm Na}>0} \sigma_n^{\rm (two\ center)} + \sum_{n:\epsilon_n^{\rm Ps}>0} \sigma_n^{\rm (two\ center)}, \tag{8}$$

where $\sigma_n^{\rm (two\ center)}$ is the cross section of electron transition to the nth state of the two-center calculation CCC($N_{\rm Na}$,$N_{\rm Ps}$). The CCC(116,14) calculated contributions of $\sigma_{\rm pos.form.}$ and $\sigma_{\rm breakup}$ to the sum are shown in Fig. 1 with the filled areas, where the Ps formation component is on top of the breakup one.

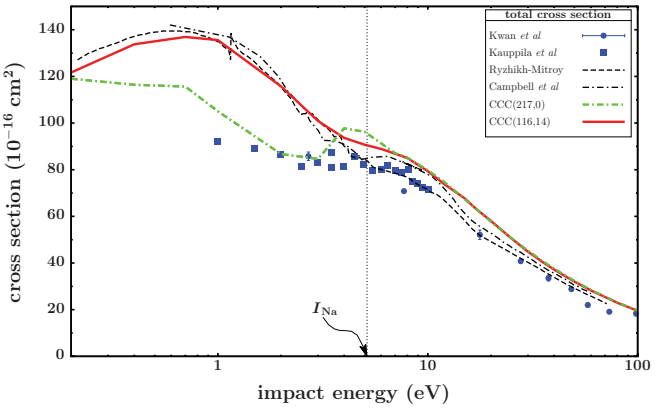

FIG. 2. (Color online) Total cross sections for positron-sodium scattering. The CCC results are compared with the theoretical data by Ryzhikh and Mitroy [19] and Campbell *et al*. [20]. The experimental points are due to Kwan *et al*. [25] and Kauppila *et al*. [26].

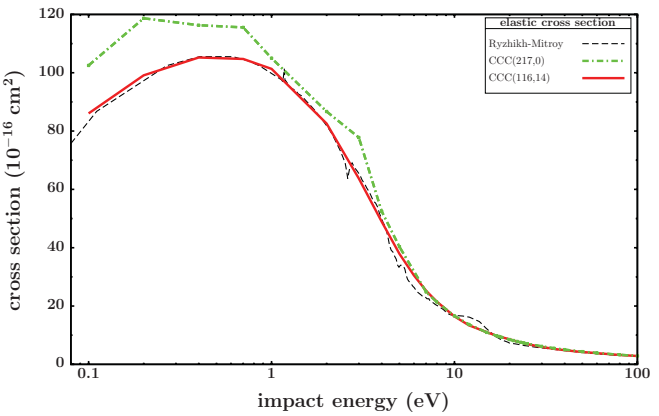

FIG. 3. (Color online) Same as Fig. 2 but for elastic cross section.

Note that due to the absence of positive-energy Ps pseudostates, there is no contribution to breakup from the second term of (14). However, though not present, when such states are included the results are only marginally affected. We see that the cross sections obtained with the use of the two different wave-function expansions are in a very good agreement for energies above ∼10 eV. For smaller energies, the results of the CCC(116,14) and CCC(217,0) calculations differ significantly. This is because the one-center approach can only be accurate above the ionization threshold. With a much larger expansion, the single center calculation could be made to rise even more rapidly past the ionization threshold. However, it will always be wrong below this threshold (for sodium). Its usefulness lies instead as a consistency check of both calculations, which gives us great confidence in the accuracy of the two-center calculation at all energies. Also, one should note that electron exchange was treated exactly in the one-center calculations. This validates the use of the local-exchange approximation in the two-center calculations.

Figure 2 shows the total cross section calculated with the use of both one-center and two-center expansions. Also shown with dashed and dotted lines are calculations by Ryzhikh and Mitroy [19] and Campbell *et al*. [20], respectively. As expected from Fig. 2, we see that the CCC(217,9) and CCC(116,14) calculations are on top of each other above ∼10 eV. Above the ionization threshold, our calculations are a little above the results of Campbell *et al*. [20] and Ryzhikh and Mitroy [19]. The agreement between the one- and two-center CCC calculations gives us considerable confidence in the accuracy of the CCC results in this region. Note that the ionization channels were not taken into account by Ryzhikh and Mitroy [19]. Below the I_{Na} threshold, the CCC(217,0) calculation is presented for completeness, but has little meaning as it is not convergent, being unable to account for Ps formation. However, CCC(116,14) agrees well with other two-center calculations. Unfortunately, all two-center theories disagree with the experiment.

The elastic cross section for positron-sodium scattering is shown in Fig. 3. Our calculations are compared with each other and the results by Ryzhikh and Mitroy [19]. We see again good quantitative agreement between the two-center calculations supported by the one-center theory above ∼10 eV.

Figure 4 shows the CCC results of the positronium formation cross section together with the experimental points [17,18] and the data of the other theoretical works [19–21]. We see from Fig. 4 that the CCC cross sections are in overall qualitative agreement with the results of other theories. This agreement indicates also that the dielectric correlation due to the electron-positron potential modification in the vicinity of the ion core [21] has only a marginal effect on the Ps formation. The theoretical calculations are all systematically lower than experiment. The fact that theory predicts higher total cross sections and yet lower Ps formation cross sections, at energies where the elastic and Ps formation are the only two open channels, suggests that the theoretical elastic cross section would need to be very wrong, too. In our opinion, the discrepancies identified here warrant new experimental investigation.

IV. SUMMARY

The one- and two-center CCC calculations have been conducted for positron scattering with sodium atoms on a broad range of energies of practical interest. For energies above 10 eV we found good agreement between the data obtained

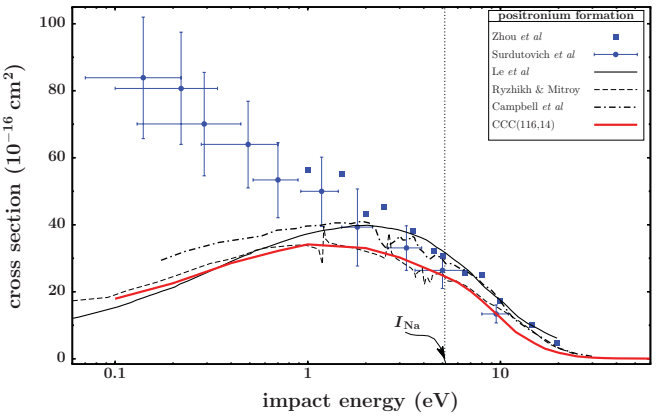

FIG. 4. (Color online) Total positronium formation cross section for e^+-Na along with the experimental points [17,18] and theoretical calculations [19–21].

with the use of these two methods providing an important consistency check. At low energies, two-center results are in good agreement with the other theoretical works, but not with the available experimental data. We would appreciate further experimental and theoretical investigation to see if the present discrepancy with experiment can be resolved.

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