PHYSICAL REVIEW A, VOLUME 61, 012502

S-, *P*-, and *D*-wave resonances in positronium–lithium-atom scattering

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(Received 27 October 1998; revised manuscript received 5 May 1999; published 8 December 1999)

We investigate ortho-positronium–lithium-atom (Ps-Li) scattering using static-exchange and three-Ps-state coupled-channel calculations. The present three-Ps-state scheme, while closely agreeing with the resonance and binding energies in the Ps-H system, predicts *S*-, *P*-, and *D*-wave resonances at 4.25 eV, 4.9 eV, and,,, 5.25 eV, respectively, in the electronic spin-singlet channel of Ps-Li scattering. The present calculation also yields a Ps-Li binding in this attractive singlet channel with an approximate binding energy of 0.218 eV, which is in adherence with the recent findings of a chemically stable PsLi system using stocastic variational and quantum Monte Carlo calculations. We further report elastic, Ps$(2s)$-, and Ps$(2p)$-excitation cross sections at low to medium energies (0.068–30 eV).

PACS number(s): 36.10.Dr

Positronium (Ps), having an internal charge and mass symmetry, is believed to be capable of providing interesting and new dynamical information from its scattering with matter after the fundamental electron and positron impact studies [1]. Positronium-beam studies now play an important role in the domain of both physics and chemistry and especially in the study of condensed-matter physics and surface physics [2,3]. The neutral character of Ps and the intimate interaction affinity of its positron with matter make it attractive as a probe. However, to have a reliable conclusion of these studies one needs to have a fair understanding of the positron and positronium interaction dynamics with the atomic species including the resonance behavior [4–7] and the formation of Ps or Ps-target bound states [6–18], respectively.

Among positronium impact studies, Ps-H is the mostly visited system that is found to form resonance [4–7] in the *S*-wave singlet channel of two electrons (of Ps and of H) and form a chemically stable positronium hydride (PsH) bound state [6–10,13,14,16]. The resonance formation in Ps-H has been interpreted, by Drachman [8], as a consequence of the attachment of the Rydberg states of the positron to the singlet H^- ion. Recently, *P*- and *D*-wave resonances have also been reported [6] in the singlet channel of Ps-H scattering, in addition to the *S*-wave resonance reported earlier in several calculations [4,5]. On the other hand, the next highly visited system is Ps-He [19–22], where the attractive electronic spin-singlet scattering channel does not exist and no resonance or binding aspect has been reported in this closed-shell atom [23] and also in Ne and Ar [24]. After hydrogen, the next open-shell atom is lithium. In recent studies, using stochastic variational and quantum Monte Carlo calculations, lithium is reported to form a bound state with Ps [11,12,15,17]. Also there are other calculations as well in the Ps-Li system [25,26] investigating its chemical stability. The existing singlet or triplet channel of the four electrons of the ortho-Ps$(1s)$–Li$(1s^2 2s)$ system basically corresponds to the singlet or triplet channel of the pair containing the valence electron of lithium and the electron of Ps, since the core of Li$(1s^2 2s)$ is in a singlet state. In that sense the dynamics of the ortho-Ps-Li scattering could bear close resemblance to the Ps-H case and could lead to resonance and binding features in the attractive singlet channel of four electrons (one of Ps and three of Li). We devote the present work to study the binding and the possibility of associated resonances of the ortho-Ps-Li system employing a coupled channel formalism in the framework of the momentum-space Lippmann-Schwinger equation.

In the calculations for ortho-Ps scattering from a hydrogen atom, the resonance is found to be manifested with the inclusion of Ps-excitation channels in a coupling scheme [6,7]. It is also found that no resonance appears in a coupled-channel calculational scheme with the target excitation channels taken as a basis set [7,27]; nor are the resonances get destroyed with the addition of target-excitation channels in the Ps-state coupling scheme [7]. However, the inclusion of target excitation channels in the Ps-state expansion scheme has been found to improve the Ps-H binding energy by about 7–8 %, and their effect on the resonance position and low-energy elastic cross section is not very significant compared to the inclusion of Ps-excitation channels [7]. This is quite a reasonable feature owing to the high polarizability of $36a_0^3$ for the Ps atom. The recent finding of a correlation between resonance and binding energies in PsH using coupled-channel Lippmann-Schwinger equations with model exchange [7] and the consistency of these results with the measurements and variational predictions on resonance and binding energies prompts us to visit the Ps-Li system for a similar study of resonance and binding and the scattering dynamics.

