Findings in Ps-H scattering

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The best three-channel projectile-inelastic close-coupling approximation (CCA) is used to study the resonances in positronium (Ps) and hydrogen (H) scattering at the energy region below the inelastic threshold. The s-wave elastic phase shifts and s-wave elastic cross sections are studied using the static-exchange, two- and three-channel projectile-inelastic CCA for both the singlet (+) and triplet (−) channels. The singlet resonances detected using different CCA schemes confirm previous predictions [Drachman and Houston, Phys. Rev. A **12**, 885 (1975); Page, J. Phys. B. **9**, 1111 (1976)]. We report a resonance in the triplet channel too using the present three-channel CCA scheme.

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I. INTRODUCTION

In collision physics, resonance is an important phenomenon. When a microscopic moving object that is a wave enters into the scattering chamber near the target, it faces interactions. When it comes out of the scattering zone, the original incident wave gathers a phase shift and the new wave is known as the scattered wave. The change in phase (phase shift) is the parameter that carries the information about the scattering process. A rapid change in phase shift by π rad in a very narrow energy interval of the incident wave is an indication of the existence of a resonance. It carries information about a bound system if it is in the s-wave elastic scattering and below the threshold of excitation.

The phase shift δ_l can be decomposed as

$$\delta_l = \xi_l + \eta_l.$$

ξ_l corresponds to the hard-sphere scattering or nonresonant part; it does not depend on the shape and depth of the potential. The term η_l depends on the details of the potential. The quantities ξ_l and η_l vary in general slowly and smoothly with the incident particle energy. But in certain cases η_l may vary rapidly in a small energy interval of width Γ about a given energy value E_R such that we can write

$$\eta_l = \eta_l^R = \tan^{-1}\frac{\Gamma}{2(E_R - E)}.$$

In that energy interval the phase shift is therefore given approximately by

$$\delta_l \simeq \xi_l + \eta_l^R.$$

The physical significance of a narrow resonance can be inferred by examining the amplitude of the radial wave function inside the interaction region. The probability of finding the scattered particle within the potential is much larger near the resonance energy $E = E_R$, so that in that case the particle is nearly bound in the well. Thus the resonance may be considered as a metastable state whose lifetime τ, which is much longer than a typical collision time, can be related to the resonance width Γ by using the uncertainty relation $\Delta t \Delta E \gtrsim \hbar$. Thus, with $\Delta t \simeq \tau$ and $\Delta E \simeq \Gamma$, we have $\tau \simeq \hbar / \Gamma$.

The shape of the cross-section curve near a resonance as a function of energy depends on the nonresonant phase shift ξ_l. For the s-wave scattering it is

$$\sigma_l = \frac{\sin^2\xi_l (E_R - E)^2 + \cos^2\xi_l \Gamma^2 + \sin 2\xi_l (E_R - E)\Gamma/2}{(E_R - E)^2 + \Gamma^2/4}$$

Two limiting cases for a nonresonant phase shift are 0 and $\pi/2$. In the first case the above equation becomes

$$\sigma_l = \frac{\Gamma^2}{(E_R - E)^2 + \Gamma^2/4},$$

which is symmetric and represents a rise in cross section at the resonance energy. In the other case,

