S-wave Ps-Li and Ps-Na scattering

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Projectile-elastic, target-elastic, and full close-coupling approximation models have been employed to investigate scattering of *ortho*-positronium off Li and Na atoms at low energies. Nine different basis sets for each system have been used to find the relative importance of atomic (target and projectile) states on the elastic scattering parameters and the convergence of the predicted results with added eigen- and pseudostates. The *s*-wave elastic phase shifts, scattering lengths and cross sections of both the systems are reported upto the incident energy $k=0.5$ a.u. and compared with the corresponding existing theoretical predictions. It has been found that the van der Waals and higher order long-range interactions play a crucial role in predicting *s*-wave elastic parameters for Ps–alkali-metal-atom systems at low energies.

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INTRODUCTION

Interest on the scattering of positronium (Ps) by atoms and molecules has been renewed after the measurements on these systems were carried out by the University College of London (UCL) group [1]. They have reported the total cross sections of Ps-atom (He, Ar) and Ps-molecule (H_2,O_2) scattering at medium energies. Apart from these experiments, zero- or near-zero-energy total cross sections of the Ps-He system have been measured by different groups using various experimental techniques [2]. These measured data on Ps-He scattering differ significantly amongst themselves. Theoretically, Ps-atom scattering has been investigated using different forms of coupled-state models. Ps-H is the simplest and most extensively studied system [3]. Due to the nonavailability of the experimental results, accuracy of the theoretical predictions cannot be judged for this system. Theoreticians are then engaged to investigate Ps-He scattering mainly to test their models. Predictions of Ps-He scattering parameters at zero- or near-zero-incident energy differ amongst themselves, like measured data. However, very recently, theoretically reported cross sections are in fair agreement amongst themselves [4]. Experiments on Ps–alkali-metal atom scattering are expected to be performed in the near future. As a natural choice, theoreticians are interested in investigating Ps–alkali-metal scattering as an alkali-metal atom may be visualized as a quasi-one-electron system.

Ps-atom scattering is much more complicated than the electron/positron-atom scattering owing to the evaluation of the exchange matrix element that involves multicentered and multidimensional integrals. Moreover, Ps–alkali-metal atoms have their special academic interest. The ionization threshold of the Ps atom is always greater than the corresponding threshold of alkali-metal atoms. In Ps-H scattering the first excitation threshold is at 5.1 eV (opening with $n=2$ states of the Ps atom) whereas in the Ps-Li system the first excitation threshold is due to the opening of the $2p$ state of the Li atom (about 1.8 eV). Moreover, the excited state ($n=2$) of Ps and the ground state of the Li atom are of comparable size. Therefore, it is expected that both the atoms interact more rigorously than the corresponding interactions of Ps with H and He atom systems. We hasten to add that the alkali-metal atom is a highly polarizible target having polarizibility about 30 times higher than that of H and the induced dipole polarizibilty of a Ps atom is also higher than that of a H atom. It is expected that the long-range van der Waals interaction, which arises out of a dipole-dipole interaction, will be prominent and will influence the scattering parameters very significantly at low energies. Therefore, it is obvious that the dynamics of Ps–alkali-metal-atom systems will be different from the corresponding Ps-H/He systems.

Previously, the Ps-Li system has been investigated by Biswas [5] using a phenomenologically tuned model nonlocal exchange potential within the framework of target-elastic close-coupling approximation (CCA). He has used two target-elastic models; a static exchange, and a three-state CCA [Ps($1s,2s,2p$)+Li($2s$)], to predict different elastic and inelastic scattering parameters. He has also reported *s*-, *p*-, and *d*-wave resonances in Ps-Li scattering. Ray [6] has investigated the same problem using static exchange and a two-state CCA [Ps($1s$)+Li($2s,2p$)] models. Adhikari and Mandal [7] have studied Ps-Na and Ps-K scattering using target-elastic three-state CCA [Ps($1s,2s,2p$) +Na($3s$)/K($4s$)], in which the exchange matrix element has been represented by the nonlocal-tuned model potential. They have predicted the scattering parameters up to the incident energy 50 eV and reported *s*-, *p*-, and *d*-wave resonances for the Ps-Na and Ps-K systems. The most elaborate coupled-state calculations for the Ps-Li system has been carried out by Chakraborty *et al.* [8]. They have employed target-elastic and projectile-elastic CCA models having different basis sets. The most elaborate target-elastic and projectile-elastic CCA models used for lithium target are [Ps($1s,2s,2p,3s,3p,3d$)+Li($2s$) and Ps($1s$) +Li($2s,2p,3s,3p,3d,4s,4p,4d$)], respectively. For the

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Ps-Na system, the most elaborate target-elastic and projectile-elastic CCA calculations [Ps$(1s,2s,2p,3s,3p,3d)$+Na$(3s)$ and Ps$(1s)$+Na$(3s,3p,4s,3d,4p)$] have been performed by Sinha *et al.* [9]. Apart from these investigations Mitroy *et al.* [10] have studied Ps–alkali-metal-atom systems and they have reported the break-up energy of alkali-Ps bound states using the stochastic variational method. The long-range van der Waals interaction, which is of key importance in atom-atom scattering, has not been considered in any calculation carried out so far. Mitroy and his co-workers have included the effect of van der Waals interaction implicitly.