The Ps-Li scattering has the most complications of a many-body problem, but few-body techniques can be employed for its solution. As already mentioned in previous works [6,7,22,24,28,29], the underlying charge and mass symmetry of the Ps atom renders the elastic and all even-parity state Ps-excitation channel potentials zero and reinforces the exchange interaction to play a predominant role in its low-energy scattering from a neutral target. Nevertheless, polarizability of Ps is very high $(36a_0^3)$ and it is of crucial importance to include Ps-excitation channels in any of its calculational schemes to get a reliable prediction. We address the present work to study the resonances and binding in the electronic singlet channel of the ortho-Ps-Li system. Also, we focus our attention on whether the shifting of the binding energy towards a lower value, with the growing size of the target from hydrogen to lithium, associates with any shifting of the *S*-wave singlet resonance position or not. In the present work we restrict ourselves to target elastic processes, keeping the target frozen to its initial state, and we employ static-exchange and three-Ps-state models. This truncation of the expansion scheme, which can be justified from the vulnerability of Ps to excitation and our present motivation of addressing the possible resonances in Ps-Li and its possible correlation with the binding aspect, it should be extended in the future with the inclusion of target excitation channels for a precise determination of the medium energy total cross section, binding energy, and scattering length.

In general, expanding the Ps-Li system wave function with respect to the Ps(χ_ν) and Li(ϕ_μ) states, and antisymmetrizing it with respect to the Ps and target electron coordinates, we represent the total wave function as [6]

$$\begin{aligned}\Psi^{\pm}=\sum_{\nu}\sum_{\mu}\{&F_{\nu\mu}(\boldsymbol{\rho}_4)\chi_\nu(\mathbf{t}_4)\phi_\mu(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\\&+(-1)^{S_{41}}F_{\nu\mu}(\boldsymbol{\rho}_1)\chi_\nu(\mathbf{t}_1)\phi_\mu(\mathbf{r}_4,\mathbf{r}_2,\mathbf{r}_3)\\&+(-1)^{S_{42}}F_{\nu\mu}(\boldsymbol{\rho}_2)\chi_\nu(\mathbf{t}_2)\phi_\mu(\mathbf{r}_1,\mathbf{r}_4,\mathbf{r}_3)\}\\&+(-1)^{S_{43}}F_{\nu\mu}(\boldsymbol{\rho}_3)\chi_\nu(\mathbf{t}_3)\phi_\mu(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_4),\end{aligned}$$

where $\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3$ are the electron coordinates of the lithium and $\mathbf{x},\mathbf{r}_4$ are the coordinates of the positron and electron of the Ps atom. Indices S_{4j}, $j=1,2,3$, represent the total spin of the pair of electrons $\mathbf{r}_4$ and $\mathbf{r}_j$ and $\mathbf{t}_i=\mathbf{x}-\mathbf{r}_i$, $\boldsymbol{\rho}_i=(\mathbf{x}+\mathbf{r}_i)/2$. The spin of the positron will conserve separately and the electron exchange profile of the Ps-Li system corresponds exactly to the $e^- -$Li system. In the above expression, spin parts of the wave function are not explicitly shown.

Averaging over spin-states, we recast the time-independent Schrödinger equation into the following momentum-space Lippmann-Schwinger (LS) scattering integral equation [30]:

$$\begin{aligned}f^{\pm}_{\nu'\mu',\nu\mu}&(\mathbf{k}_f,\mathbf{k}_i)\\&=B^{\pm}_{\nu'\mu',\nu\mu}(\mathbf{k}_f,\mathbf{k}_i)-\frac{1}{2\pi^2}\sum_{\nu''}\sum_{\mu''}\\&\quad\times\int d\mathbf{k}''\frac{B^{\pm}_{\nu'\mu',\nu''\mu''}(\mathbf{k}_f,\mathbf{k}'')f^{\pm}_{\nu''\mu'',\nu\mu}(\mathbf{k}'',\mathbf{k}_i)}{k^2_{\nu''\mu''}-k''^2+\mathrm{i}0},\end{aligned}\tag{1}$$

