Positronium–alkali-ion scattering in the close-coupling approximation

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We present results for low- and medium-energy elastic and capture cross sections for positronium-atom–alkali-ion scattering using the coupled static close-coupling approximation.

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I. INTRODUCTION

We study low- and medium-energy positronium–alkali-ion scattering in the coupled-static close-coupling approximation (CCA). In particular, we study the Ps-proton, Ps-Li^+, and Ps-Na^+ scattering, where Ps stands for the positronium atom. These systems are effective three-particle systems with some unique interesting properties, which makes this study of general theoretical interest. The Born term for the elastic scattering in the CCA vanishes and the static elastic cross section is identically zero. The Ps-Li^+ and Ps-Na^+ systems are rearrangements of the positron-Li and positron-Na systems. However, the elastic Ps-Li^+ and Ps-Na^+ thresholds are lower than the elastic positron-Li and positron-Na thresholds. Hence the study of the elastic Ps-Li^+ and Ps-Na^+ scattering below the elastic positron-Li and positron-Na thresholds should yield information on these systems in a energy region not accessible by the elastic positron-Li and positron-Na processes.

To a first approximation, the alkali atoms are treated as a single-active-electron atom where the unique electron outside the closed shell is considered to be dynamically active, as this electron could be easily extracted to participate in ionization and Ps formation. The identities of the closed-shell electrons are easily taken into consideration, but they are considered to be dynamically inactive and do not participate in ionization or Ps formation. The alkali ions are singly charged positive ions with closed-shell electrons. In this model the Born term for the elastic positronium–alkali-ion scattering is zero and this scattering proceeds via coupling to the other channel(s). Such a study should reveal the effect of coupling to the rearrangement channel. Being a very heavy particle, the proton or the alkali ion is considered fixed in the center-of-mass frame, which significantly simplifies the mathematical treatment.

Electrons, positrons, and neutral atoms and molecules are often used as a probe of solid surfaces. Neutral atoms and molecules like He and H_2 interact mainly with surface atoms, but the available low-energy beams of few MeV are not energetic enough to probe small scale surface structure. Because of the smaller mass of the Ps atom it has a much larger velocity than an ordinary atom for a given energy. Hence Ps atoms will interact more intimately with various forms of matter than heavier atoms and molecules, ranging from electrons, protons, and alkali ions, to atoms, molecules, solid surfaces, and plasmas and will provide important information about the target medium [1,2]. So the Ps atom is now considered to be a better probe of matter than the usual neutral atoms. Scattering involving Ps atoms, as in the present article, should reveal the interaction of Ps atoms with matter, which should be of value in probing solid surfaces. Also, with the recent availability of the monoenergetic positronium beam [1,2], Ps-atom scattering seems feasible in the future, which will make this study of interest to experimentalists too. The possibility of studying ionic crystals of alkali atoms by a Ps-atom beam has been considered in Ref. [1]. In such a study free Ps-Li^+ and Ps-Na^+ scattering, as considered in this paper, should play a vital role.

The CCA provides a practical framework for dealing with electron-atom and positron-atom scattering. It deals with rearrangement and elastic channels in a unified way and provides results for elastic and rearrangement cross sections. This approach has been frequently used in e^+-H and other positron-atom scattering problems [3–11]. We shall use the following basis sets in the present study: Ps($1s$)+H($1s$) (Ps-proton), Ps($1s$)+Li($2s$) (Ps-Li^+), and Ps($1s$)+Na($3s$) (Ps-Na^+).

In the present treatment, instead of the coupled integro-differential equations we consider the equivalent coupled Lippmann-Schwinger-type integral equations of the CCA. We report here S-, P-, D-, and F-wave elastic and rearrangement cross sections for Ps-proton, Ps-Li^+, and Ps-Na^+ scattering. The rearrangement transitions lead to e^+-H, e^+-Li, and e^+-Na in the final states, respectively. We also report the partial wave summed total cross sections for Ps-proton, Ps-Li^+, and Ps-Na^+ scattering. We present the CCA equations in Sec. II, and the numerical results in Sec. III.