Considering these, we plan to study the scattering of *ortho*-Ps off Li and Na atoms using full CCA in which internal degrees of freedom of both the atoms have been considered. The present models include the van dar Waals interaction and the effect of exchange of electrons explicitly by antisymmetrized total wave function of the system.

THEORY

The position vectors of the electron and the positron of the incident positronium atom are denoted by $\vec{r}_1$ and $\vec{x}$ and that of the valence electron of the alkali atom as $\vec{r}_2$. All the distances are measured from the target nucleus. The total interaction Hamiltonian of the Ps–alkali-metal-atom system may be expressed as

$$H = -\frac{1}{4}\nabla^2_{R_1} + H_{\rm Al}(\vec{r}_2) + H_{\rm Ps}(\vec{\rho}_1) + V_{\rm int}(\vec{x},\vec{r}_1,\vec{r}_2), \qquad (1)$$

where $H_{\rm Al}(\vec{r}_2)$ and $H_{\rm Ps}(\vec{\rho}_1)$ are the Hamiltonians of the target alkali-metal atom and positronium atom, respectively. $V_{\rm int}(\vec{x},\vec{r}_1,\vec{r}_2)$ is the interaction potential. In post form it can be expressed as

$$V_{\rm int}(\vec{x},\vec{r}_1,\vec{r}_2) = \frac{1}{x} - \frac{1}{r_2} - \frac{1}{|\vec{x}-\vec{r}_1|} + \frac{1}{|\vec{r}_1-\vec{r}_2|}. \qquad (2)$$

In the close-coupling approximation, the antisymmetrized total wave function is expressed in terms of the bound states of atomic subsystems as

$$\psi^{\pm}(\vec{r}_1,\vec{r}_2,\vec{x}) = \frac{1}{\sqrt{2}}\sum_{\nu\eta}(1 \pm {\rm P}_{12})\phi_\eta(\vec{r}_2)\omega_\nu(\vec{\rho}_1)F^{\pm}_{\nu\eta}(\vec{R}_1), \quad (3)$$

where

$$\vec{R}_i = \frac{\vec{x}+\vec{r}_i}{2}, \quad \vec{\rho}_i = \vec{x}-\vec{r}_i \quad (i=1,2). \qquad (4)$$

P_{12} is an exchange operator and $F^{\pm}_{\nu\eta}(\vec{R}_i)$ represents the outgoing projectile atom. $\phi_\eta(\vec{r}_2)$ and $\omega_\nu(\vec{\rho}_1)$ define the wave functions of the alkali-metal atom and the Ps atom, respectively. The superscript "+" denotes the spin singlet scattering while "−" is used for the triplet case.

The total wave function of the scattering system must satisfy the Schrödinger equation

$$H\psi^{\pm}(\vec{r}_1,\vec{r}_2,\vec{x}) = E\psi^{\pm}(\vec{r}_1,\vec{r}_2,\vec{x}). \qquad (5)$$

In the integral representation, one can recast the Schrödinger equation into a Lippman-Schwinger-type equation in momentum space as

$$f^{\pm}_{\nu'\eta';\nu\eta}(\vec{k}',\vec{k}) = f^{B\pm}_{\nu'\eta';\nu\eta}(\vec{k}',\vec{k}) - \frac{1}{2\pi^2}\sum_{\nu''\eta''}\int d\vec{k}'' \times \frac{f^{B\pm}_{\nu'\eta';\nu''\eta''}(\vec{k}',\vec{k}'')f^{\pm}_{\nu''\eta'';\nu\eta}(\vec{k}'',\vec{k})}{k^2_{\nu''\eta''} - k''^2 + i\epsilon}, \qquad (6)$$

where $\vec{k}$ and $\vec{k}'$ are the momenta of the projectile atom in the initial and the final states, respectively, and are related (in magnitude) as

$$\frac{1}{4}k^2 - \epsilon^{\rm Ps}_\nu - \epsilon^{\rm Al}_\eta = \frac{1}{4}k'^2 - \epsilon^{\rm Ps}_{\nu'} - \epsilon^{\rm Al}_{\eta'}. \qquad (7)$$

The first-order scattering amplitudes, $f^{B\pm}$, are given by

$$f^{B\pm}_{\nu'\eta';\nu\eta}(\vec{k}',\vec{k}) = f^{B}_{\nu'\eta';\nu\eta}(\vec{k}',\vec{k}) \pm g^{B}_{\nu'\eta';\nu\eta}(\vec{k}',\vec{k}). \qquad (8)$$

