

Positronium formation in positron-Li and positron-Na collisions at low energies

Anh-Thu Le,^{*} M. W. J. Bromley,[†] and C. D. Lin

Department of Physics, Cardwell Hall, Kansas State University, Manhattan, Kansas 66506, USA

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We present the positronium formation cross sections for a positron colliding with lithium and sodium for the collision energies from 0.01 eV up to 20 eV by the hyperspherical close-coupling method. For Li, our results agree with the experimental data and with other calculations. Our results for Na remain in agreement with previous close-coupling calculations, but do not support the latest experimental data for Na below 1 eV. To validate our model potentials and method in the low-energy regime, the binding energies of positronic lithium and positronic sodium as well as the s -wave scattering lengths for positronium scattering from Li^+ and Na^+ are also presented.

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I. INTRODUCTION

It is well known that positronium (Ps) formation plays an important role in the collision of positrons with alkali-metal atoms at very low energies since the Ps channel is open at zero collision energy for all alkali-metal atoms. It is therefore not surprising that the presence of Ps channels must be included in the calculations of positron-alkali-metal atoms at relatively low collision energies [1,2]. While such calculations are challenging to perform, reasonable agreement between experiment and theory has been achieved for almost all the alkali-metal atoms. The notable exception to this is for sodium, where measurements of the Ps formation cross section [3,4] disagree strongly with the most elaborate close-coupling (CC) calculations [1,2].

The most recent positronium formation cross sections measured by Surdutovich *et al.* [4], in fact, were in good agreement with recent theoretical calculations for lithium, but not for sodium, for energies near and below 1 eV. Below about 1 eV the measurements showed that, as the energy is decreased, the positronium formation cross section increases for sodium but levels out or even decreases for lithium. In contrast, independent CC calculations by the Belfast group [2,5] and by Ryzhikh and Mitroy [1] suggest that the positronium formation cross sections should behave similarly for both of these alkali-metal atoms and drop at energies below about 1 eV. A recent calculation for e^+ -Na collisions, to complicate the situation further, based on an optical potential approach [6], predicts that as the collision energy is reduced, the positronium formation cross section rises *more rapidly* than the experiment.

Speculation on the possible inadequacy of the CC calculations arose [4] because both lithium and sodium have recently been shown to be positronic atoms [7–10] (i.e., atoms that can form bound states with positrons; see Ref. [11] for a review). There remains the hypothesis that previous calculations of both lithium and sodium were simply not converged

at low energies since the positronic bound states were not taken into account and/or the low-energy Ps formation cross sections may be dependent on the precise details of the model potentials.

In this paper, we report the results of hyperspherical close-coupling (HSCC) calculations for positron scattering from sodium and lithium at the energy range from 0.01 eV up to 20 eV. The HSCC has been employed in numerous papers for three-body collisions involving particles with different combination of masses. Here, we use the HSCC variant developed initially for ion-atom collisions [12], which has been successfully applied to various ion-atom collision systems (see, for example [13], and references therein) as well as for collisions involving different combinations of masses such as antiproton-H [14] and muon transfer [15]. In the HSCC method, the collision is treated as a dynamic process and the hyperradius is considered as an adiabatic variable in a similar manner as in the Born-Oppenheimer (BO) approach for molecules. Any effect of the positronic bound states, therefore, is automatically incorporated in the calculations, provided that the appropriate channels supporting the bound states of $e^+\text{Na}$ and $e^+\text{Li}$ are included.

The paper is organized as follows. In Sec. II we describe the HSCC method and the use of our model potentials. The results are presented in Sec. III. First, to validate our calculations, the binding energies of the positron-atom bound states and the s -wave scattering lengths for $\text{Ps}(1s)\text{-Li}^+$ and $\text{Ps}(1s)\text{-Na}^+$ interactions are presented. Second, we present the positronium formation cross sections. We find good agreement for lithium with both experiments and other theories. For the sodium case, at energies below about 1 eV, we find continuing agreement with the other close-coupling calculations and strong disagreement with the experimental data. The last section contains a summary and conclusion.