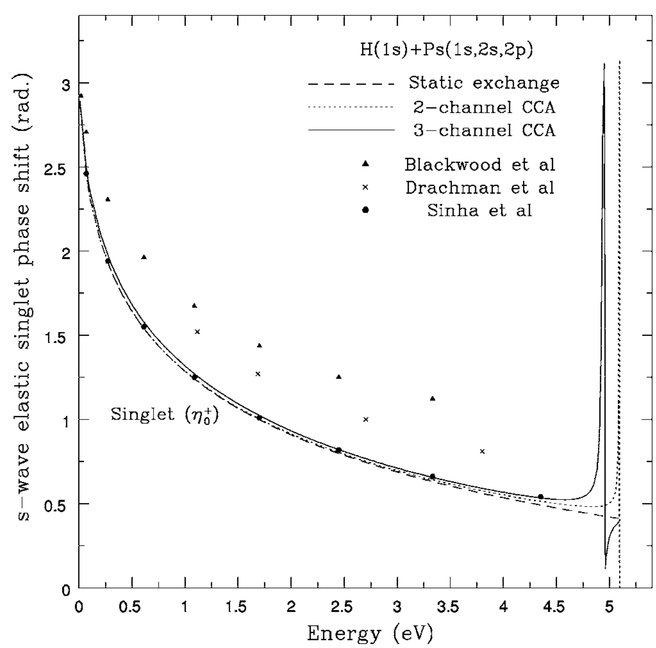

FIG. 1. The singlet (+) s-wave elastic phase shifts.

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$$\sigma_l = \frac{(E_R - E)^2}{(E_R - E)^2 + \Gamma^2/4},$$

which is also symmetric but goes down to zero at the resonance energy. If the nonresonant phase shift gets some other value then other forms of the cross section can occur.

Resonance in the singlet channel in positronium (Ps) and hydrogen (H) scattering was reported by many workers using different approaches [1–14]. It was first predicted by Drachman and Houston [1] using a Feshbach formalism with stabilization and complex rotation methods. But no such resonance was reported using the close-coupling approximation (CCA) [15–22].

The CCA is the best theory to study low-energy scattering phenomena. It is based on the very basic principle of quantum mechanics known as eigenstate expansion methodology. It takes into account the coupling effect of different channels by adopting the conservation of total angular momentum quantum numbers J and M. The coupling effect is more pronounced for the channels that are energetically closer. We employ different projectile-inelastic CCA schemes to investigate Ps-H scattering. We perform exact calculations for all the direct and exchange matrix elements, considering all the possible Coulomb interactions, but the direct first Born amplitudes vanish if the parity of Ps remains unaltered. Our objective is to investigate the resonances in the present system. It is a very difficult task since a large number of fine mesh points are required in a very narrow energy interval $\sim 10^{-2}$ to 10^{-3} eV. We study s-wave elastic phase shifts and s-wave elastic cross sections in the energy region below the inelastic threshold.

II. THEORY

The wave function of the system is

$$\Psi^{\pm}(\mathbf{r}_p,\mathbf{r}_1,\mathbf{r}_2) = \frac{1}{\sqrt{2}}(1 \pm P_{12}) \sum_{n_t l_t n_p l_p L J_1 J M} \frac{F_{\Gamma_0 n_t l_t n_p l_p L J_1 J M}(\mathbf{k},\mathbf{k}',R_1)}{R_1} \frac{U_{n_t l_t}(r_2)}{r_2} \frac{V_{n_p l_p}(\rho_1)}{\rho_1} \times \sum_{m_t m_p M_L} \begin{pmatrix} L & l_p & J_1 \\ M & m_p & M_1 \end{pmatrix} \times \begin{pmatrix} J_1 & l_t & J \\ M_1 & m_t & M \end{pmatrix} Y_{LM_L}(\hat{\mathbf{R}}_1) Y_{l_p m_p}(\hat{\rho}_1) Y_{l_t m_t}(\hat{\mathbf{r}}_2) \quad (1)$$

with the Hamiltonian of the system as

$$H = -\frac{1}{2}\nabla_p^2 - \frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 + \frac{1}{|\mathbf{r}_p|} - \frac{1}{|\mathbf{r}_1|} - \frac{1}{|\mathbf{r}_2|} - \frac{1}{|\mathbf{r}_p - \mathbf{r}_1|} - \frac{1}{|\mathbf{r}_p - \mathbf{r}_2|} + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}. \quad (2)$$

