

High partial wave resonances in positron hydrogen scattering

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In this work, we present results for high-angular-momentum resonances in positron-hydrogen scattering obtained by using the method of complex-coordinate rotations. Resonance states with angular momenta of $L = 3$ to 6 are calculated using highly correlated Hylleraas-type wave functions. Furthermore, for the $L=0$ and 1 states, we present our updated results. Comparisons with other calculations are made.

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I. INTRODUCTION

The atomic system that consists of a positron and a hydrogen atom has attracted considerable interest. This system contains three distinct particles: a positron, an electron, and a proton, but they do not form a bound state. However, there exist many quasibound states that lie in the e^+ -H scattering continua. There has been a long history on investigations of the existence of resonances in e^+ -H scattering. There are similarities and differences between resonances in e^- -H scattering and those in e^+ -H scattering. It is well known that the resonances below the H ($N=2$) threshold in e^- -H scattering are the result of the $2s$ - $2p$ degeneracy of the excited $N=2$ states of the target hydrogen atom [1]. Mittleman [2] pointed out that the attractive dipole potential, which behaves like r^{-2} asymptotically in e^+ -H scattering, would be the same as that in e^- -H scattering, and such resonances in e^+ -H scattering should also exist. In the latter case, there exists a lower-lying positronium formation channel. However, since the opening of this channel is of short-range effect, it will not affect the existence of such dipole resonances even though the positions and widths may change. The first definitive calculation to establish that S -wave resonances exist in e^+ -H scattering below the H ($N=2$) threshold was carried out by Doolen *et al.* [3] using the method of complex-coordinate rotation (see Ref. [4] and references therein). They used Pekeris functions that include explicitly the coordinates for positronium atoms. Choo *et al.* [5] and Trembl [6] have provided the theoretical justification for the existence of resonances lying below the H ($N=2$) threshold. The method of complex-coordinate rotation has also been used to calculate the S -wave resonances in

e^+ -H scattering associated with higher thresholds of the hydrogen and positronium atoms [7]. In addition to the S -wave resonances, P - and D - wave resonances have also been calculated by using different methods. The earlier investigation of P -wave resonances below the H ($N=2$) threshold was a three-state ($1s$ - $2s$ - $2p$) close-coupling calculation [8]. However, in Ref. [8] the lower-lying positronium formation channel was not included. In recent years, several methods have been used to calculate resonances in e^+ -H scattering, including the method of complex-coordinate rotation [9,10]. Other recent work includes the close-coupling method [11], the use of hyperspherical functions [12,13], and the Harris-Nesbet variational method [14]. The complex-coordinate results can be used as an assessment of merit for these calculations. While the resonances in e^+ -H scattering have yet to be observed in laboratories, theoretical activity on this fundamental system has been the subject of several reviews [15]. There has also been considerable interest in the investigations of resonances in another few-body positronic system, positronium hydride (PsH) [16–19].

In this work, we present results for high-angular-momentum resonances in positron-hydrogen scattering obtained by using the method of complex-coordinate rotation. Resonance states with angular momentum of $L=3$ (F states) to 6 (I states) are calculated by using highly correlated Hylleraas-type wave functions. To the best of our knowledge, such high-angular-momentum resonance states in the e^+ -H system have not been reported in the literature until now. As for the $L=0$ to 1 states, we present our updated results. Comparisons with other calculations are made.

TABLE I. States with total angular momentum L .

State	L	(l_1, l_2)	Ω	Total N
S	0	(0,0)	20	1771
P	1	(1,0);(0,1)	21	$2 \times 1771 = 3542$
D	2	(2,0);(1,1);(0,2)	20	$3 \times 1330 = 3990$
F	3	(3,0);(2,1);(1,2);(0,3)	19	$4 \times 969 = 3876$
G	4	(4,0);(3,1);(2,2);(1,3);(0,4)	19	$5 \times 816 = 4080$
H	5	(5,0);(4,1);(3,2);(2,3);(1,4);(0,5)	19	$6 \times 680 = 4080$
I	6	(6,0);(5,1);(4,2);(3,3);(2,4);(1,5);(0,6)	19	$7 \times 560 = 3920$

TABLE II. *S*-wave resonances in e^+ -H scattering. In the column for widths, $a[-b]$ implies $a \times 10^{-b}$.