II. MODEL POTENTIALS AND THE HSCC METHOD

The e^+ -alkali-metal collision system is approximated as consisting of a positively charged core, an electron, and a positron. The effective interaction among the three charged particles is given by $V=V_{12}+V_{13}+V_{23}$ where we use indexes

^{*}Electronic address: atle@phys.ksu.edu

[†]Faculty of Technology, Charles Darwin University, Darwin, NT 9090, Australia.

1, 2, and 3 to denote the core, the positron, and the electron, respectively.

In this paper, we employ model potentials based on a semiempirical ansatz that has been used in the description of positronic lithium and positronic sodium [9]. The electron-core interaction V_{13} is the sum of a static, a localized exchange potential and an induced dipole core-polarization potential. In brief, the recipe proceeds as follows: the static core potential is first obtained from a Hartree-Fock calculation [16]; the effects of electron-core exchange are treated with the addition of a local potential such that agreement is reached with an exact exchange calculation of the lowest ns and np one-electron energy levels [9] (including core orthogonality). Finally, the polarization potential is added, which is of the form

$$V_{pol}(r) = -(\alpha_d/2r^4)\{1 - \exp[-(r/\rho_c)^6]\}, \quad (1)$$

where $\alpha_d=0.1923a_0^3$ and $0.998a_0^3$ are the dipole polarizabilities of the Li^+ and Na^+ cores [17,18], respectively. The cut-off radius for each atom was chosen as $\rho_c=0.825a_0$ for Li^+ and $\rho_c=1.15a_0$ for Na^+ so that the lowest few energy levels agreed with experiment.

For the positron-core interaction V_{12} , the static part of the potential is the same as in V_{13} but with opposite sign; there is no exchange term, and the polarization potential is chosen to the same as in V_{13} [with $\rho_c(e^+) = \rho_c(e^-)$]. For the interaction between the positron and electron, V_{23} , besides the interparticle Coulomb potential, we also include the so-called dielectronic correction

$$V_{diel} = 2 \cos(\theta_{23})\sqrt{V_{pol}(r_p)V_{pol}(r_e)}, \quad (2)$$

where θ_{23} is the angle between the positron and electron with respect to the core. This term has the effect of providing the correct asymptotic description of the interaction between the two “bare” charges and the core [19]. This model potential will be denoted in the paper as FCLX_{pol} (frozen core + local exchange + polarization).

To provide some sense of the sensitivity of the positronium formation with respect to the model sodium potential we also employ a simple model potential, suggested by Schweizer *et al.* [20]. The electron-core interaction V_{13} is taken in the form

$$V_{SFG}(r) = -\frac{1}{r}[1 + 10 \exp(-a_1 r) + a_2 r \exp(-a_3 r)], \quad (3)$$

where $a_1=7.902$, $a_2=23.51$, and $a_3=2.688$. This model potential will be denoted in the paper as SFG (Schweizer-Faßbinder-Gonzalez-Ferez). Note that using this potential we are unable to unravel the different potential contributions, and thus we simply use the positron-core interaction to be the same [i.e., $V_{12}=V_{SFG}(r)$]. The SFG positron-core potential thus includes an unwanted exchange-like potential contribution, as well as being unable to include any dielectronic correction. This potential was chosen, however and furthermore, as it can be used to trivially benchmark future calculations against the present.

To determine the positronium formation cross sections, we use the HSSC method. Given the model potentials described above, the three-body problem is then solved in the mass-weighted hyperspherical coordinates. In the “molecular” frame, the first Jacobi vector $\boldsymbol{\rho}_1$ is chosen to be the vector from the core to the positron, with reduced mass μ_1 , and the second Jacobi vector $\boldsymbol{\rho}_2$ goes from the center of mass of the core and the positron to the electron, with reduced mass μ_2 . The hyperradius R and hyperangle ϕ are defined as

$$R = \sqrt{\frac{\mu_1}{\mu} \rho_1^2 + \frac{\mu_2}{\mu} \rho_2^2}, \quad (4)$$

$$\tan \phi = \sqrt{\frac{\mu_2 \rho_2}{\mu_1 \rho_1}}, \quad (5)$$

where μ is arbitrary. In this paper we chose $\mu = \sqrt{\mu_1 \mu_2}$. We further define an angle θ as the angle between the two Jacobi vectors.

