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A resonant state and the ground state of positronium hydride

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The lowest-lying resonance occurring in S-wave positronium-hydrogen scattering is reinvestigated, using the complex-rotation method. By employing a generalized Hylleraas-type wave function that includes all six interparticle coordinates, a very accurate value of the resonance position E_r is obtained, along with a good value of the width. The present result for E_r (-1.205 ± 0.001 Ry) is lower than the previous result of Drachman and Houston, who omitted the interelectronic coordinate r_{12} in their trial function. In addition, the lowest ground-state energy of positronium hydride is obtained by using 210 terms in the trial wave function. The effect of the r_{12} coordinate and others on both the resonant energy and the binding energy of PsH is discussed.

I. INTRODUCTION

The system consisting of a positronium and a hydrogen atom in a total S state has been investigated theoretically in recent years. The binding energy of the particle-stable ground state of the system (called positronium hydride) has been calculated by several authors.[1-4] The problem of elastic scattering has been examined by Fraser and his co-workers[5-8] and recently by Drachman and Houston.[9-11] A possible resonance in the positronium-hydrogen elastic scattering was first discussed by Drachman and Houston[9,10] and recently by Page.[8] The former authors,[9] who employed the stabilization method,[12] pointed out that below the excitation threshold of positronium there is a stabilized eigenvalue and suggested that a resonance occurs at a scattering energy of 4.5 eV, about 0.6 eV below the excitation threshold. They[10] also used the complex-rotation method[13,14] to confirm the existence of the resonance and found that its width is about 0.06 eV. Recently Page[8] used a numerical algebraic Kohn method and confirmed such resonance at about 4.45 eV with a smaller width of 0.05 eV. In Refs. 9 and 10, however, the authors used a less complete Hylleraas-type wave function in which the r_{12} coordinate—the correlation between two electrons—was omitted. That omission caused an almost 33% reduction in the binding energy, as demonstrated by Page and Fraser.[3]

In this work we examine the resonance by using a generalized Hylleraas-type wave function such that the six interelectronic coordinates are included. Although Page[8] did include all the coordinate factors including the product terms of r_{12} and r_{1p},[15] his agreement with Ref. 10 is probably partly coincidental, since he only used a small number of correlation terms (35 terms without r_{12} and 15 terms with r_{12} coordinate). Generally the resonance position will be lower if more correlation terms are used. In the present calculation, we use the complex-rotation method[13] to determine the resonance parameters. In addition, we study the effect of the individual correlation factors of the six coordinates by omitting each of them in turn from the trial wave function.

II. CALCULATIONS AND RESULTS

In this work, we use a generalized ($L=0$, S-wave) Hylleraas-type wave function similar to the calculation of the binding energy of PsH[3] and, for the problem of positron attachment to ^3S helium state,[16]

$$\Psi = \sum_{k,l,m,n \geq 0}^{N} C_{klmn} e^{-\gamma r_p} r_p^m r_{12}^k \times \left(e^{-\alpha r_1 - \beta r_2} r_1^l r_{1p}^n + e^{-\beta r_1 - \alpha r_2} r_2^l r_{2p}^n\right), \tag{1}$$

where k, l, m, n are integers such that $k+l+m+n \leqslant \omega$. For the resonance calculation we use up to $\omega=5$ which corresponds to $N=126$ terms. The technique used to estimate the resonance parameters is the complex-rotation method.[13,14] The complex-rotation method "rotates" the nonrelativistic Hamiltonian $H(r)$ into a complex energy plane by transforming r into $re^{i\theta}$ for $\theta > 0$ and real. One is able to obtain the resonant parameters by solving the complex eigenvalue equation:

$$|\langle \Psi | H(r,\theta) - W | \Psi \rangle| = 0, \tag{2}$$

where

$$H(r,\theta) = Te^{-2i\theta} + Ve^{-i\theta} \tag{3}$$

(for pure Coulombic interactions) and

$$W = E_r - \tfrac{1}{2} i \Gamma. \tag{4}$$

In Eq. (3), T and V are the kinetic and potential energy operators, respectively. Doolen[14] observed that in the complex energy plane, as the rotational angle θ increased, the nonresonant eigenvalues rotated uniformly away from the real axis while the resonant eigenvalue rotated "toward" the reso-