Here, f^B and g^B are the first Born and Born-Oppenheimer scattering amplitudes and are given by

$$f^{B}_{\nu'\eta';\nu\eta}(\vec{k}',\vec{k}) = \frac{2\mu}{Q^2}\int d\vec{\rho}_1\omega^*_{\nu'}(\vec{\rho}_1)\{e^{\frac{i}{2}\vec{Q}\cdot\vec{\rho}_1} - e^{-\frac{i}{2}\vec{Q}\cdot\vec{\rho}_1}\}\omega_\nu(\vec{\rho}_1)\int d\vec{r}_2\phi^*_{\eta'}(\vec{r}_2)\{1 - e^{-i\vec{Q}\cdot\vec{r}_2}\}\phi_\eta(\vec{r}_2) \qquad (9)$$

and

$$g^{B}_{\nu'\eta';\nu\eta}(\vec{k}',\vec{k}) = -\frac{\mu}{2\pi}\int d\vec{r}_1\int d\vec{r}_2\int d\vec{x}\phi^*_{\eta'}(\vec{r}_1)\omega^*_{\nu'}(\vec{\rho}_2) \times e^{-i\vec{k}'\cdot R_2}e^{i\vec{k}\cdot\vec{R}_1}(H-E)\phi_\eta(\vec{r}_2)\omega_\nu(\vec{\rho}_1), \quad (10)$$

with μ denoting the reduced mass of the system.

The evaluations of the direct first-order matrix elements are straight forward. On the other hand, the exchange elements are very complicated as these involve muticentered and multidimensional integrals.

The total angular momentum, J, of the scattering system is a constant of motion. We express the scattering amplitude in partial wave decomposed form as

$$f^{\pm}_{\nu'\eta';\nu\eta}(\vec{k}',\vec{k}) = \frac{1}{\sqrt{kk'}}\sum_{JM}\sum_{J_1M_1}\sum_{J'_1M'_1}\sum_{LM_L}\sum_{L'M'_L}\begin{pmatrix} L' & l'_p & J'_1 \\ M'_L & m'_p & M'_1\end{pmatrix} \times \begin{pmatrix} J'_1 & l'_t & J \\ M'_1 & m'_t & M\end{pmatrix} \times Y^*_{L'M'_L}(\hat{k}')T^{J\pm}(\tau'k';\tau k)Y_{LM_L}(\hat{k}) \times \begin{pmatrix} L & l_p & J_1 \\ M_L & m_p & M_1\end{pmatrix}\begin{pmatrix} J_1 & l_t & J \\ M_1 & m_t & M\end{pmatrix}, \qquad (11)$$

and a similar expression for $f^{B\pm}$ with $T^{J\pm}$ on the right side of Eq. (11) is replaced by $B^{J\pm}$. Here l_p and l_t are the angular

momenta of the bound projectile and the target atoms, respectively, and L represents the angular momentum of the the moving positronium atom. τ represents the set of quantum numbers $(n_p, l_p, n_t, l_t, J_1, L)$. The corresponding final state quantum numbers are denoted by primes. After partial wave analysis, Eq. (6) becomes a one-dimensional coupled equation for unknown amplitudes $T^{J\pm}$ as

$$T^{J\pm}(\tau' k'; \tau k) = B^{J\pm}(\tau' k'; \tau k) - \frac{1}{2\pi^2} \sum_{\tau''} \int dk'' k'' \frac{B^{J\pm}(\tau' k'; \tau'' k'') T^{J\pm}(\tau'' k''; \tau k)}{k^2_{\nu''\eta''} - k''^2 + i\epsilon}. \tag{12}$$

To solve these equations one needs $B^{J\pm}$'s as input. With a knowledge of $f^{B\pm}$ one can get

$$B^{J\pm}(\tau' k'; \tau k) = \frac{\sqrt{kk'}}{(2J+1)} \sum_{M M_L M'_L} \sum_{m_t m'_t} \sum_{m_p m'_p} \begin{pmatrix} L' & l'_p & J'_1 \\ M'_L & m'_p & M'_1 \end{pmatrix} \times \begin{pmatrix} J'_1 & l'_t & J \\ M'_1 & m'_t & M \end{pmatrix} \begin{pmatrix} L & l_p & J_1 \\ M_L & m_p & M_1 \end{pmatrix} \times \begin{pmatrix} J_1 & l_t & J \\ M_1 & m_t & M \end{pmatrix} \int d\hat{k} \int d\hat{k}' Y^*_{L'M'_L}(\hat{k}') \times f^{B\pm}_{\nu'\eta';\nu\eta}(\vec{k}', \vec{k}) Y_{LM_L}(\hat{k}). \tag{13}$$

Equation (12) is solved by a matrix inversion method and sufficient care has been taken for evaluation of the principal value part. For the Jth partial wave scattering at incident momentum k_0, the real part of the elastic phase shift is given as

$$\delta_J(k) = \frac{1}{2} \tan^{-1} \left(\frac{\mathrm{Re}[T^J(\tau_0 k_0; \tau_0 k_0)]}{2\pi - \mathrm{Im}[T^J(\tau_0 k_0; \tau_0 k_0)]} \right), \tag{14}$$

where τ_0 designates the initial states of both the atoms and the angle integrated Jth partial wave elastic cross section is given by

$$\sigma^{el}(J) = \frac{(2J+1)}{4\pi k_0^2} |T^J(\tau_0 k_0; \tau_0 k_0)|^2. \tag{15}$$