The HSCC treats the hyperradius R as a slow variable in the similar way the BO approximation treats the internuclear distance. Thus we first solve the adiabatic equation with hyperradius R fixed to obtain adiabatic channel functions $\Phi_{\nu I}(R; \Omega)$ and adiabatic potential energies $U_{\nu I}(R)$. Here ν is the channel index and I is the absolute value of the projection of total angular momentum \mathbf{J} along the body-fixed z' axis, taken to be the axis between the core and positron. We solve this equation by using B-spline basis functions. Typically about 160 and 80 grid points are used for ϕ and θ , respectively. Special care was taken so that more grid points were distributed near the singularities of the Coulomb interactions among the three particles.

In the next step we solve the coupled hyperradial equations using a combination of the R -matrix propagation [21] and slow and smooth variable discretization (SVD) [22] techniques. The hyperradius range was divided into sectors and the SVD was used in each sector. The SVD has the advantage of avoiding the tedious calculations of the non-adiabatic couplings. It is therefore very suitable for the case when there are numerous avoided crossings in the potential curves. The R matrix is then propagated from one sector to the next up to a large hyperradius where the solutions are matched to the known asymptotic solutions to extract the scattering matrix. The calculations were carried out for each partial wave until a converged cross section is reached. We refer the reader to Liu *et al.* [12] for more details of the method.

III. RESULTS AND DISCUSSIONS

Before presenting the Ps-formation cross sections, we present calculations validating the present HSCC calculations at low energies.

A. Validations

The first few adiabatic potential curves for $J=0$ are shown in Fig. 1 for $e^+ - \text{Li}$ and in Fig. 2 for $e^+ - \text{Na}$. Note that there are no major apparent differences between the sets of curves

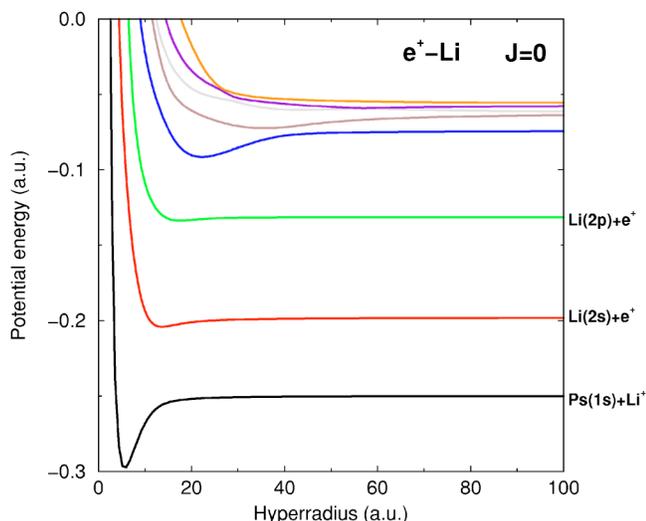


FIG. 1. (Color online) $J=0$ hyperspherical potential curves for the e^+ -Li system.

for these two alkali-metal atoms. Note that not shown are the curves corresponding to the forbidden core states, which are neglected throughout the HSCC calculations.

We examined the existence of bound states for both positronic lithium and positronic sodium. Table I shows the binding energies in a one-channel approximation which uses just the lowest potential curve in Figs. 1 and 2. These values are consistent with the one-channel results of Yuan *et al.* [10]. Table I also includes the binding energy resultant from a three-channel approximation, which improves the agreement with the latest stochastic variational method (SVM) and frozen-core SVM results by Mitroy and collaborators [11,23,24].