where $f^{\pm}$ represent the singlet (+) and triplet (−) amplitudes corresponding to the four-electron Ps-Li system. $k^2_{\nu''\mu''}=2m/\hbar^2(E-\epsilon_{\nu''}-\Upsilon_{\mu''})$ with $\epsilon_{\nu''}$ and $\Upsilon_{\mu''}$ are the binding energies of the intermediate Ps and Li states; *m* is the reduced mass of Ps and *E* is the total energy of the system. As the core of the lithium ground state is in a singlet state and we are not considering any excitation of Li, the four-electron system could be either in a singlet or in a triplet state depending on whether the pair containing the Ps electron and the valance electron of Li is in a singlet or triplet state, respectively. In the summation over final spin states, the two-electron singlet-state exchange terms of the Ps electron with any core electron leading to the core excitation of Li are excluded as the lithium excitation will not be considered in this calculation. To analyze the effect of the core, for this neutral Ps projectile, we also present results for the 3-Ps-state model where the exchange with the core, which is a purely repulsive potential here in the absence of any target excitation (exchange between like spins), is neglected. This will give an estimation of the effect of the core in the binding and resonance feature. In the above equation, $B^{\pm}$ are the potentials for the singlet (+) and triplet (−) channels, respectively. The direct amplitudes of this equation are exactly the Born amplitudes given by

$$\begin{aligned}B^{D}_{\nu'\mu',\nu\mu}(\mathbf{k}_f,\mathbf{k}_i)=-\frac{1}{\pi}\int&d\mathbf{r}_1d\mathbf{r}_2d\mathbf{r}_3d\mathbf{r}_4d\mathbf{x}\,e^{-i\mathbf{k}_f\cdot\boldsymbol{\rho}_4}\\&\times\chi^*_{\nu'}(\mathbf{t}_4)\phi^*_{\mu'}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)V_{\text{int}}\\&\times\chi_\nu(\mathbf{t}_4)\phi_\mu(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)e^{i\mathbf{k}_i\cdot\boldsymbol{\rho}_4}.\end{aligned}\tag{2}$$

In the present case we shall not consider excitation of lithium, and both the indices μ and μ' would correspond to the Li($1s\,^22s$) ground state; V_{int} is the Coulomb interactions between Ps and Li and is given by

$$V_{\text{int}}=\frac{1}{x}-\sum_{j=1}^{3}\frac{1}{|\mathbf{x}-\mathbf{r}_j|}-\frac{1}{r_4}+\sum_{j=1}^{3}\frac{1}{r_{4j}},$$

where $\mathbf{r}_{4j}=\mathbf{r}_4-\mathbf{r}_j$ and the total Hamiltonian is given by

$$H=H_{\text{Ps}}+H_{\text{Li}}+V_{\text{int}}.$$

Changing the set of variables $\{\mathbf{x},\mathbf{r}_4\}$ to $\{\boldsymbol{\rho}_4,\mathbf{t}_4\}$ and integrating the Born amplitude over $\boldsymbol{\rho}_4$, we can rewrite it as [31,32]

$$\begin{aligned}B^{D}_{\nu'\mu',\nu\mu}(\mathbf{k}_f,\mathbf{k}_i)=\frac{4}{q^2}\langle\phi_{\mu'}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)|&3\\&-\sum_{j=1}^{3}e^{i\mathbf{q}\cdot\mathbf{r}_j}|\phi_\mu(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\rangle\\&\times\langle\chi_{\nu'}(\mathbf{t}_4)|e^{i\mathbf{q}\cdot\mathbf{t}_4/2}-e^{-i\mathbf{q}\cdot\mathbf{t}_4/2}|\chi_\nu(\mathbf{t}_4)\rangle,\end{aligned}\tag{3}$$

where $\mathbf{k}_i,\mathbf{k}_f$ are the initial and final momentum of the Ps atom with respect to the center of mass, which is fixed at the lithium nucleus, and $\mathbf{q}=\mathbf{k}_i-\mathbf{k}_f$. In the lowest-order approximation of static exchange, B^D becomes exactly zero, as can be verified from the Ps-form factor of the above equation, and the LS equation is solely governed by the nonorthogonal exchange kernel. B^D becomes also zero for other even-parity transitions ($\nu'\leftarrow\nu$) of Ps and the solution of the above LS equation becomes very slowly convergent with respect to the addition of channels due to the dominance of the nonorthogonal exchange kernel or the short-range exchange force. We overcome this situation by introducing a model exchange potential in the *ab initio* framework of CCA. In general, the model potential for a particular exchange term where the Ps electron ($\mathbf{r}_4$) undergoes exchange with a target electron ($\mathbf{r}_j$), say $\mathbf{r}_3$, is derived from