Present work		Other work	
E_r (Ry)	$\Gamma/2$ (Ry)	E_r (Ry)	$\Gamma/2$ (Ry)
Below H ($N=2$) threshold ($E_t=-0.25$ Ry)			
-0.257 374 25	6.674[-5]	-0.257 374 ^a	6.65[-5]
		-0.257 06 ^b	7.8[-5]
		-0.257 243 ^c	6.5[-5]
		-0.257 312 ^d	6.64[-5]
-0.250 399 6	3.9[-6]	-0.250 36 ^b	3.95[-6]
		-0.250 385 ^c	3.35[-6]
		-0.250 302 ^d	3.91[-6]
Below Ps ($N=2$) threshold ($E_t=-0.125$ Ry)			
-0.150 317 68	3.3397[-4]	-0.150 316 ^d	3.342[-4]
-0.131 677 5	1.63[-4]	-0.131 704 ^d	1.624[-4]
-0.126 75	6.0[-5]	-0.126 806 ^d	5.03[-5]
Below H ($N=3$) threshold ($E_t=-0.111$ 11 Ry)			
-0.116 13	6.3[-4]	-0.116 101 ^d	6.161[-4]
-0.112 125	1.34[-4]	-0.112 100 ^d	1.300[-4]
Below H ($N=4$) threshold ($E_t=-0.0625$ Ry)			
-0.077 0876	4.74[-5]	-0.077 100 ^d	4.762[-5]
-0.067 8935	4.75[-5]	-0.067 902 ^d	4.782[-5]
-0.064 613	1.65[-5]	-0.064 625 ^d	1.625[-5]
-0.063 727	5.0[-5]	-0.063 725 ^d	4.884[-5]
-0.063 315	4.0[-6]	-0.063 304 ^d	2.7[-5]
Below H ($N=5$) threshold ($E_t=-0.04$ Ry)			
-0.047 268	8.6[-6]		
-0.043 17	6.0[-6]		
-0.042 396	1.70[-5]		
-0.041 4	2.0[-6]		
-0.040 518	6.5[-6]		
Below Ps ($N=4$) threshold ($E_t=-0.031$ 25 Ry)			
-0.034 96	9.6[-5]		
-0.032 58	4.5[-5]		

^aComplex rotation (Doolen *et al.* [3]).^b21-state close coupling (Mitroy [11]).^cHarris-Nesbet variational (Gien [14]).^dHyperspherical (Zhou and Lin [13]).

TABLE III. *P*-wave resonances in e^+ -H scattering. In the column for widths, $a[-b]$ implies $a \times 10^{-b}$.

Present work		Other work	
E_r (Ry)	$\Gamma/2$ (Ry)	E_r (Ry)	$\Gamma/2$ (Ry)
Below H($N=2$) threshold ($E_t=-0.25$ Ry)			
-0.254 113	8.0[-6]	-0.254 132 ^a	8.152[-6]
Below Ps ($N=2$) threshold ($E_t=-0.125$ Ry)			
-0.148 181	2.95[-4]	-0.148 071 ^a	2.936[-4]
-0.130 73	1.64[-4]	-0.130 666 ^a	1.480[-4]
-0.127 353	6.88[-5]	-0.127 343 ^a	6.73[-5]
Below H ($N=3$) threshold ($E_t=-0.111$ 11 Ry)			
-0.115 563	5.725[-4]	-0.115 626 ^a	5.71[-4]
-0.111 955	1.1[-4]	-0.111 953 ^a	1.167[-4]
-0.111 675	6.5[-6]	-0.111 70 ^a	6.61[-6]
-0.111 22	6.0[-5]		
Below H ($N=4$) threshold ($E_t=-0.0625$ Ry)			
-0.076 608 5	5.1[-5]	-0.076 673 ^a	5.289[-5]
-0.071 155 8	5.96[-5]	-0.071 211 ^a	5.698[-5]
-0.067 562 2	4.78[-5]	-0.067 585 ^a	4.666[-5]
-0.064 460	1.3[-5]	-0.064 520 ^a	1.31[-5]
-0.064 280	2.86[-5]	-0.064 360 ^a	2.81[-5]
-0.063 274	1.0[-5]		
-0.063 161 5	2.3[-5]		
Below Ps ($N=3$) threshold ($E_t=-0.055$ 55 Ry)			
-0.059 804	4.3[-4]		
-0.056 912	1.325[-4]		
Below H ($N=5$) threshold ($E_t=-0.04$ Ry)			
-0.047 115 5	8.2[-6]		
-0.045 074 2	5.62[-5]		
-0.043 061 5	6.1[-6]		
-0.042 182	1.48[-5]		
-0.041 725	2.85[-5]		
-0.0413	5.0[-6]		
-0.040 61	1.9[-5]		
-0.040 445	6.0[-6]		
Below Ps ($N=4$) threshold ($E_t=-0.031$ 25 Ry)			
-0.037 11	2.34[-4]		
-0.034 808	8.8[-5]		
-0.034 26	1.8[-4]		
-0.032 499	4.8[-5]		
-0.031 867	4.5[-5]		

^aHyperspherical coordinates (Zhou and Lin [13]).