We have also calculated the s -wave scattering length for elastic Ps($1s$) scattering from both Li^+ and Na^+ , as it is very sensitive to the form of the potential. We first calculated the phase shifts, finding excellent visual agreement with the data

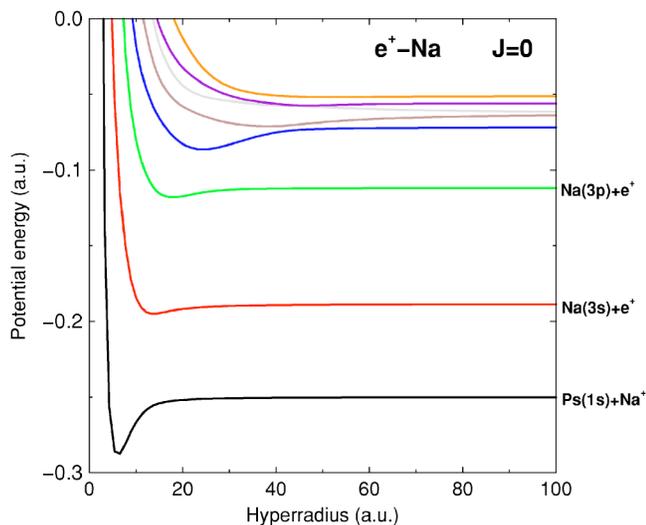


FIG. 2. (Color online) $J=0$ hyperspherical potential curves for the e^+ -Na system.

TABLE I. Theoretical binding energies ϵ of positronic lithium and positronic sodium [in units of millihartrees relative to the $\text{Ps}(1s)-\text{Li}^+$ and $\text{Ps}(1s)-\text{Na}^+$ dissociation threshold of $E=-0.25$ hartree]. The column ϵ_1 gives the single-channel results, while ϵ_3 gives the three-channel results. The column A gives the s -wave scattering length (in a_0) for elastic $\text{Ps}(1s)$ scattering from the two alkali-metal ions.

Model	ϵ_1	ϵ_3	A
Li present	2.04	2.47	13.1
Li YEML [10]	2.14		
Li SVM/FCSVM [24,25]	2.482		12.9
Na present	0.263	0.453	27.9
Na YEML [10]	0.255		
Na FCSVM [23,25]	0.473		28.5

of Mitroy and Ivanov [25], and use the same modified effective-range theory (MERT) [26] fitting to extract the scattering length A using

$$k \cot \delta(k) = -\frac{1}{A} + \frac{\alpha_d \pi k}{3A^2} + \frac{2\alpha_d k^2}{3A} \ln \frac{\alpha_d k^2}{16} + Bk^2 + Ck^3 + O(k^4), \quad (6)$$

where $k = \sqrt{2m_{red}E}$ is the momentum and $\alpha_d = 72a_0^3$ is the *effective* polarizability of $\text{Ps}(1s)$ [25] (determined from low-energy calculations of Ps -proton scattering [27]). The MERT is used instead of the effective-range theory because of the long-range polarization of the Ps atom interacting with the positive ion. From our phase shifts in the range $k = 0a_0^{-1} - 0.2a_0^{-1}$, we obtained the values of the scattering length shown in Table I. These compare very well with the results of Mitroy and Ivanov [25]. The computed s -wave phase shifts and the MERT fits are shown in Fig. 3 together with the data from Mitroy and Ivanov [25]. The fact that the HSCC and the independent SVM-based calculations agree so well in the low-energy region gives us confidence in the calculations we next present.

B. Positronium formation

To calculate the positronium formation cross sections for the e^+ -Li collision, we used up to 19 channels for $l=0$, 12 channels for $l=1$, 6 channels for $l=2$ and two channels for $l=3$. To obtain total positronium cross sections, partial waves up to $J=30$ have been calculated. For smaller energies few partial waves are needed. In fact, for energies below 1 eV, mainly $J \leq 5$ contribute. We match the solutions to the asymptotic solutions at different hyperradii at $R=200a_0$ and $R=400a_0$ to ensure the stability of the cross sections with respect to the matching radius.