$$g^{E(3)}_{\nu'\mu',\nu\mu}(\mathbf{k}_f,\mathbf{k}_i)=-\frac{1}{\pi}\int d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3 d\mathbf{r}_4 d\mathbf{x}\, e^{-i\mathbf{k}_f\cdot\boldsymbol{\rho}_3} \times\chi^*_{\nu'}(\mathbf{t}_3)\phi^*_{\mu'}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_4)\frac{1}{\mathbf{r}_{43}} \times\chi_\nu(\mathbf{t}_4)\phi_\mu(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)e^{i\mathbf{k}_i\cdot\boldsymbol{\rho}_4}. \tag{4}$$

The development of a nonlocal model exchange potential from the above expression has been elaborated in Ref. [22], and here we quote the final result for such a term leading to a general exchange between $\mathbf{r}_4$ and $\mathbf{r}_j$:

$$B^{E(j)}_{\nu'\mu',\nu\mu}(\mathbf{k}_f,\mathbf{k}_i)=\frac{4(-1)^{l+l'}}{Q_j^2} \times\langle\phi_{\mu'}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)|e^{i\mathbf{q}\cdot\mathbf{r}_j}|\phi_\mu(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\rangle \times\langle\chi_{\nu'}(\mathbf{t}_j)|e^{i\mathbf{q}\cdot\mathbf{t}_j/2}|\chi_\nu(\mathbf{t}_j)\rangle, \tag{5}$$

where $Q_j^2=(k_f^2+k_i^2)/8+C^2\{[\alpha^2_{\mu'}(j)+\alpha^2_\mu(j)]/2+(\beta^2_{\nu'}+\beta^2_\nu)/2\}$. Superfix $j=1,2,3$ runs over target electrons. Indices l and l' are the orbital angular momenta of the initial and final Ps states. Expressions $\alpha^2_\mu(j)/2$, $\alpha^2_{\mu'}(j)/2$ represent the binding energies of the μth and μ'th slater orbital of the jth target electron in atomic units, respectively; $\mu(\mu')$ corresponds to quantum states. Expressions β^2_ν, $\beta^2_{\nu'}$ are the binding energies of the initial and final Ps states in atomic units (a.u.), respectively. C is the only parameter of the model exchange potential which is normally equal to 1 and can be varied from unity to yield a precise fitting of any low-energy scattering parameter. In the present case of Ps-Li scattering, we keep the normal value of $C=1$ as there were no precise low-energy scattering data available for the system until the submission of this work.

We use exact wave function for the Ps atom and for lithium we use the Hartree-Fock wave functions of Clementi and Roetti [33]. After a partial-wave decomposition of the three-dimensional LS equation, the coupled equations for the singlet and triplet channels are solved by the method of matrix inversion [30]. The maximum number of partial waves included in the calculation is eighteen ($L=0\rightarrow17$). A contribution of higher partial waves to the cross sections was included by corresponding partial wave Born terms. It should be mentioned here that the convergence of the results with respect to partial wave contributions is very slow compared to the corresponding Ps-H case. For example, at 0.068 eV, the lowest energy considered, the Ps-H system result converges up to the fourth significant digit with a contribution from only one partial wave ($L=0$), whereas for the Ps-Li system it requires two partial waves ($L=0,1$) to achieve the same level of convergence. At 30 eV, the Ps-H results converge up to the fourth significant digit with $L_{\max}=11$, whereas for the present Ps-Li case, the same level of convergence requires $L_{\max}=18$.