Here P_{12} stands for the exchange operator and $\mathbf{R}_i = \frac{1}{2}(\mathbf{r}_p + \mathbf{r}_i)$ and $\boldsymbol{\rho}_i = \mathbf{r}_p - \mathbf{r}_i$, $i=1,2$; $\mathbf{r}_1$ and $\mathbf{r}_2$ are the position vectors of the electrons belonging to Ps and H, respectively, and $\mathbf{r}_p$ is that of the positron with respect to the center of mass of the system. $U_{n_t l_t}(\mathbf{r})/r$ and $V_{n_p l_p}(\boldsymbol{\rho})/\rho$ are the radial parts of the wave functions of H and Ps, respectively, and $F_{\Gamma_0 \Gamma}(\mathbf{k},\mathbf{k}',R)/R$ is the radial part of the continuum wave function of the moving Ps atom; Γ_0 indicates all the quantities $n_t l_t n_p l_p L J_1 J M$ of Γ at the initial channel.

Projecting the Schrödinger Eq. (1) just as in the Hartree-Fock variational approach and integrating over the desired coordinates, we can get a set of integro-differential equations which can be transformed into integral equations like the Lippmann-Schwinger equations by applying asymptotic boundary conditions. These coupled integral equations can be formed either in momentum space or in configuration space. Fraser *et al.* used the configuration space approach [23] whereas we are using the momentum space formalism [24]. The set of coupled integral equations obtained for the scattering amplitudes is as follows:

$$f^{\pm}_{n'l',nl}(\mathbf{k}',\mathbf{k}) = B^{\pm}_{n'l',nl}(\mathbf{k}',\mathbf{k}) - \frac{1}{2\pi^2}\sum_{n''} \int d\mathbf{k}'' \frac{B^{\pm}_{n'l',n''l''}(\mathbf{k}',\mathbf{k}'') f^{\pm}_{n''l'',nl}(\mathbf{k}'',\mathbf{k})}{k^2_{n''l''} - k''^2 + i\epsilon}. \quad (3)$$

$B^{\pm}$ indicates the Born-Oppenheimer [25] scattering amplitudes; plus (+) is for the singlet channel and minus (−) for the triplet channel. The formulation for the Born matrix element is available in our previous papers [26–32]. Similarly $f^{\pm}$ indicates the unknown scattering amplitudes for the singlet and the triplet channels, respectively. The summation over $n''l''$ is to include various channels. The two sets of coupled integral equations of scattering amplitudes in momentum space for the singlet (+) and triplet (−) channels, respectively, are solved separately for each partial wave (L).

III. RESULTS AND DISCUSSION

We report our singlet (+) s-wave elastic phase shifts in Fig. 1 and corresponding cross sections in Fig. 2 using the present two- and three-channel projectile-inelastic CCA schemes. Similarly we report our triplet (−) s-wave elastic phase shifts and cross sections in Figs. 3 and 4. We have presented the corresponding static-exchange data [15–18] in all the four figures. The present phase shifts are again compared with other theoretical data for the singlet

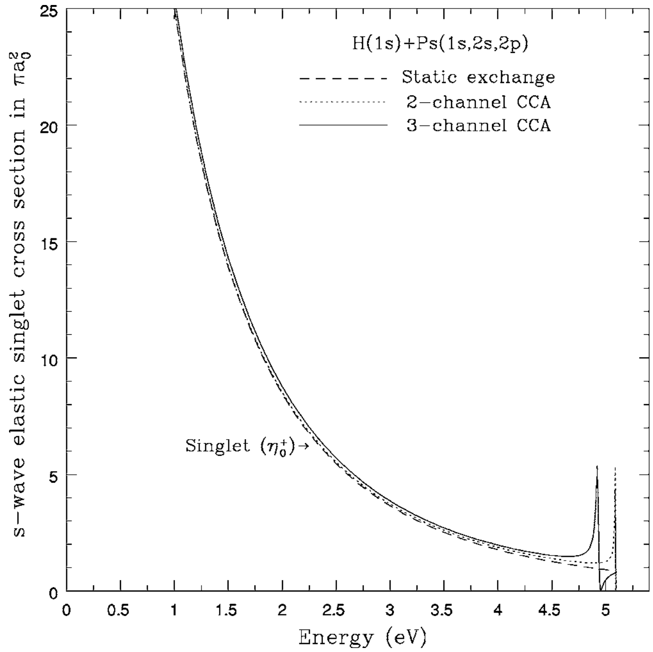

FIG. 2. The singlet (+) s-wave elastic cross sections.