II. CCA EQUATIONS

In the following we give the details of the e^+-Li ($\rightarrow$Ps-Li^+) equations we use. In the case of e^+-H ($\rightarrow$Ps-H^+) and e^+-Na ($\rightarrow$ Ps-Na^+) scattering the equations can be similarly written down. In the CCA the total wave function for the e^+-Li (Ps-Li^+) system is written as [3,6–8]

$$\Psi(\vec{r}_1,\vec{r}_2,\vec{r}_3,\vec{x}) = \sum_i \Phi_i(\vec{r}_1,\vec{r}_2,\vec{r}_3) F_i(\vec{x}) + \sum_\nu \Phi^+_{1s}(\vec{r}_1,\vec{r}_2)\,\eta_\nu(\rho) G_\nu(\vec{R}), \quad (1)$$

with

$$\rho=|\vec{x}-\vec{r}_3|, \quad R=|\vec{r}_3+\vec{x}|/2, \tag{2}$$

where $\vec{r}_i$ $(i=1,2,3)$ are the coordinates of the atomic electrons and $\vec{x}$ is the positron coordinate. Here $\Phi_i(\vec{r}_1,\vec{r}_2,\vec{r}_3)$ and $\eta_\nu(\vec{\rho})$ are the ith and νth eigenstates of the lithium and the Ps-atom systems, respectively. The ground-state wave function of the lithium ion is described by $\Phi^+_{1s}(\vec{r}_1,\vec{r}_2)$, $F_i(\vec{x})$ describes the motion of the incident positron, and $G_\nu(\vec{R})$ describes the relative motion between the positronium and the lithium ions. In our treatment we include only one term in each sum of Eq. (1), e.g., the ground states of both lithium and Ps atoms. The CCA calculation involving one term in each sum of expansion (1) is termed coupled static.

The coupled scattering integral Lippmann-Schwinger-type equations of the CCA are written as

$$f_{\beta\alpha}(\vec{k}',\vec{k})=f^B_{\beta\alpha}(\vec{k}',\vec{k})-\frac{1}{4\pi^2\mu_\nu}\sum_\nu \times\int_0^\infty d\vec{k}''\frac{f^B_{\beta\nu}(\vec{k}',\vec{k}'')f_{\nu\alpha}(\vec{k}'',\vec{k})}{E_\nu+i0-E''}. \tag{3}$$

Here $f_{\beta\alpha}(\vec{k}',\vec{k})$ is the scattering amplitude for the transition from channel α to channel β, $\vec{k}$ and $\vec{k}'$ are the relevant relative momenta in these channels, μ_ν is the reduced mass in channel ν, and $f^B_{\beta\alpha}(\vec{k}',\vec{k})$ is the corresponding Born amplitude. The partial wave expansion of $f_{\beta\alpha}(\vec{k}',\vec{k})$ from the initial state $|nlm\rangle$ of the target atom to the final state $\langle n'l'm'|$ of the target atom is given by

$$f_{\beta\alpha}(\vec{k}',\vec{k})=\frac{1}{(kk')^{1/2}}\sum_{JM}\sum_{L,M_L}\sum_{L',M_{L'}}\langle L'l'M_{L'}m'|JM\rangle \times\langle LlM_Lm|JM\rangle \times T^J_{\beta\alpha}(\tau'k',\tau k)Y^*_{L'M_{L'}}(\hat{k}')Y_{LM_L}(\hat{k}), \tag{4}$$

where L and M_L are the orbital angular momentum and projection of the incident projectile state, n, l, and m are the principal quantum number, orbital angular momentum, and projection of the initial target-atom state, J and M are the total angular momentum and projection, and $\langle LlM_Lm|JM\rangle$ is the usual Clebsch-Gordan coefficient. The primed variables refer to the final state. A similar partial wave expansion holds for the Born term. Also, τ stands for the collective quantum numbers (n,l,m).