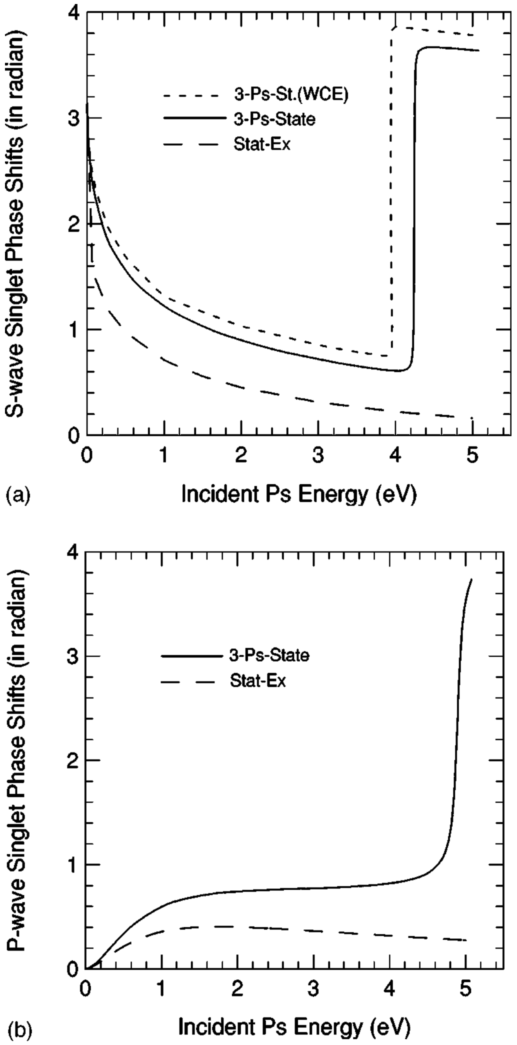

FIG. 1. *S*- and *P*-wave singlet phase shifts (in radians) versus incident Ps energy (in eV). The jump in the phase shift by π radian at Ps energy of 4.25 eV and 3.95 eV (a) and at 4.9 eV (b) corresponds to Ps-Li resonances for the *S*- and *P*-wave scatterings, respectively. Stat-Ex stands for static exchange; WCE stands for without core exchange.

First we analyze the phase shifts for resonances and binding aspects. In Figs. 1(a) and 1(b), we display the present *S*- and *P*-wave singlet phase shifts for Ps-Li using static-exchange and 3-Ps-state models. As anticipated, from the very similarity of the Ps-Li system with the Ps-H system, resonances appear in both the *S*- and *P*-wave phase shifts for the 3-Ps-state model. In Fig. 1(a) we also plot the *S*-wave singlet phase shift for the 3-Ps-state model where the repulsive exchange term with the core is dropped from the scheme. This shifts the resonance position to lower energies of 3.95 eV and we shall see in the next paragraph that it simultaneously shifts the binding energy towards higher values (more negative value). Compared to the nature of the corresponding resonances in Ps-H scattering, present *S*-wave resonance in Ps-Li is very sharp. The *P*-wave resonance is less sharp compared to the *S*-wave one. We also obtain a *D*-wave resonance but this is more diffused, as in the case of the Ps-H system [6]. So, we plot the corresponding singlet

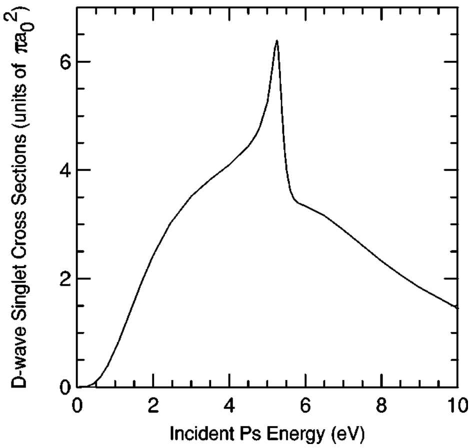

FIG. 2. *D*-wave singlet cross sections (in units of πa_0^2) versus incident Ps energy (in eV). The jump in the cross section around 5.25 eV corresponds to resonance in the *D*-wave Ps-Li scattering.

cross section in Fig. 2. The sharp structure in the cross section around 5.2 eV corresponds to the resonant behavior of the *D*-wave phase shifts. The *S*-, *P*-, and *D*-wave resonances are found at 4.25 eV, 4.90 eV, and 5.25 eV, respectively. The accurate *S*-wave resonance position in Ps-H is at 4.01 eV and the newly reported *P*- and *D*-wave resonance positions in Ps-H are at 4.88 eV and 5.28 eV, respectively [6]. In Ps-Li, this is the first prediction on resonance and we could not compare these positions as no other prediction was available.