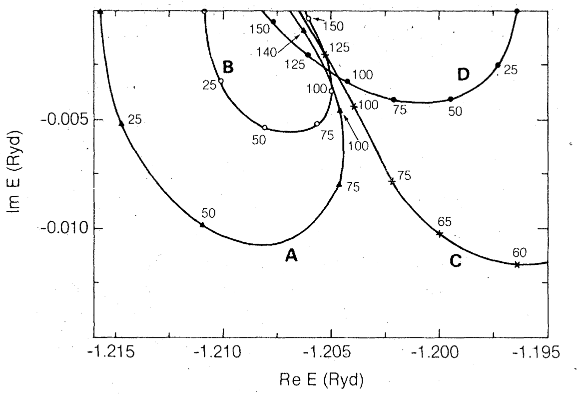

FIG. 1. Rotational paths for the resonance in the Ps-H elastic scattering. The rotation angle θ is shown in milliradians near each eigenvalue. In this figure, 126 terms ($\omega=5$) are used. Curve A: $\alpha=0.65$, $\beta=1.0$, $\gamma=0.59$; curve B: $\alpha=0.75$, $\beta=1.0$, $\gamma=0.50$; curve C: $\alpha=0.63$, $\beta=1.0$, $\gamma=0.59$; curve D: $\alpha=0.65$, $\beta=1.03$, $\gamma=0.50$.

nant position, "slowed down," and then rapidly rotated away. For small changes in the nonlinear parameters [Eq. (1)], the resonant eigenvalue simply rotates from different directions but eventually "converges" to the same position, provided that the wave function is good enough to represent the system. In the present calculation we employ the same technique as that of Doolen.[14]

A typical result (for $\omega=5$) is shown in Fig. 1, in which four different sets of nonlinear parameters are used. We estimate the resonance parameters to be

$$E_r=-1.205\pm0.001\ \text{Ry},\qquad \Gamma=0.0055\pm0.0020\ \text{Ry}. \tag{5}$$

These results may be compared with those of Ref. 10, which were also obtained by the complex-rotation method:

$$E_r=-1.1726\pm0.0007\ \text{Ry},\qquad \Gamma=0.0046\pm0.0010\ \text{Ry}. \tag{6}$$

Although the two values of Γ obtained are consistent, the present value of E_r lies lower by 0.032 Ry, outside the estimated errors of the two calculations. Noting that a major component of the resonant wave function must be the configuration $e^+\text{H}^-$, one may suspect that much of the difference between the two values of E_r concerns the accuracy with which the H^- ion is represented. In fact, the binding energy of H^- is underestimated by 0.0266 Ry when the r_{12} coordinate is omitted; this accounts for about 80% of the above discrepancy. To clarify in detail the sensitivity of E_r and Γ to the various correlation terms, the complex-rotation calculation was repeated with each omitted in turn.

The results are shown in Table I along with previous results. They can be summarized as follows: First, product terms of the form $r_{12}r_{1p}$ are not very important (column 2), and their omission simplifies and speeds the computation greatly. Second, when all r_{12} terms are removed (column 3), the results of Ref. 10 are recovered. Finally, when the r_{1p} terms are removed (column 4), it is found that no reasonable value for Γ can be obtained, although E_r is hardly affected. Here we used the stabilization technique[12] to estimate the resonance position E_r.

This last situation can be understood as follows: The width of the resonance is due to the decay of the resonant state through the Ps-H channel, the only open channel at this energy. If we omit the r_{1p} terms in the trial function, we are unable to represent the decay channel properly and so are unable to calculate Γ. The trial function with r_{1p} terms omitted thus resembles a Q-projected function in the Feshbach sense, with the width due to coupling with the open channel.