After partial wave analysis the coupled integral equations have the following form:

$$T_{\beta\alpha}(p_\beta,k_\alpha)=B_{\beta\alpha}(p_\beta,k_\alpha)+1/(2\pi^2)\sum_\nu \times\int_0^\infty q_\nu^2 dq_\nu B_{\beta\nu}(p_\beta,q_\nu) \times(q_\nu^2-k_\nu^2-i0)^{-1}T_{\nu\alpha}(q_\nu,k_\alpha). \tag{5}$$

In this equation $B_{\beta\alpha}$ is the partial wave projection of the CCA Born term. The channel subscripts α, β, etc., are supposed to contain information about the atomic states involved and from now on the J and τ indices are dropped for simplicity. The variables k_ν, etc., are on-shell wave numbers for channel ν.

The lithium atom wave function is given by

$$\Phi_{2s}(\vec{r}_1,\vec{r}_2,\vec{r}_3)=u_{1s}(\vec{r}_1)u_{1s}(\vec{r}_2)u_{2s}(\vec{r}_3), \tag{6}$$

where the atomic orbitals for the $1s$ and the $2s$ electrons are given by

$$u_{ns}(\vec{r})=\sum_{i=1}^{6} a_i(ns)r^{(m_i-1)}e^{-\lambda_i r}Y_{00}(\hat{r}). \tag{7}$$

The lithium-ion wave function is taken to be given by

$$\Phi_{\mathrm{Li}^+}(\vec{r}_1,\vec{r}_2)=u^+_{1s}(\vec{r}_1)u^+_{1s}(\vec{r}_2), \tag{8}$$

where the atomic orbitals are given by

$$u^+_{1s}(\vec{r})=\sum_{i=1}^{4} a^+_i(1s)e^{-\lambda_i r}Y_{00}(\hat{r}). \tag{9}$$

The constants for this wave function are taken from Ref. [12]. In the case of Na the atomic wave function is taken to be that of a hydrogenlike atom with only one electron in the $3s$ state given by

$$u_{3s}(r)=\frac{1}{\sqrt{(4\pi)}}\sum_{i=1}^{8} c_i(3s)r^{(m_i-1)}e^{-\lambda_i r}. \tag{10}$$

The constants of the wave functions are taken from Ref. [12].

III. NUMERICAL RESULTS

The CCA integral equations were solved by standard numerical techniques [13]. We calculated the elastic and rear-

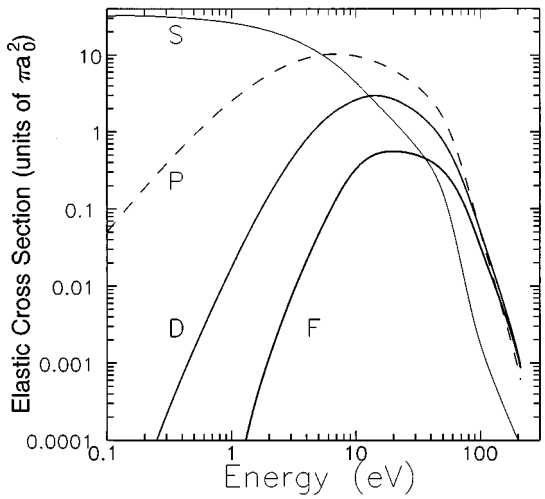

FIG. 1. S-, P-, D-, and F-wave elastic Ps-proton scattering cross sections, denoted, respectively, by S, P, D, and F, in units of πa_0^2 versus incident Ps-atom energies.

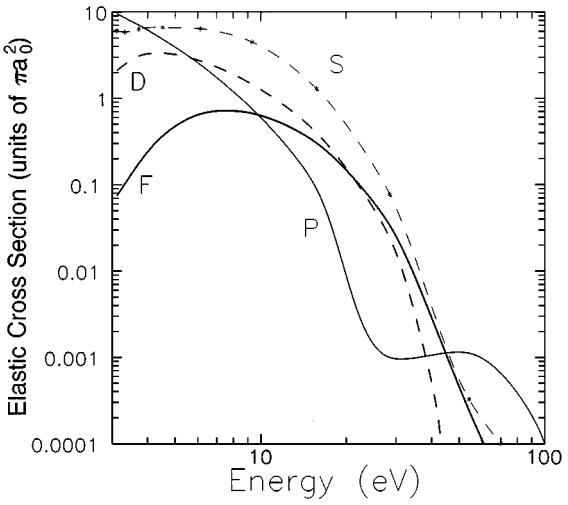

FIG. 2. Same as Fig. 1 for the Ps-Li^+ system.