To have a credible understanding of the variation of phase shifts from the binding aspect of PsLi, we therefore plot $k\ \cot(\delta_0^+)$ and ik versus k^2 in Fig. 3 (δ_0^+ is the *S*-wave singlet phase shifts). This plot immediately suggests a chemically stable PsLi system as was recently found by Ryzhikh and Mitroy using a variational calculation [11,12], and by Yoshida and Miyako [15] and Bressanini *et al.* [17] and Carl *et al.* [23] using quantum Monte Carlo (QMC) calculations. From a negative energy extrapolation, and from the *t*-matrix pole condition, $k\cot(\delta_0^+)-ik=0$, we obtain the binding energy of the PsLi system as 0.218 eV for the 3-Ps-state coupling model compared to the variational prediction of 0.316 eV [12]. Results for the binding energy improve significantly from almost zero-level (0.008 eV) at the static-exchange approximation to 0.218 eV for the 3-Ps-state coupling, indicating the importance of the inclusion of the highly polarizable Ps states in the coupling scheme. The singlet and triplet channel scattering lengths for these phase shifts are $8.05a_0$ and $1.86a_0$, respectively. In another study, to estimate the effect of the core, we drop the exchange term with the core of Li, which is purely repulsive in the absence of core excitation. In this case, we get the singlet and triplet channel scattering lengths as $6.90a_0$ and $1.73a_0$, respectively. The binding energy arising from the phase shifts of this later model neglecting exchange with core electrons is 0.318 eV, which is incidentally very close to the fixed core SVM (stochastic variational method) prediction of 0.316 eV by Rizhikh and Mitroy [12].

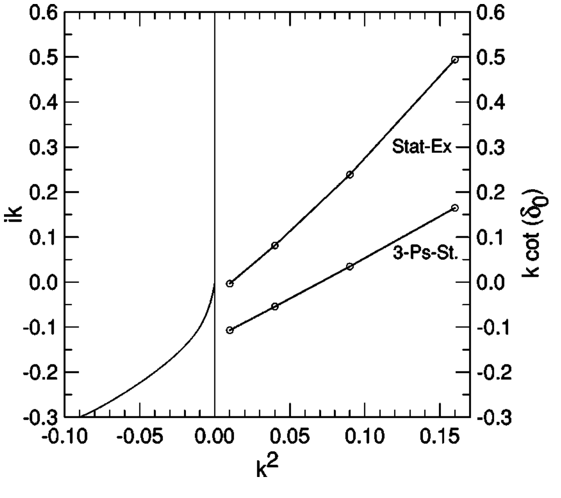

FIG. 3. $k\cot\delta$ and ik (in units of a_0^{-1}) versus k^2 (in units of a_0^{-2}). The corresponding abscissa of the meeting point of negative energy extrapolation of $k\cot\delta$ curve with ik curve represents the binding energy of the Ps-Li system for breaking into Ps and Li in a.u. (Energy $=6.8k^2$ eV.)

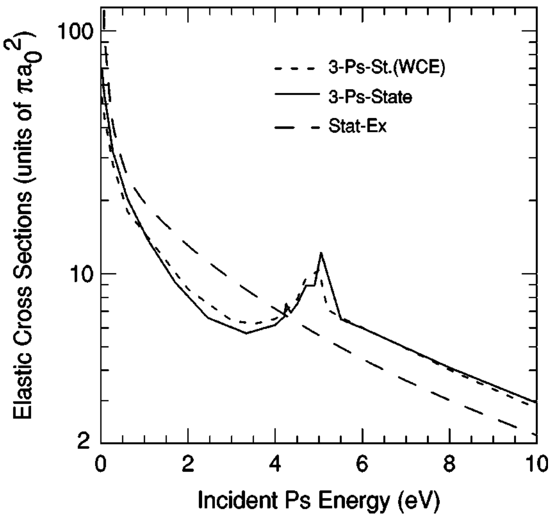

FIG. 4. Elastic cross sections for Ps-Li scattering using static-exchange (Stat-Ex), three-Ps-state coupling (3-Ps-state), and three-Ps-state coupling without core exchange [3-Ps-st.(WCE)] versus incident Ps energy.