In these calculations we employ the following nine models for Ps-Li and Ps-Na scattering:

(1) Ps$(1s)$+Li$(2s)$,
(2) Ps$(1s,2s,2p)$+Li$(2s)$,
(3) Ps$(1s,2s,2\overline{p})$+Li$(2s)$,
(4) Ps$(1s)$+Li$(2s,2p)$,
(5) Ps$(1s)$+Li$(2s,2p,3s,3p,3d)$,
(6) Ps$(1s,2s,2p)$+Li$(2s,2p)$,
(7) Ps$(1s,2s,2\overline{p})$+Li$(2s,2p)$,
(8) Ps$(1s,2s,2p)$+Li$(2s,2p,3s,3p,3d)$,
(9) Ps$(1s,2s,2\overline{p})$+Li$(2s,2p,3s,3p,3d)$;

and

(1) Ps$(1s)$+Na$(3s)$,
(2) Ps$(1s,2s,2p)$+Na$(3s)$,
(3) Ps$(1s,2s,2\overline{p})$+Na$(3s)$,
(4) Ps$(1s)$+Na$(3s,3p)$,
(5) Ps$(1s)$+Na$(3s,3p,3d,4s,4p)$,
(6) Ps$(1s,2s,2p)$+Na$(3s,3p)$,
(7) Ps$(1s,2s,2\overline{p})$+Na$(3s,3p)$,
(8) Ps$(1s,2s,2p)$+Na$(3s,3p,3d,4s,4p)$,
(9) Ps$(1s,2s,2\overline{p})$+Na$(3s,3p,3d,4s,4p)$, respectively.

Here, $2\overline{p}$ is the pseudostate of the Ps atom taken from Damburg and Karule [12]. The wave function of the ground and excited states of Li and Na are taken from Nielsen *et al.* [11]. The relative importance of each state included in the expansion scheme can be judged from the results of the different models. Moreover the physical insight of using various basis sets will be discussed in the next section.

RESULTS AND DISCUSSION

We investigate the *s*-wave elastic scattering of *ortho*-Ps atoms off atomic lithium and sodium targets up to the incident energy 1.5 eV (which corresponds to $k=0.5$ a.u.). For each system, nine CCA models (static-exchange, two target-elastic, two projectile-elastic, and four full CCA) have been employed. We solve numerically one-dimensional coupled integral Eq. (12) by the matrix inversion method. As a check of the program we reproduce all the phase shifts as obtained by Chakraborty *et al.* [8] and Sinha *et al.*, [9] with our present numerical code. This study reports the *s*-wave elastic scattering parameters for both spin alignments. We would like to mention that in Ps-Li scattering Chakraborty *et al.* have employed four models (models a, f, b, and c), which correspond to our models (models 1, 2, 4, and 5). On the other hand, for the Ps-Na system, our models 1, 2, and 5 have been already employed by Sinha *et al.* (their models a, f, and c). It is to be noted that the models employed by Chakraborty *et al.* and Sinha *et al.* are static-exchange, target-elastic, and projectile-elastic CCA. In earlier works, Ray [6] has used projectile-elastic CCA, and Biswas [5] and Adhikari *et al.* [7] have employed target-elastic CCA. The van der Waals and higher order interactions can be included dynamically in the calculation if and only if excitations of both the colliding atoms to *p* and higher angular momentum states are retained in the expansion scheme. Therefore, all the calculations carried out so far have not been included the van der Waals and higher order long-range interactions.

In the pictorial representation, out of nine models we include the results of the static-exchange (model 1), the most elaborate target-elastic (model 3) and projectile-elastic (model 5) results together with four full CCA models (models 6–9). Figure 1 presents the *s*-wave singlet elastic phase shifts for Ps-Li scattering using seven models up to the incident energy $k=0.5$ a.u., out of which two sets of phase shifts (of models 1 and 5) are due to Chakraborty *et al.* We avoid providing the other two sets of results to make the figure distinct. We hasten to add that model 5 is an elaborate projectile-elastic CCA model. The present models 6–9 retain the excitations to nonzero angular states of both the colliding atoms. These models include dynamically the long-range interactions (van der Waals and higher order) to a different extent. Model 6 includes the van der Waals interaction partially whereas the major part of the van der Waals and higher order $(1/R^8)$ interactions have been considered in model 9.