rangement cross sections in different partial waves for Ps-proton, Ps-Li^+, and Ps-Na^+ systems at low and medium energies. We also calculated in each case the capture cross sections for the present and reverse rearrangement processes Ps-proton$\rightarrow e^+$-H and e^+-H$\rightarrow$Ps-proton, Ps-$Li^+\rightarrow e^+$-Li and e^+-Li$\rightarrow$Ps-Li, and Ps-$Na^+\rightarrow e^+$-Na and e^+-Na$\rightarrow$Ps-Na. The underlying t matrices in these two cases were related by time-reversal invariance. In each partial wave such cross sections are related by

$$k_\alpha^2 \sigma_{\alpha\beta} = k_\beta^2 \sigma_{\beta\alpha},$$

where σ represents the partial wave cross section. In numerical calculations this identity was verified to an estimated error of less than 1%. This valuable check assures us of the numerical accuracy of the method, since different t matrix sets were used for the two cross sections.

Of the three problems commented on above the Ps-proton system deserves special mention. Many accurate calculations have been performed for the positron-hydrogen [14] and Ps-

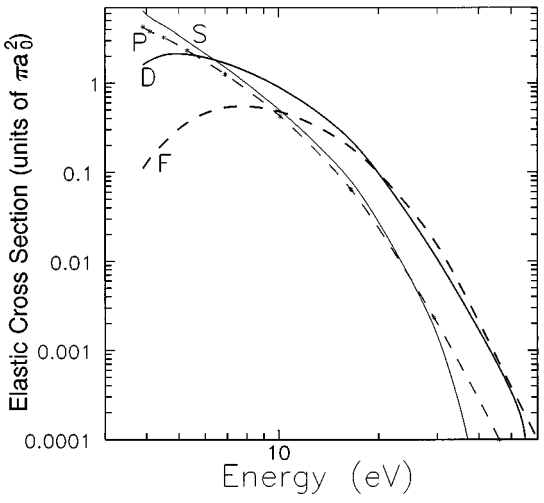

FIG. 3. Same as Fig. 1 for the Ps-Na^+ system.