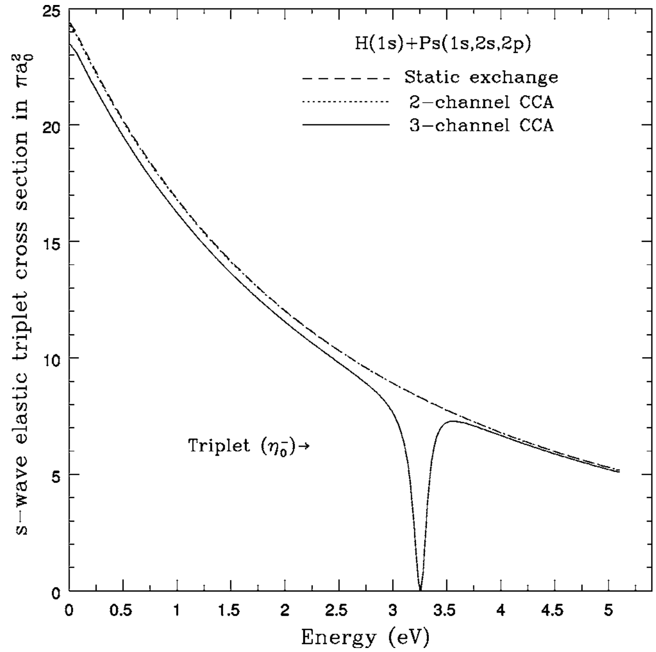

FIG. 4. The triplet (−) s-wave elastic cross sections.

channel [1,9,18] in Fig. 1 and for the triplet channel [3,9,18] in Fig. 3.

We find resonances in the singlet channel using two- and three-channel projectile-inelastic CCA schemes both in phase shift and in cross section at the energy region very close to the inelastic threshold. The position and width have both been changed by adding the target-elastic Ps($2p$) channel after the target-elastic Ps($2s$) channel. The position of the resonance is shifted toward lower energy away from threshold and the width increases. All these findings are quite consistent with the existing physics [1–14]. Our nonresonant phase shift near the resonance energy region is ~ 0.5 rad,

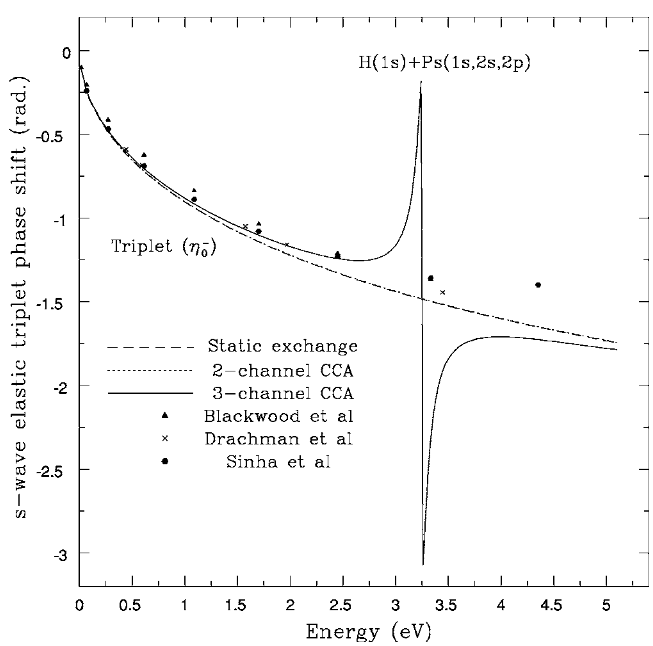

FIG. 3. The triplet (−) s-wave elastic phase shifts.

which is responsible for the peak appearing in partial cross sections and in reasonable agreement with the above discussed Breit-Wigner-like formulation.