In Fig. 4 we compare our Li results with the experimental data from Surdutovich *et al.* [4] as well as the theoretical results by Hewitt *et al.* [28] and McAlinden *et al.* [5]. The agreement among the theories and experiment is seen to be very good across the range of energies. The cross sections of the close-coupling calculations by Hewitt *et al.* [28] seem to

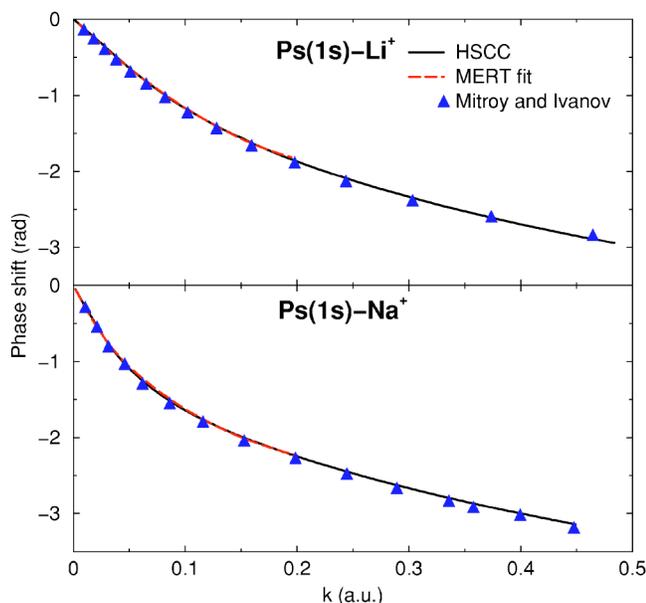


FIG. 3. (Color online) s -wave phase shifts for $\text{Ps}(1s)\text{-Li}^+$ (upper panel) and $\text{Ps}(1s)\text{-Na}^+$ (lower panel).

be a bit higher at low energies. This is probably due to the fact that their basis set was not large enough.

To obtain the positronium formation cross sections for the sodium case, we used up to 17 channels for $l=0$, 10 channels for $l=1$, 5 channels for $l=2$, and one channel for $l=3$. In Fig. 5 we show our results for the positronium formation cross sections together with the experimental data from Surdutovich *et al.* [4] as well as the theoretical results from recent close-coupling calculations. Our results agree very well with the two CC calculations by Ryzhikh and Mitroy [7] and Campbell *et al.* [2] for the whole range of energy considered. In other words, our calculations also do not reproduce the experimental data of Surdutovich *et al.* and our approach is

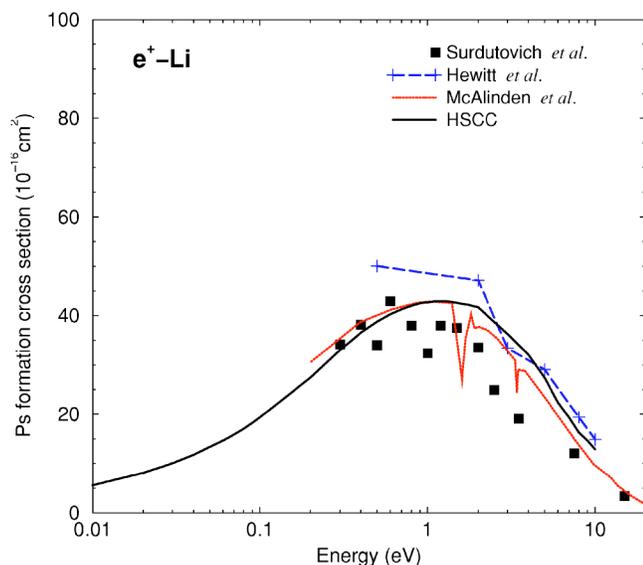


FIG. 4. (Color online) Ps formation cross sections for $e^+\text{-Li}$. The lower limits of the experimental results as given in [4] are shown.