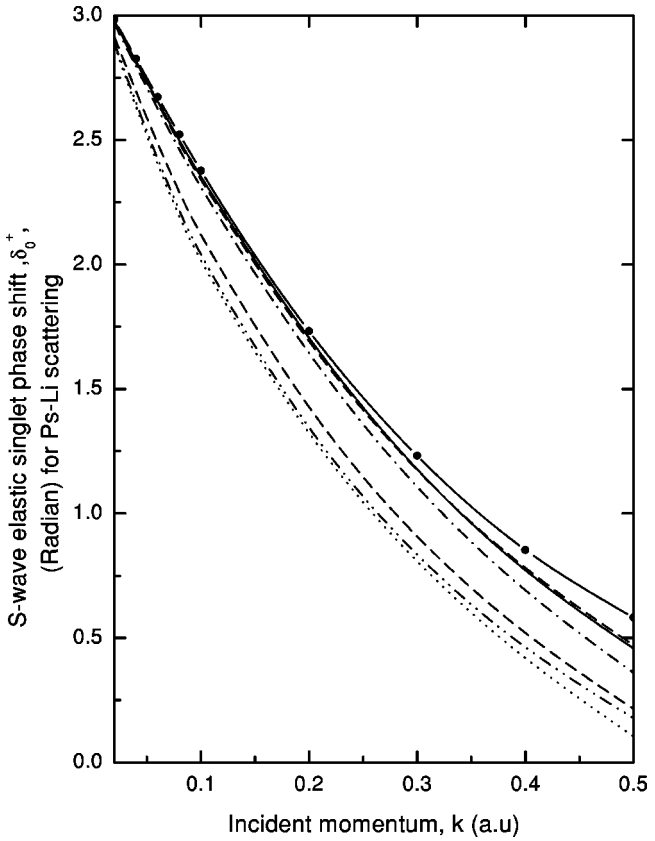

FIG. 1. *s*-wave singlet elastic phase shift (radian) for Ps-Li scattering. Curves: dotted, model 1; short dashed, model 3; dash dot dotted, model 5; dash dotted, model 6; solid, model 7; dashed, model 8; solid + closed circle, model 9.

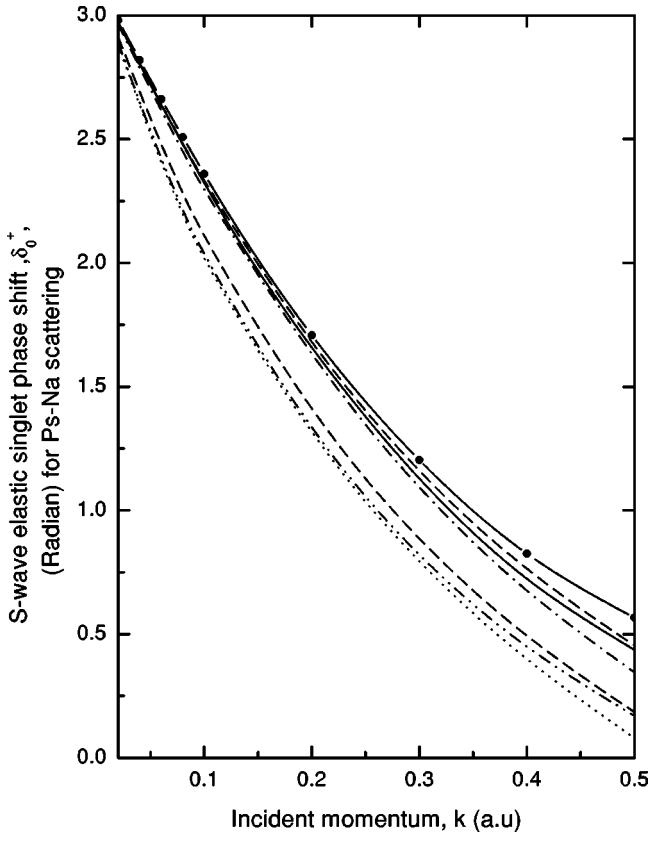

FIG. 2. *s*-wave singlet elastic phase shift (radian) for Ps-Na scattering. Curves: dotted, model 1; short dashed, model 3; dash dot dotted, model 5; dash dotted, model 6; solid, model 7; dashed, model 8; solid + closed circle, model 9.

Moreover, models 7 and 9 include the effect of the continuum of the Ps atom via the pseudostate $2\overline{p}$. The effect of long-range force is apparent from Fig. 1. All the phase shifts obtained by using full CCA (6–9) models are quantitatively different from earlier models (1–5) in which long-range forces have not been considered. The effect of the eigenstates beyond the first *p* state of target atom can be visualized by comparing the results of models 6 and 8 and/or from the results of models 7 and 9. The present phase shifts become more positive with added states, i.e., variationally consistent. We conclude that the predicted *s*-wave singlet phase shifts are nearly convergent at very low incident energies (below $k=0.1$ a.u.) with added eigen and pseudostates. It is evident from Fig. 1, that the long-range forces ($1/R^6$ and higher orders) influence the elastic singlet phase shifts very significantly at low energies (up to $k=0.5$ a.u.) for Ps-Li scattering.

The situation in the case of the Ps-Na system is not very much different from that of Ps-Li scattering. The *s*-wave elastic singlet phase shifts (Fig. 2) here also are found to be variationally consistent. The van der Waals and higher order long-range interactions are found to be very much crucial in predicting *s*-wave elastic singlet phase shifts. It can be easily understood from the results of models 6–9 when compared with those of the other models. The effect of the pseudostate of the Ps atom can be judged by comparing the predictions of models 2 and 3, 6 and 7, and 8 and 9. The *s*-wave elastic singlet phase shifts of Ps-Na scattering is also nearly convergent with added eigen and pseudostates at low energies.

