

Triply excited autodissociating resonant states of positronium hydride

Y. K. Ho

Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803-4001
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Triply excited autodissociating resonant states of positronium hydride are investigated by using a method of complex-coordinate rotation. States with which the positron is attaching to the doubly excited $2s^2\ ^1S^e$ state of the H^- ion are calculated. Resonance parameters (both positions and widths) are obtained by employing elaborated Hylleraas-type wave functions in which all six interparticle coordinates are included.

INTRODUCTION

We present here a calculation of triply excited autodissociating resonant states in a positronium hydride, a system consisting of a positronium atom and a hydrogen atom. These states are a result of the positron attaching to the doubly excited $2s^2\ ^1S^e$ state of the H^- ion. In previous investigations, it has been shown that Rydberg series do exist as a result of the positron attaching to the ground state of the H^- ion. Such Rydberg states, with the exception of the lowest S -wave state, which also lies below the $Ps + H$ threshold and becomes the ground state of PsH , would appear as resonances in $Ps-H$ scattering.

Studies of positronium hydride are of continuous interest. Ore¹ first showed that this system does form a bound state. Over the years²⁻⁶ calculations of its binding energy have been improved and the latest calculation⁶ indicated that the binding energy is 0.077 89 Ry against the dissociation into positronium and hydrogen atoms. Calculations of two-photon annihilation rates are also of interest.³⁻⁶ Resonance states of PsH have been studied theoretically. The resonance parameters for the lowest S -wave resonance state in $Ps-H$ scattering have been studied by using the stabilization method⁷ and a method of complex coordinates.^{5,8} Higher resonance states of PsH converging on the ground state of H^- were studied by Drachman⁹ from the point of view that these are Rydberg states between a positively charged positron and a negatively charged H^- ion.

This work extends the investigation to the energy region below the lowest doubly excited state of H^- . A method of complex-coordinate rotation¹⁰ is used. Elaborate Hylleraas-type wave functions are employed. Figure 1 shows the energy levels of this four-particle system. In previous studies published in the literature, autodissociating resonant states of PsH below the ground state of the $H^-(1s^2)$ threshold were investigated. These states converge on the $e^+ + H^-$ threshold at -1.0555 Ry. The present investigation concentrates on the energy region below the threshold of the doubly excited $2s^2\ ^1S^e$ state at -0.297 Ry.¹¹

HAMILTONIAN AND WAVE FUNCTIONS

The Hamiltonian for this system is

$$H = -\nabla_1^2 - \nabla_2^2 - \nabla_p^2 - \frac{2}{r_1} - \frac{2}{r_2} + \frac{2}{r_p} - \frac{2}{r_{1p}} - \frac{2}{r_{2p}} + \frac{2}{r_{12}}, \tag{1}$$

where 1, 2, and p denote electrons 1, 2, and positron, respectively. The interparticle coordinate r_{1p} represents the distance between the electron 1 and the positron, and r_1 the electron 1 and the nucleus, etc. Atomic units are used in this work with energy expressed in rydbergs. The coordinate system of PsH is shown in Fig. 2.

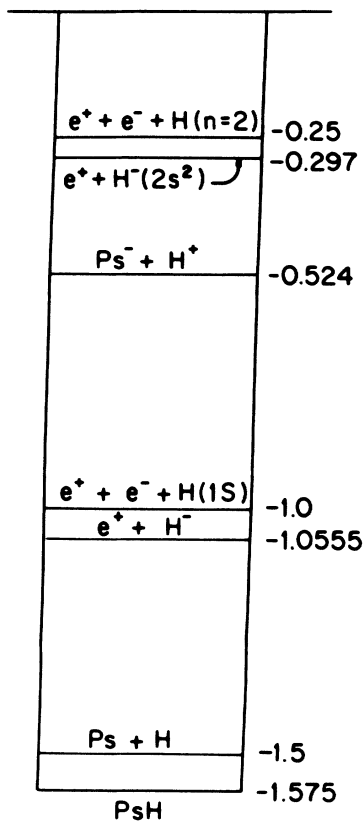


FIG. 1. Energy levels (in rydbergs) of positronium hydride.