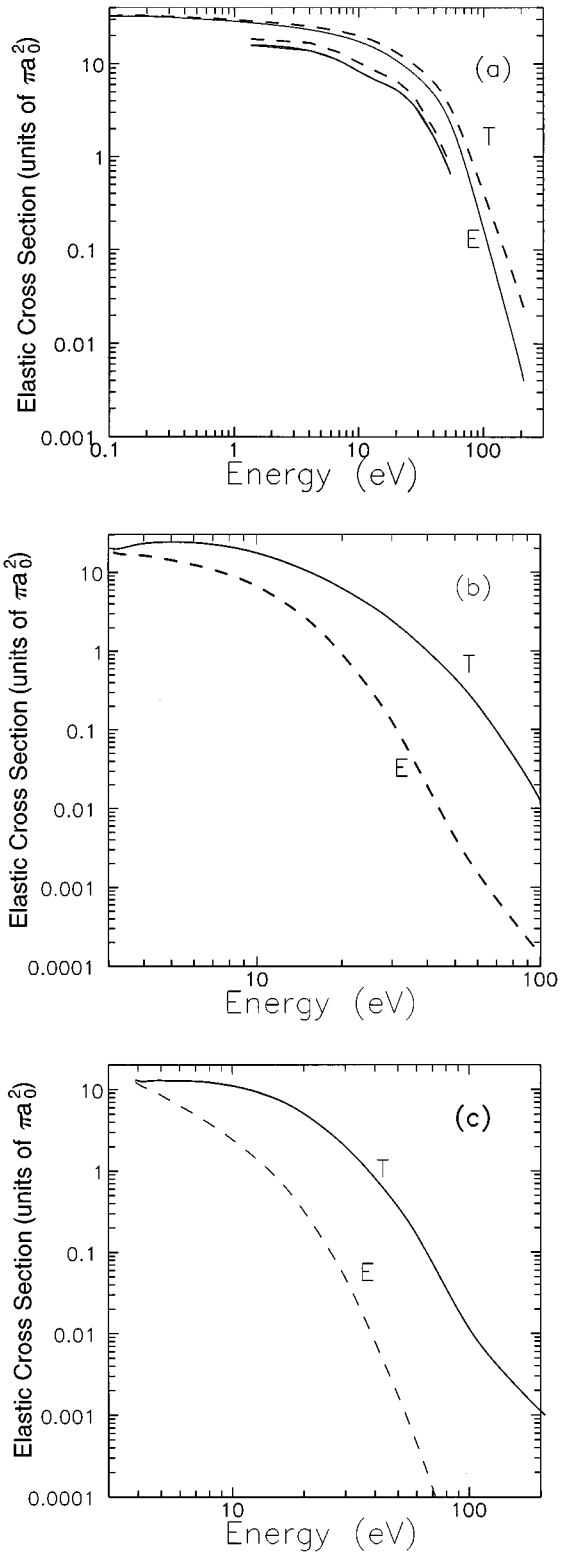

FIG. 4. Partial wave summed elastic (full line denoted E) and total [dashed line denoted T (=elastic+capture)] cross sections in units of πa_0^2 for (a) Ps-proton, (b) Ps-Li^+, and (c) Ps-Na^+ systems at different incident Ps-atom energies. In (a) the short curves are results of elastic (full line) and total [elastic + capture to the H(1s) state denoted by dashed line] cross sections of a six-state CCA calculation taken from Ref. [15].

proton [15] systems. These calculations should serve as the testing ground for approximation schemes. In the present study we are interested in the scattering of Ps-Li^+ and Ps-Na^+ systems using the coupled-static CCA scheme. A more accurate calculation in this case seems to be complicated at present, so one can naturally question the reliability of the present approximation scheme. In order to check the usefulness of the coupled-static CCA scheme in studying the elastic and rearrangement scattering, we have compared below the present results for the Ps-proton system with the six-state CCA calculation [15] and find the present results to be in good qualitative agreement with results of Ref. [15]. Also, in positron-hydrogen scattering [14] the coupled-static CCA model provides a good description of elastic scattering. These checks in the Ps-proton and positron-hydrogen scattering give us confidence in the reliability of the present coupled-static study of Ps-Li^+ and Ps-Na^+ scattering, where it is much more difficult to obtain an improved calculation.

First, we exhibit the results of elastic scatterings for S, P, D, and F partial waves in Figs. 1–3. The partial wave summed elastic and total (elastic+capture) cross sections for these systems are plotted in Figs. 4(a)–4(c), respectively. In Fig. 4(a) we have also plotted the results for elastic and total [elastic+capture to H(1s) state] cross sections of Mitroy and Stelbovics using a six-state CCA [15] scheme and their result is in qualitative agreement with ours. The short curves in this figure are from Ref. [15].

From Figs. 1–3 we can see that at very low incident Ps-atom energies ($E<1$ eV) the partial wave cross section decreases as the angular momentum increases for all three systems. At intermediate energies there is no definite relation between cross sections of different partial waves. For each system we have a different trend, as can be seen from Figs. 1–3. In the case of Ps-proton and Ps-Li^+ systems the partial wave elastic cross sections are of the same order of magnitude, whereas in the case of the Ps-Na^+ system it is smaller.

From Fig. 4 we can find that in the case of Ps-proton the capture cross section represented by (Ps+proton $\rightarrow$positron+H) is very small; the capture cross section is the difference between two curves labeled T and E. In the cases of Ps-Li^+ and Ps-Na^+ systems this difference is larger and so are the capture cross sections represented by (Ps+Li^+ $\rightarrow$positron+Li) and (Ps+$Na^+\rightarrow$positron+Na), respectively.

In summary, we report results for the coupled-static CCA calculation for scattering between Ps atom and alkali ions. We present results for partial wave elastic cross sections for Ps-proton, Ps-Li^+, and Ps-Na^+ scattering at various incident-Ps-atom energies. We also present results for total elastic and capture cross sections for these three systems.

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