The *s*-wave elastic triplet phase shifts up to incident energy $k=0.5$ a.u. for Ps-Li scattering are shown in Fig. 3 and the corresponding results for the Ps-Na system are plotted in Fig. 4. Model 5 for both the systems are the elaborate projectile-elastic CCA models employed by Chakraborty *et al.* (Fig. 3) and Sinha *et al.* (Fig. 4) for Ps-Li and Ps-Na scattering, respectively. The triplet phase shifts are found to be variationally consistent with added eigen and pseudostates for both the systems. Qualitative feature of triplet *s*-wave phase shifts is found to be more or less similar to the corresponding singlet phase shifts for both the systems. For *s*-wave elastic triplet scattering, the potentials other than $1/R^6$ (which are included in models 8 and 9) are found to play a significant role. At very low energies (below $k=0.1$ a.u.) the triplet phase shifts of models 8 and 9 for both the systems coalesce with each other. It indicates that the results are convergent with added eigen- and pseudostates.

Tables I and II present the scattering lengths and effective ranges for Ps-Li and Ps-Na systems, respectively. For the Ps-Li system the singlet scattering length a_0^+ obtained in the static-exchange model is $13.13a_0$ and the result of model 5 (of Chakraborty *et al.*) is $12.69a_0$. When the long-range forces are included, scattering length reduces drastically (models 6–9). When the first *p* state of both the colliding atoms are included (model 6) the value of the *s*-wave singlet scattering length is $8.63a_0$, which is reduced by 32% from

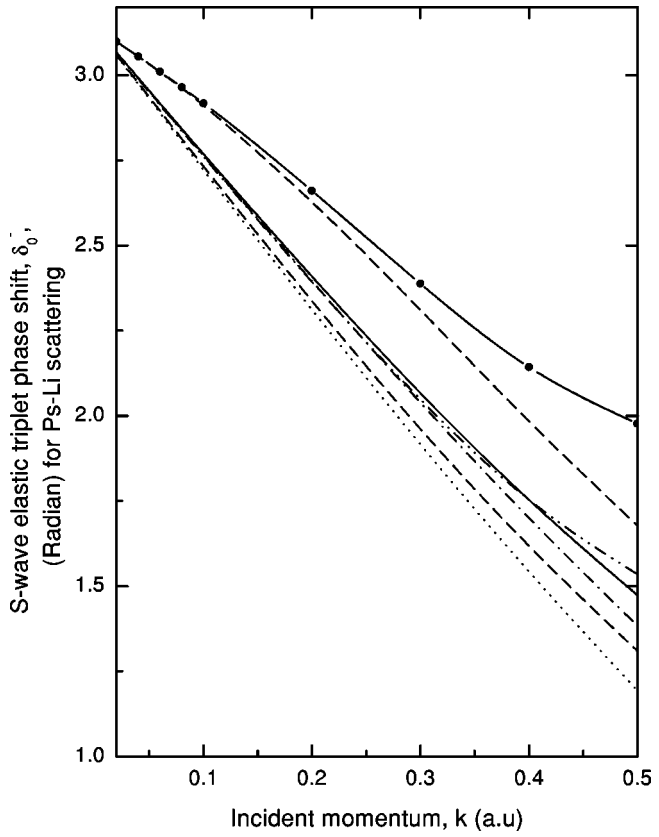

FIG. 3. *s*-wave triplet elastic phase shift (radian) for Ps-Li scattering. Curves: dotted, model 1; short dashed, model 3; dash dot dotted, model 5; dash dotted, model 6; solid, model 7; dashed, model 8; solid + closed circle, model 9.