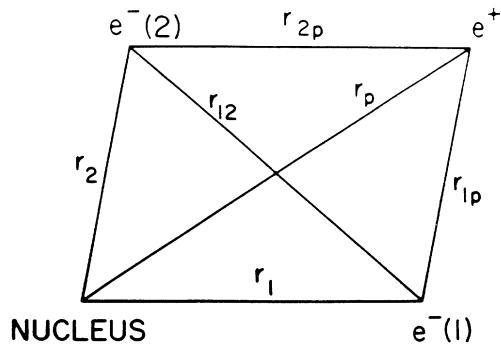


FIG. 2. Coordinate system of positronium hydride.

A general form of wave function for positronium hydride is

$$\Psi = \sum_{\substack{i,j,k \\ l,m,n}} C_{ijklmn} [r_1^i r_2^j r_p^k r_{12}^l r_{1p}^m r_{2p}^n e^{-\alpha r_1 - \beta r_2 - \gamma r_p} + (1 \leftrightarrow 2)], \quad (2)$$

where k, m, n , etc., are non-negative integers, with $\omega \leq i + j + k + l + m + n$, and $(1 \leftrightarrow 2)$ represents terms similar to those preceding but with 1 and 2 interchanged.

CALCULATIONS AND RESULTS

The method of complex-coordinate rotation (see, for example, a review by Ho¹⁰) is used to study resonance phenomena in PsH. The use of this method would provide parameters for both resonance energy positions and widths. We employ Hylleraas-type wave functions in which all six interparticle coordinates are included. A total of $N = 500$ terms are used in the present investigation.

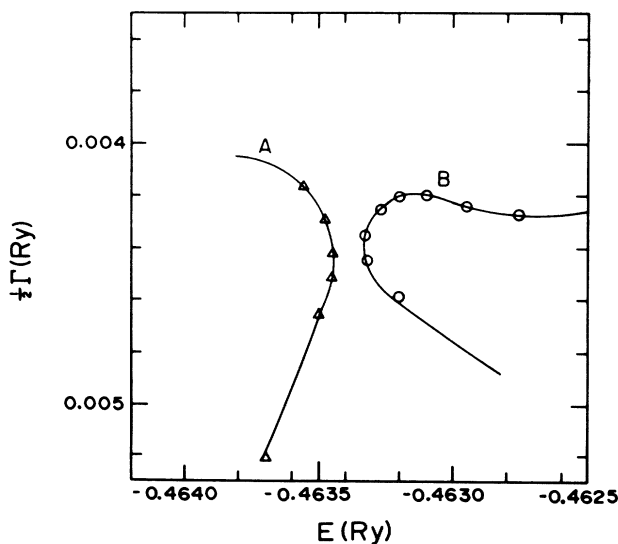


FIG. 3. Complex stabilization behavior of the $2s^2 2s\bar{s}$ state. Curve A: $\alpha = \beta = 0.5, \gamma = 0.23$. Curve B: $\alpha = \beta = 0.5, \gamma = 0.25$. The complex eigenvalues shown here are calculated as a function of θ in the increment of 0.025 rad.

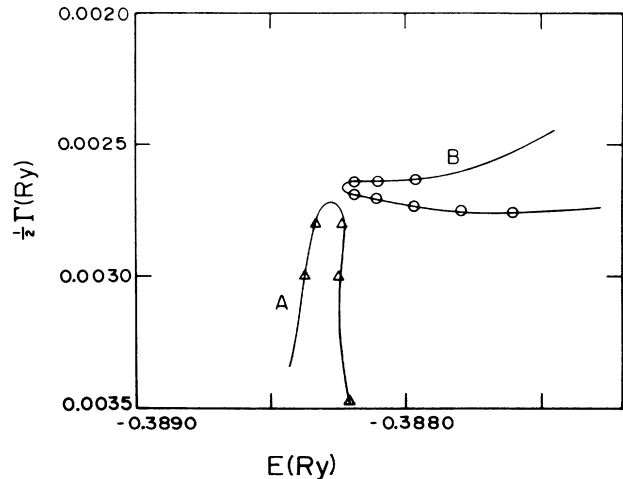


FIG. 4. Complex stabilization behavior of the $2s^2 3s\bar{s}$ state. Curve A: $\alpha = \beta = 0.5, \gamma = 0.25$. Curve B: $\alpha = \beta = 0.5, \gamma = 0.23$. The complex eigenvalues shown here are calculated as a function of θ in the increment of 0.025 rad.