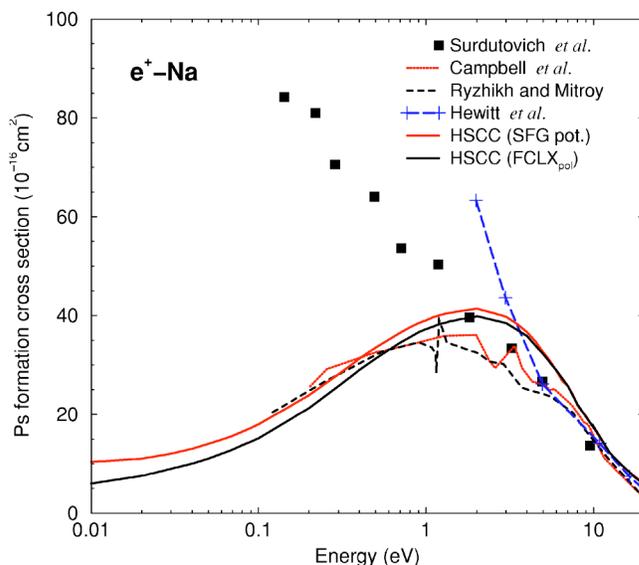


FIG. 5. (Color online) Ps formation cross sections for $e^+\text{-Na}$. The lower limits of the experimental results as given in [4] are shown.

rather different from these two other close-coupling calculations.

Our calculations have been checked with a smaller basis set, and we have convinced ourselves that the present cross sections are converged to better than 5% over the entire energy region presented. In particular, the convergence at smaller energies below 1 eV is much better, as the higher channels are not expected to contribute significantly.

Even though the calculation of Hewitt *et al.* [28] suggests that the cross section continues to rise with decreasing energies, these results are not supported by calculations with larger basis sets [2,7] and therefore should not be considered to be converged. Not shown in the figure are the results of Ke *et al.* [6] using the optical potential approach, where they predicted a dramatic increase of cross sections for energies below about 3 eV. This method employs some approximations which have not been justified nor tested for other systems, and thus their results should not currently be considered to support the experimental results.

To check the stability of the cross sections with respect to the model potential we slightly modified the cutoff ρ_c in Eq. (1) and found that the cross sections are indeed quite stable. Furthermore, we also employed the simple SFG model potential, as given by Eq. (3). The cross sections are plotted as the red solid curve in Fig. 5. For future reference, the SFG cross sections at energies of 0.1, 1, and 10 eV were $18.0 \times 10^{-16} \text{ cm}^2$, $39.1 \times 10^{-16} \text{ cm}^2$, and $17.3 \times 10^{-16} \text{ cm}^2$. Above 0.1 eV, the SFG results are within 20% of the FCLX_{pol} results. For collision energies higher than about 5 eV, the two calculations are almost identical, indicating that the potential details such as the exchange potential and dielectronic correction are not important for the Ps formation cross sections in that energy region. The differences between the two potentials become more pronounced as collision energy decreases. At 0.01 eV, the SFG cross section is about factor of 2 larger than the FCLX_{pol} result.

Based on these comparisons, it is clear that our results tend to support the conclusions from the close-coupling calculations and that the experimental results showing an increase at lower collision energies below 1 eV for e^+ +Na cannot be reproduced by any current elaborate calculations. It appears that further experiments are needed to resolve the discrepancy for this system.

IV. SUMMARY AND CONCLUSIONS

We have presented the results of hyperspherical close-coupling calculations for the positron-lithium and positron-sodium collisions at low energies. A large number of channels and high partial waves were included to ensure the convergence of the cross sections. For the positronium formation cross sections, we found good agreement with recent theoretical calculations for both lithium and sodium systems across the energy range from about 0.1 eV to 20 eV. Whereas the agreement with the available experimental data is very good for e^+ -Li and for e^+ -Na at energies above about 1 eV, it is unsatisfactory for e^+ -Na at the lower energies.

The binding energies of e^+ Li and e^+ Na as well as the s-wave scattering lengths for Ps(1s)-Li⁺ and Ps(1s)-Na⁺

interactions have also been calculated using the present HSCC method and they are in agreement with other elaborate theoretical calculations. This supports our conclusion that the model potential used in the present calculation is adequate and that the positronium formation cross sections we obtained at low energies should be reliable. Note that the present HSCC calculations are expected to be more accurate for lower energies. Further positron-sodium experiments in the difficult low-energy region appear to be needed to resolve the discrepancy.

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