The analogy with the Feshbach method should not be overemphasized, however, since the lowest S-wave resonance with r_{1p} omitted is not the lowest eigenvalue. To examine the properties of the ground state of PsH, the effect of the omission of certain correlation terms on the lowest eigenvalue was also studied and is shown in Table II.

The results of Table II can be summarized as

TABLE I. Effect on resonance of PsH due to different correlation factors (results are in Ry).

	Present calculation ($\omega=5$)				Previous calculations	
N	126	91	56	56		
Terms omitted from Eq. (1)		$r_{1p}r_{12}$	r_{12}	r_{1p}	Drachman-Houston[10]	Page[8]
E_r	-1.205 ± 0.001	-1.204 ± 0.001	-1.173[a]	-1.204[b]	-1.1726 ± 0.007	-1.1738
Γ	0.0055 ± 0.0020	0.0055 ± 0.0020	0.0046[a]	$\cdots$[b]	0.0046 ± 0.001	0.0035

[a] Result of Ref. 10 is qualitatively reproduced.

[b] Determined from stabilization method; also see text.

TABLE II. Effect on ground-state energy of PsH due to different correlation factors. The nonlinear parameters ($\alpha=0.63$, $\beta=0.986$, $\gamma=0.59$) are nearly optimized at $\omega=5$ (126 terms).

	Present calculation						Previous calculations			
ω	6	5	5	4	5	5	PF[3]	C[4]	NSL[2]	HD[1]
N	210	126	91	55	56	56				
Terms omitted from Eq. (1)			$r_{1p}r_{12}$	$r_{1p}r_{12}$	r_{12}	r_{1p}				
$-E$ (Ry)	1.57505	1.57472	1.57124	1.57020	1.54634	1.41832	1.5736	1.5684	1.5584	1.5496
E_a (eV)[a]	1.02112	1.01663	0.96928	0.95513	0.63049		1.0014	0.9306	0.7946	0.6748

[a] $R_\infty = 13.60580$ eV

follows: When all r_{1p} terms are omitted (column 6), thus effectively removing any reference to the Ps-H configuration, the lowest eigenvalue does not even correspond to a bound state, although, as seen before, the resonant energy was given well in this approximation. The next most important type of correlation term is r_{12}; including it increases the binding energy over that in Ref. 1 by more than 40%. Less important are the product terms of the form $r_{12}r_{1p}$ (columns 3 and 4), which contribute about 5% to the binding energy. The present result for $\omega=6$, $N=210$ (column 1) improves upon the best previous result[3] for the binding energy of PsH, giving a value of 1.02112 eV against dissociation into Ps + H.

III. DISCUSSION AND CONCLUSION

We have performed a calculation of a resonant eigenvalue of the positronium-hydride by the complex-rotation method and also provided the best variational ground state energy of PsH. We have found that the resonant position is significantly different from the previous calculation, and an explanation has been suggested. The contribution to the resonant position and the ground-state energy from different interelectronic coordinates have been tested. Although the marked effect of the r_{12} terms is clear for the resonance position and the r_{1p} terms are important to determine the width, we believe, however, that the width we obtained is not conclusive. We feel that in the terminology of the complex-rotation method, the rotational paths do not "slow down" enough when they come across the resonance position. Other methods to determine resonant parameters may be worthwhile to try. For example, the calculation of Ref. 8 should be extended to include more correlation terms. In particular, one must include both r_{12} and r_{1p} factors. But at the same time, one can afford to omit the product terms of r_{12} and r_{1p} and still get quite accurate results. As demonstrated in this work, such product terms only produce a small contribution to the resonance position (although they are important for accurate calculation of the binding energy). It is practical to omit such product terms in resonance calculations since they will consume the most computing time.

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[15] Throughout this text, r_{1p} implies both r_{1p} and its symmetric part r_{2p}. They represent the correlations between the electrons and positron.

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