TABLE IV. *F*-wave resonances in e^+ -H scattering. In the column for widths, $a[-b]$ implies a $\times 10^{-b}$.

E_r (Ry)	$\Gamma/2$ (Ry)
Below Ps ($N=2$) threshold ($E_t=-0.125$ Ry)	
-0.137 694 1	4.73[-5]
-0.126 776	1.75[-5]
Below H ($N=3$) threshold ($E_t=-0.111$ 11Ry)	
-0.113 062 8	2.313[-4]
-0.111 28	7.0[-5]
Below H ($N=4$) threshold ($E_t=-0.0625$ Ry)	
-0.074 226 5	7.54[-5]
-0.067 999	8.8[-5]
-0.065 992	4.95[-5]
-0.063 635	1.9[-5]
-0.063 207	1.95[-5]
Below Ps($N=3$) threshold ($E_t=-0.055$ 55 Ry)	
-0.058 055	1.98[-4]
Below H ($N=5$) threshold ($E_t=-0.04$ Ry)	
-0.046 352 3	5.1[-6]
-0.044 149 5	6.98[-5]
-0.042 548	5.5[-6]
-0.041 648	3.9[-5]
-0.041 245	3.5[-5]
-0.041 167	1.9[-5]
Below Ps ($N=4$) threshold ($E_t=-0.031$ 25 Ry)	
-0.036 52	2.3[-4]
-0.034 435	8.0[-5]
-0.034 03	8.7[-5]
-0.033 75	1.8[-4]
-0.032 3	1.3[-4]
-0.031 735	4.5[-5]

II. HAMILTONIAN AND WAVE FUNCTIONS

The total Hamiltonian H for the e^+ -H system, with the energy expressed in Rydberg units, is given by

$$H = T + V, \tag{1}$$

with

TABLE V. *G*-wave resonances in e^+ -H scattering. In the column for widths, $a[-b]$ implies a $\times 10^{-b}$.

E_r (Ry)	$\Gamma/2$ (Ry)
Below Ps ($N=2$) threshold ($E_t=-0.125$ Ry)	
-0.130 279	3.15[-5]
Below H($N=3$) threshold ($E_t=-0.111$ 11 Ry)	
-0.111 442 6	2.35[-5]
Below H ($N=4$) threshold ($E_t=-0.0625$ Ry)	
-0.072 351	7.4[-5]
-0.065 704 8	9.71[-5]
-0.064 872 7	2.85[-5]
-0.063 115	1.1[-5]
-0.062 65	6.0[-6]
Below Ps ($N=3$) threshold ($E_t=-0.055$ 55 Ry)	
-0.056 963	2.68[-4]
Below H ($N=5$) threshold ($E_t=-0.04$ Ry)	
-0.045 738 2	6.2[-6]
-0.043 423 4	6.05[-5]
-0.042 157	5.4[-6]
-0.040 923	3.7[-5]
-0.040 839	2.5[-5]
-0.040 82	1.0[-5]
-0.040 491	3.0[-5]
Below Ps ($N=4$) threshold ($E_t=-0.031$ 25 Ry)	
-0.036 025	1.85[-4]
-0.033 795	1.05[-4]
-0.033 53	1.0[-4]
-0.033 278	9.0[-5]

$$T = -\nabla_1^2 - \nabla_2^2 \tag{2}$$

and

$$V = -\frac{2}{r_1} + \frac{2}{r_2} - \frac{2}{r_{12}}, \tag{3}$$

where the indices 1 and 2 refer to the coordinates of the electron and the positron. Throughout this work an infinite nuclear mass is used. The basis set is constructed using Hylleraas coordinates

TABLE VI. H -wave resonances in e^+ -H scattering. In the column for widths, a[-b] implies $a \times 10^{-b}$.