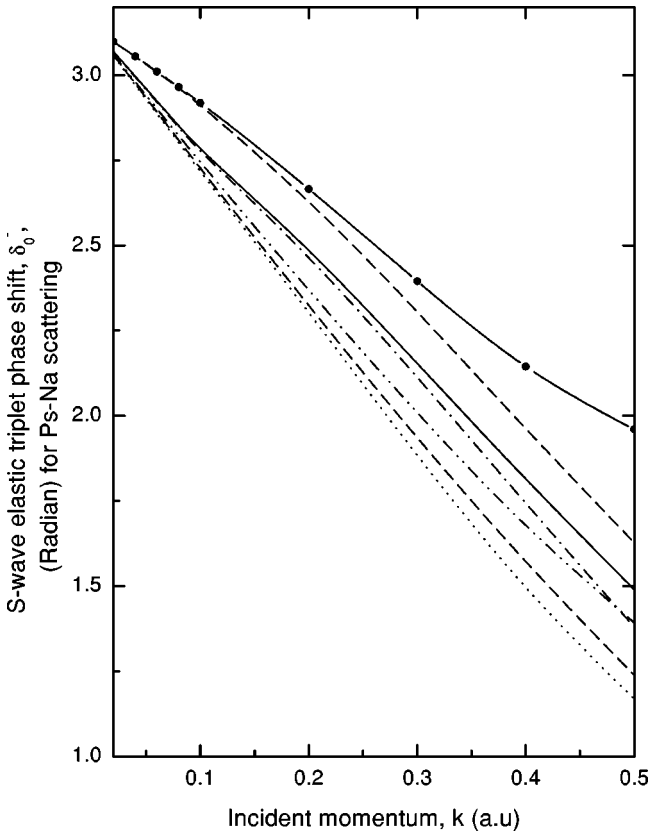

FIG. 4. *s*-wave triplet elastic phase shift (radian) for Ps-Na scattering. Curves: dotted, model 1; short dashed, model 3; dash dot dotted, model 5; dash dotted, model 6; solid, model 7; dashed, model 8; solid + closed circle, model 9.

the result of Chakraborty *et al.* The effect of the pseudostates of the Ps atom can be noticed by comparing the scattering lengths of model 6 with that of 7 and of model 8 with 9. We would like to mentioned that the *s*-wave singlet scattering length for Ps-Li system is reduced by about 40% using model 9 from the corresponding prediction of static-exchange model whereas the triplet scattering length is reduced by 49%. In the case of Ps-Na system, features of the singlet and triplet scattering lengths are very much similar both quantitatively and qualitatively with those of the Ps-Li system. Singlet and triplet scattering lengths differ from the corresponding values of the static-exchange model by about 38 and 49%, respectively.

Stability of the scattering length is of key importance to justify a model. We have calculated the scattering lengths in the different domain of energy using our final model. It has been found in both the cases that the variation of scattering lengths for both the systems and for different domains of energy lie within 0.1%.

In Fig. 5 spin-averaged *s*-wave elastic cross sections for Ps-Li scattering are plotted. The first three models 1, 3, and 5, are the static-exchange, projectile-elastic, and target-elastic predictions. When the van der Waals interaction is included, situations differ and cross sections reduce significantly as noticed in the case of phase shifts and scattering lengths. The value of the *s*-wave elastic cross section is approximately one-third of the corresponding static-exchange value. A similar feature is found in the case of the *s*-wave elastic cross sections of the Ps-Na system (Fig. 6). This shows the importance of the effect of the van der Waals and higher order long-range forces in investigating elastic *s*-wave Ps–alkali-metal scattering at low incident energies.

TABLE I. The *s*-wave scattering length, $a_0^{\pm}$ (in a.u.), and effective range, $r_0^{\pm}$, (in a.u.) for Ps-Li scattering.

Models	Singlet scattering length, a_0^+	Singlet effective range, r_0^+	Triplet scattering length, a_0^-	Triplet effective range, r_0^-
1	13.13	6.03	4.22	2.66
2	12.42	5.84	4.10	2.58
3	11.41	5.64	4.12	2.53
4	12.78	5.99	3.98	2.32
5	12.69	5.99	3.80	2.30
6	8.63	4.79	3.54	1.85
7	8.07	4.50	3.48	1.59
8	8.38	4.72	2.16	6.28
9	7.91	4.44	2.16	4.83

TABLE II. The *s*-wave scattering length, $a_0^{\pm}$ (in a.u.), and effective range, $r_0^{\pm}$ (in a.u.), for Ps-Na scattering.

Models	Singlet scattering length, a_0^+	Singlet effective range, r_0^+	Triplet scattering length, a_0^-	Triplet effective range, r_0^-
1	13.01	6.12	4.26	2.68
2	12.16	5.84	4.15	2.40
3	11.53	5.74	4.17	2.59
4	12.76	6.09	4.00	2.37
5	12.67	6.08	4.04	1.87
6	8.91	4.98	3.69	2.31
7	8.51	4.78	3.64	2.18
8	8.46	4.75	2.17	6.09
9	8.10	5.51	2.16	4.59

CONCLUSION

The scattering of Ps atoms off Li and Na atoms has been investigated at low energies using static-exchange, projectile-elastic, target-elastic and full close-coupling models. We employed nine basis sets to find the relative importance of each eigen- or pseudostate on the elastic scattering.