Our triplet results using the two-channel projectile-inelastic CCA are in reasonable agreement with previous calculations of Sinha *et al.* [18]. In their three-channel CCA scheme, Sinha *et al.* [18] excluded the intermediate target-elastic $\mathrm{Ps}(2p) \rightarrow \mathrm{Ps}(2p)$ channel that is responsible for the nonadiabatic or dynamic effects [33]. Including that channel with exact exchange in our three-channel CCA scheme, we find a resonance in the triplet channel too. Our three-channel CCA results are different from theirs [18] only in the energy region near and above the resonance. We find a dip in the triplet cross section. It is again consistent with a Bright-Wigner-like formulation. In this case our nonresonant phase shift near the resonance energy region is $\sim -\pi/2$ rad; it satisfies the above mentioned second criterion of the cross section. In both Figs. 1 and 3, the solid triangles are the phase shift data obtained by Blackwood *et al.* [9], crosses are the data obtained by Drachman and Houston [1,3], and solid squares are the three-channel projectile-inelastic CCA results calculated by Sinha *et al.* [18]. However, not enough theoretical data are available to compare the present results near and above both the resonances [1–14]. So we welcome special attention in this energy region.

In addition, the present triplet phase shift data fit nicely with the nonresonant part as

$$\xi_0 = -1.4053 + 0.1295E - 0.04613E^2$$

and provide the width $\Gamma = 0.15173$ eV and resonance position $E_R = 3.2630$ eV.

An interesting question is the reality of these resonances, i.e., if we increase the basis set do the resonances still exist? Resonances above threshold were reported by Higgins and Burke [34,35] and Sarkar *et al.* [36,37] which were reported later as untrue by Zhou and Lin [38]. So the subject of above-threshold resonances needs more investigation. We discuss below-threshold resonances. According to the literature the van der Waals interaction should be important in Ps-atom scattering. In our calculation, although the van der Waals interaction has been omitted, all the Coulomb interactions are taken into account exactly in evaluating all the matrix elements required in the calculation. In addition the major quantum-mechanical effect of channel coupling from the closest excitation channels, e.g., $\mathrm{H}(1s)+\mathrm{Ps}(1s)\rightarrow\mathrm{H}(1s)+\mathrm{Ps}(2s)$ and $\mathrm{H}(1s)+\mathrm{Ps}(1s)\rightarrow\mathrm{H}(1s)+\mathrm{Ps}(2p)$ on the elastic channel $\mathrm{H}(1s)+\mathrm{Ps}(1s)\rightarrow\mathrm{H}(1s)+\mathrm{Ps}(1s)$ is considered. The target excitation channels, or the excitation of both atoms, which are responsible for the van der Waals interaction, are energetically far away from the elastic channel. Thus, according to quantum-mechanical concepts, the effect of these target excitations and both excitation channels is expected to be less important in Ps-H scattering.

However, the target-elastic $\mathrm{Ps}(3s)$ and $\mathrm{Ps}(3p)$ channels are energetically closer to the elastic channel than other channels. So calculations using these two further target-elastic projectile excitation channels in the CCA scheme are very useful for future investigation.

IV. CONCLUSION

We perform a complete and exact three-channel projectile-inelastic CCA calculation for both the singlet and triplet channels in Ps-H scattering. We study s-wave elastic phase shifts and cross sections below the inelastic threshold. We report singlet resonances using two- and three-channel projectile-inelastic CCA schemes that confirm earlier predictions [1,2]. We report a resonance in the triplet channel using the best three-channel projectile-inelastic CCA scheme.

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