E_r (Ry)	$\Gamma/2$ (Ry)
Below H ($N=4$) threshold ($E_t=-0.0625$ Ry)	
-0.070 038 5	5.1[-5]
-0.063 798 5	2.70[-5]
-0.063 182	4.1[-5]
Below Ps ($N=3$) threshold ($E_t=-0.05555$ Ry)	
-0.055 95	3.35[-4]
Below H ($N=5$) threshold ($E_t=-0.04$ Ry)	
-0.044 975	1.3[-5]
-0.042 527	4.3[-5]
-0.041 697	9.0[-6]
-0.040 56	2.0[-5]
-0.040 52	1.6[-5]
-0.040 10	1.8[-5]
Below Ps ($N=4$) threshold ($E_t=-0.031 25$ Ry)	
-0.035 4	1.35[-4]
-0.033 1	1.0[-4]
-0.032 83	5.8[-5]
-0.032 58	9.5[-5]

TABLE VII. I -wave resonances in e^+ -H scattering. In the column for widths, a(-b) implies $a \times 10^{-b}$.

E_r (Ry)	$\Gamma/2$ (Ry)
Below H ($N=4$) threshold ($E_t=-0.0625$ Ry)	
-0.067 337	1.67[-5]
-0.062 83	2.3[-5]
Below Ps ($N=3$) threshold ($E_t=-0.055 55$ Ry)	
-0.0549	3.0[-4]
Below H ($N=5$) threshold ($E_t=-0.04$ Ry)	
-0.044 078	2.8[-5]
-0.041 504 4	3.45[-5]
-0.041 19	1.35[-5]
Below Ps ($N=4$) threshold ($E_t=-0.031 25$ Ry)	
-0.034 65	1.75[-4]

TABLE VIII. Resonances in e^+ -H scattering below the H ($N=2$) threshold.

State	L	E_r (Ry)	$\Gamma/2$ (Ry)
S	0	-0.257 374 25	6.674[-5]
P	1	-0.254 113	8.0[-6]
D	2	-0.250 095 9	1.4[-6]

$$\{\chi_{ijk}(\alpha, \beta) = r_1^i r_2^j r_{12}^k e^{-\alpha r_1 - \beta r_2} y_{l_1 l_2}^{LM}(\hat{r}_1, \hat{r}_2)\}, \quad (4)$$

where $y_{l_1 l_2}^{LM}(\hat{r}_1, \hat{r}_2)$ is the vector coupled product of solid spherical harmonics for the electron and the positron forming an eigenstate of total angular momentum L defined by

$$y_{l_1 l_2}^{LM}(\hat{r}_1, \hat{r}_2) = \sum_{m_1 m_2} \langle l_1 l_2 m_1 m_2 | LM \rangle Y_{l_1 m_1}(\hat{r}_1) Y_{l_2 m_2}(\hat{r}_2), \quad (5)$$

and $r_{12} = |\bar{r}_1 - \bar{r}_2|$ is the distance between the electron and the positron. The explicit form of the wave functions is

$$\Psi = (\bar{r}_1, \bar{r}_2) = \sum_{ijk} a_{ijk} x_{ijk}(\alpha, \beta), \quad (6)$$

where $i+j+k+L \leq \Omega$ with i, j and k being positive integer or zero. L is the total angular momentum of a particular resonance state. Detailed evaluation of the basic integrals that appear in our calculations can be found in Ref. [20].

III. CALCULATIONS AND RESULTS

In calculations of resonance energies and widths using the method of complex-coordinate rotation [4], the radial coordinate r (r stands for r_1, r_2 , or r_{12}) is transformed into $re^{i\theta}$,

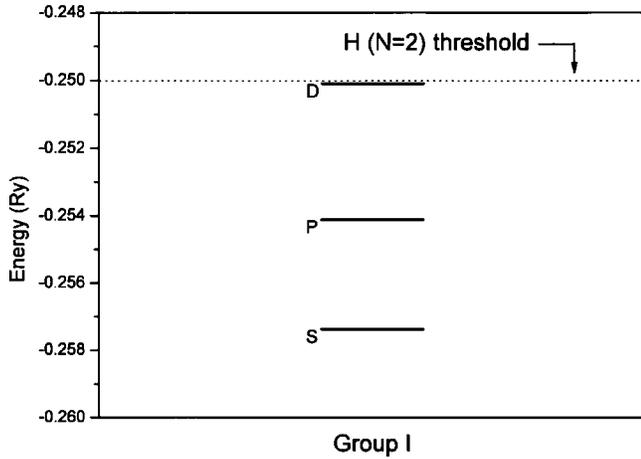


FIG. 1. A group of resonances for different angular momentum states lying below the H ($N=2$) threshold.

where θ is the rotational angle. A complex eigenvalue is determined as a resonance eigenvalue when it exhibits stabilized character with respect to changes of α and β in the wave functions [see Eq. (4)]. Furthermore, the resonance eigenvalue also shows convergence behavior when the size of the basis is increased.