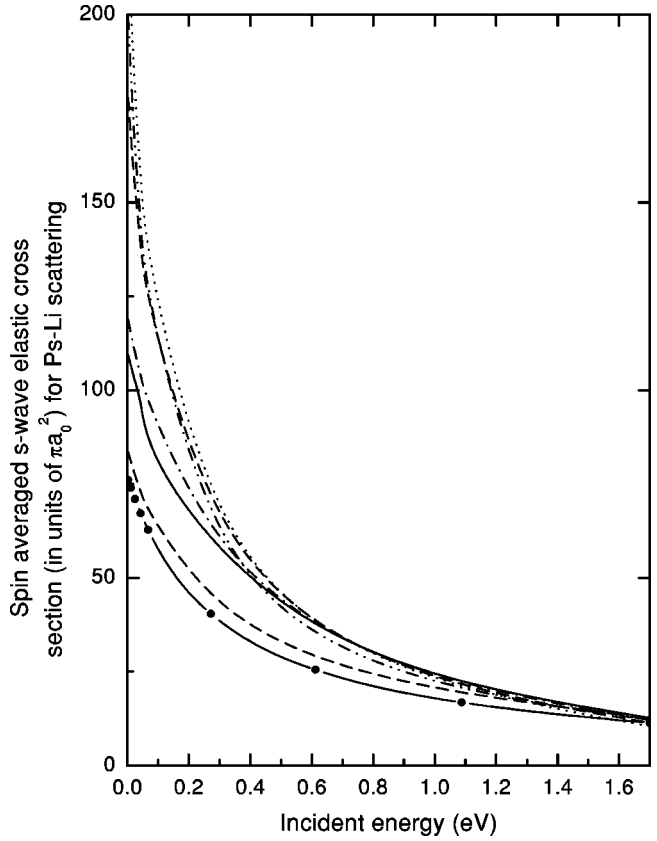

FIG. 5. Spin-averaged *s*-wave elastic cross section (in units of πa_0^2) for Ps-Li scattering. Curves: dotted, model 1; short dashed, model 3; dash dot dotted, model 5; dash dotted, model 6; solid, model 7; dashed, model 8; solid + closed circle, model 9.

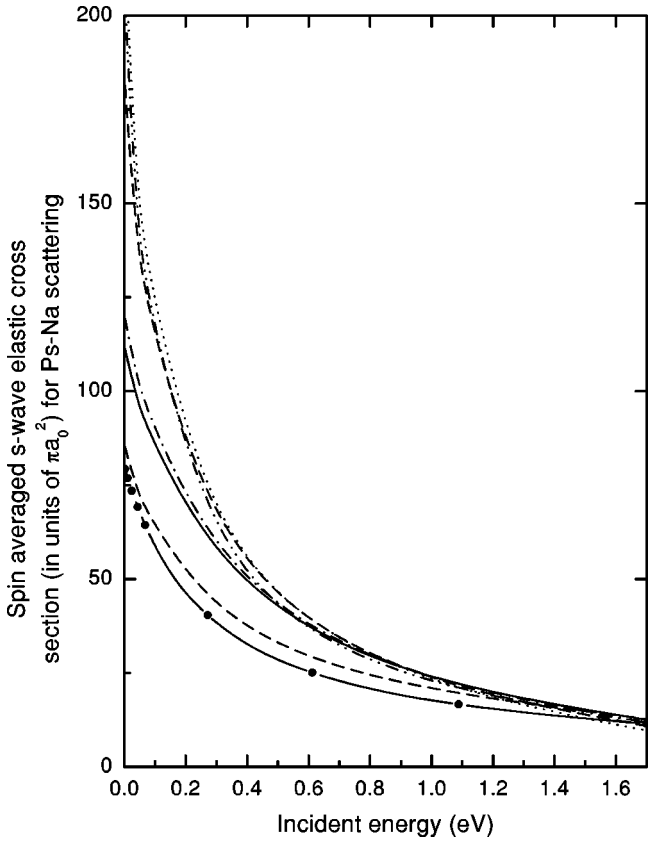

FIG. 6. Spin-averaged *s*-wave elastic cross section (in units of πa_0^2) for Ps-Na scattering. Curves: dotted, model 1; short dashed, model 3; dash dot dotted, model 5; dash dotted, model 6; solid, model 7; dashed, model 8; solid + closed circle, model 9.

In full CCA the internal degrees of freedom of both the colliding atoms have been taken into account to include van der Waals and higher order interactions via different basis sets. The effect of the continuum of the Ps atom on the elastic *s*-wave scattering has also been accounted for via pseudostates. The retention of the $2\bar{p}$ state of the Ps atom in the expansion scheme includes the full induced dipole polarizibility of Ps atom dynamically. It is well known that 98% of the induced dipole polarizibilities are taken into account if only the first *p* state of the alkali atom is retained in the basis set. The present pseudostate full CCA models incorporate major parts of the van der Waals interaction for both the systems. *s*-wave phase shifts, scattering lengths, and cross sections for both the systems are reported. By comparing our present *s*-wave scattering parameters with the static exchange and also with existing elaborate theoretical predictions (Chakraborty *et al.* and Sinha *et al.*) it is found that long-range forces have a significant contribution in predicting scattering parameters. Moreover, it has been noticed that the inclusion of the eigenstates beyond the first *p*-state of alkali-metal atoms in the expansion scheme also plays an appreciable role in estimating the scattering parameters. The phase shifts and scattering lengths are found to be variationally consistent. The scattering length using our most elaborate basis set is found to be stable. Our phase shifts are

convergent with added eigen and pseudostates at low energies (below $k=0.1$ a.u.). We conclude that in investigating Ps–alkali-metal atom scattering, van der Waals interaction plays a domimant role in predicting the *s*-wave elastic parameters at low energies. The present result may be modified on accounting the scattering space more accurately than the present one by using elaborate basis set containing higher excited states and continuum.

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