The resonance parameters, both resonance positions and total widths, are deduced from the condition that the discretized complex eigenvalue is stabilized with respect to θ , where θ is the so-called rotational angle of the complex transformation $r \rightarrow r \exp(i\theta)$, i.e.,

$$d|E|d\theta = \min,$$

together with a condition that the complex eigenvalue is stabilized with respect to changes of nonlinear parameters in the wave functions.

In this work we are concentrating on the energy region below the doubly excited $2s^2 1S^e$ state of H^- . A good representation of this doubly excited state is hence needed. By keeping the two nonlinear parameters for elec-

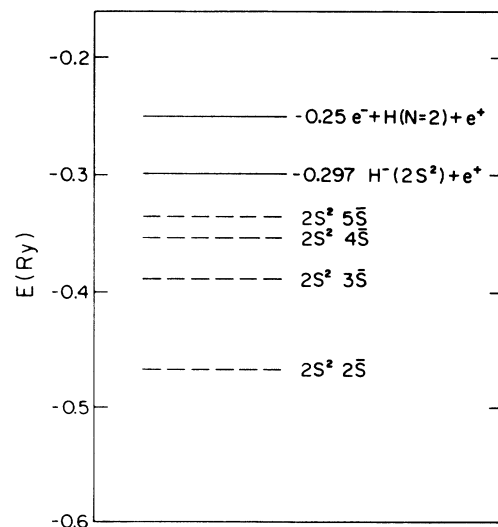


FIG. 5. Triply excited S states in PsH converging on the threshold of the doubly excited $H^-(2s^2)$ threshold.

TABLE I. Triply excited autodissociating states of PsH converging on the doubly excited $2s^2 1S^e$ state of H^- .

	E (Ry)	$\frac{1}{2}\Gamma$ (Ry)
$2s^2 2\bar{s}$	-0.4634	0.0043
$2s^2 3\bar{s}$	-0.3881	0.0027
$2s^2 4\bar{s}$	-0.3533	0.0022
$2s^2 5\bar{s}$	-0.3358	0.0017
Limit $e^+ + H^-(2s^2 1S^e)$	-0.297	

trons at $\alpha=\beta=0.5$, we have a good representation of such doubly excited state. We then vary γ as a variational parameter, and examine the complex stabilization behavior as a function of θ . Figure 3 shows the stabilization behaviors for a complex eigenvalue for two sets of nonlinear parameters. We assign this stabilized complex eigenvalue as the resonance for the $2s^2 2\bar{s}$ state. Here, the orbital with a bar on top represents that of the positron. Figure 4 shows similar complex stabilization behaviors for the $2s^2 3\bar{s}$ state. We are successful in locating four resonances below the threshold of the $H^- 2s^2 1S^e$ state (Fig. 5). The results for both resonance positions and widths are shown here in Table I. These states would appear as resonances in positron-hydrogen scattering. The resonance positions expressed in eV relative to the positronium-hydrogen scattering threshold are shown in Table II. Absent in Table I is a $2s^2 1\bar{s}$ state. We do not know where such a state, if it exists, is located. With the wave functions we used in Eq. (2) and the nonlinear parameters we employed in this work, we were unable to obtain a stabilized complex eigenvalue for such a reso-

TABLE II. Resonance positions and total widths in positronium-hydrogen scattering.

	E (eV)	Γ (eV)
$2s^2 2\bar{s}$	14.104	0.117
$2s^2 3\bar{s}$	15.128	0.073
$2s^2 4\bar{s}$	15.602	0.060
$2s^2 5\bar{s}$	15.84	0.046
Limit $e^+ + H^-(2s^2 1S^e)$	16.368	

nance. More work on this should be done in the future.

It should also be pointed out that the configuration assignment for the $2s^2 5\bar{s}$ state is tentative. It turns out that around the energy region at which this state is located, another resonance series starts to appear. These resonances belong to the $3s^2 n\bar{s}$ series, converging on the doubly excited $3s^2 1S$ state in H^- . More work should be done in the future in order to clarify the classification for this resonance at -0.3358 Ry.

In summary, we have located four triply excited autodissociating states in PsH below the threshold of the doubly excited $2s^2 1S^e$ state of H^- . The present work is the first calculation of resonances in this energy region. The resonance parameters reported here would be of interest in future theoretical and experimental work.

ACKNOWLEDGMENTS

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