The present result for the binding energy including exchange with core is expected to increase further with the inclusion of target excitation channels, as we have seen in the case of PsH [7], where it was found to increase by 7–8 %. In order to achieve further convergence for the low-energy scattering parameters, including resonance and binding energies, we need to add excited states of lithium as well in the coupling scheme. However, present investigations with and without the effect of core exchange emphasize that for Ps scattering, which possibly can move very close to lithium due to its neutral aspect, the importance of the core effect could be significant in the prediction of low-energy scattering parameters and binding energies, as has already been commented upon by Bressanini *et al.* [17]. This prevents us, for the time being, from including the Li-excitation channel in the present calculation, as the complication will be enhanced enormously with a full three-active-electron

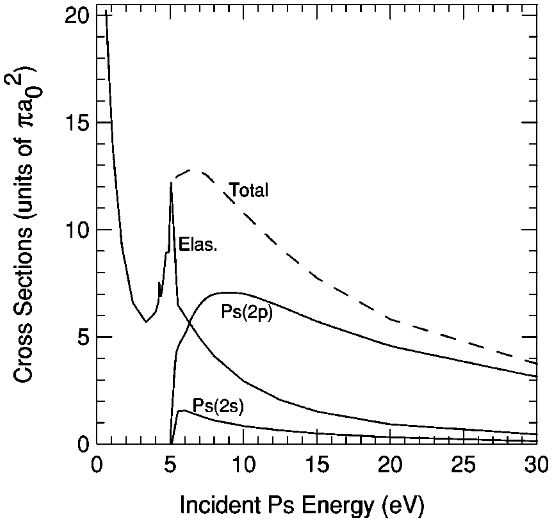

FIG. 5. Elastic and Ps$(2s)$- and Ps$(2p)$-excitation cross sections and total cross sections comprised of elastic plus Ps$(2s)$ plus Ps$(2p)$ excitations in Ps-Li scattering using the three-Ps-state model (3-Ps-state).

consideration for lithium. But we are engaged in the process and hope it will be possible in the very near future. The present study, which focuses on whether for the Ps-open-shell-atom system binding at negative energies for the *S*-wave electronic singlet channel is associated with resonance at positive energies, predicts that both resonance and binding exist for Ps-Li. This feature is already well established in the PsH system [4,6,7].

Next, we consider the angle-integrated cross sections for the elastic scattering. In Fig. 4, we present results for three sets of approximations: (i) static exchange (Stat-Ex), (ii) three-Ps-state (3-Ps-state), and (iii) three-Ps-state with neglected core exchange [3-Ps-St(WCE)]. The Stat-Ex cross sections appear highly nonconverged at low energies compared to the 3-Ps-state and 3-Ps-St(WCE) models. The structure in the elastic cross section for the 3-Ps-state and 3-Ps-St(WCE) models near 4–5 eV, compared to the Stat-Ex model, appears from the resonance behavior of the Ps-Li scattering in this energy region. A similar feature of the elastic cross section was also observed in Ps-H scattering [6,7].

In Fig. 5, we plot Ps$(2s)$ and Ps$(2p)$ excitation cross sections along with the elastic results from the 3-Ps-state model. In this figure, we also plot the total cross section (broken curve) comprising the elastic $+\mathrm{Ps}(2s)+\mathrm{Ps}(2p)$ cross sections. The total cross section agrees with the major experimental trend found in different Ps-scattering processes of having a peak around 20–25 eV and a lowering trend of the cross section thereafter with decreasing energy [34]. The different sets of theories and experiments in Ps-impact scattering collectively suggest a minimum in the cross section around the Ps-excitation threshold. This feature is also noticed in the present calculation but at lower energies. In the absence of any prediction or measurement of partial and total cross sections in Ps-Li, we could not make any direct comparison of the present cross sections.

In conclusion, we investigate Ps-Li scattering employing static-exchange and the 3-Ps-state CCA calculation using a nonlocal model exchange potential. The 3-Ps-state scheme, while closely reproducing the resonance and binding in Ps-H, predicts *S*-, *P*-, and *D*-wave resonances in the attractive singlet channel of the ortho-Ps-Li system and also adheres to the recent variational and quantum Monte Carlo predictions of a chemically stable PsLi bound state. This work suggests that for a general Ps-open-shell-atom system, the binding in the *S*-wave electronic singlet channel might be associated with resonances in the scattering solution of the corresponding channel, as has already been found and established in Ps-H [6,7]. The presence of both the binding and resonances in Ps-Li reconfirms the chemical stability of the system from the above-mentioned binding-resonance correlation. Omission of the repulsive core-exchange part from the 3-Ps-state scheme has been found to increase the binding energy and simultaneously decrease the *S*-wave resonance energy, which emphasizes the need for accounting for the effect of the core for the neutral Ps atom scattering.

The work was supported by the Fundação de Amparo à Pesquisa do Estado de São Paulo of Brazil.

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