For a state with total angular momentum $L=3$, we have four basic possible combinations to which the individual angular momenta (l_1, l_2) are coupled. Here l_1 and l_2 are the angular momenta for the electron and the positron, respectively. The possible values for (l_1, l_2) are (3,0), (2,1), (1,2), and (0,3). The higher harmonics are taken care of by the r_{ij} terms. For each sum in Eq. (6), we use basis sets up to $\Omega = 19$, leading to 969 terms for each sum. The total number of terms for $L=3$ states is hence equal to $4 \times 969 = 3876$. Table I shows the total number of terms and the individual (l_1, l_2) pairs for different angular momentum states. States with angular momentum up to $L=6$ are investigated in this work.

TABLE IX. Resonances in e^+ -H scattering below the Ps ($N=2$) threshold.

State	L	E_r (Ry)	$\Gamma/2$ (Ry)
Group I			
<i>S</i>	0	-0.150 317 68	3.3397[-4]
<i>P</i>	1	-0.148 181 0	2.95[-4]
<i>D</i>	2	-0.143 929 9	1.684[-4]
<i>F</i>	3	-0.137 694 1	4.73[-5]
<i>G</i>	4	-0.130 279 0	3.15[-5]
Group II			
<i>S</i>	0	-0.131 677 5	1.63[-4]
<i>P</i>	1	-0.130 749 1	1.507[-4]
<i>D</i>	2	-0.128 950 5	6.96[-5]
<i>F</i>	3	-0.126 776	1.75[-5]

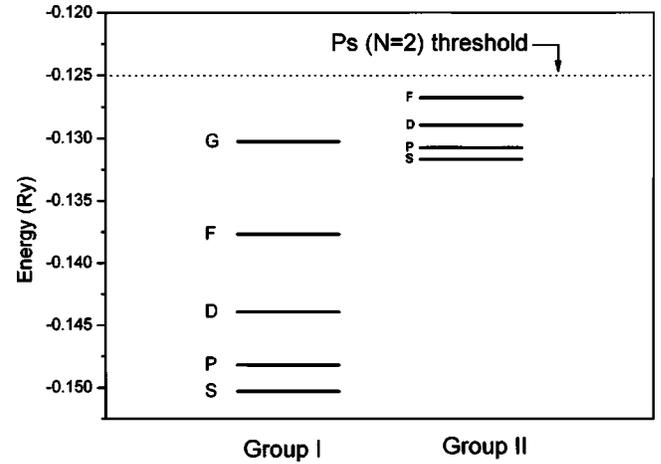


FIG. 2. Two groups of resonances for different angular momentum states lying below the Ps ($N=2$) threshold.

For G states ($L=4$), we use $\Omega=19$, which corresponds to 816 terms for the individual (l_1, l_2) pair. The total number of terms is $5 \times 816 = 4080$. For $L=5$ and 6 states, the total numbers of terms are $N=6 \times 680 = 4080$ and $N=7 \times 560 = 3720$, respectively.

For completeness, we also present our updated results for $L=0$ and 1 states in Tables II and III, respectively. Table II also shows the comparison with other calculations. For resonances below the H ($N=2$) threshold, other work includes close-coupling calculations [11], hyperspherical close-coupling calculations [13], and calculations using the Harris-Nesbet variational method [14]. For the P -wave states below the H ($N=4$) threshold, Table III also shows a comparison with the hyperspherical close-coupling calculations [14]. It is seen that the agreement is generally quite good. Table III also shows our results for resonances lying above the H ($N=4$) and below the Ps ($N=4$) threshold. To our knowledge, there are no other calculations reported for such resonances in the

TABLE X. Resonances in e^+ -H scattering below the H ($N=3$) threshold.

State	L	E_r (Ry)	$\Gamma/2$ (Ry)
Group I			
<i>S</i>	0	-0.116 13	6.3[-4]
<i>P</i>	1	-0.115 563	5.725[-4]
<i>D</i>	2	-0.114 525	4.64[-4]
<i>F</i>	3	-0.113 062 8	2.313[-4]
<i>G</i>	4	-0.111 442 6	2.35[-4]
Group II			
<i>S</i>	0	-0.112 125	1.34[-4]
<i>P</i>	1	-0.111 955	1.08[-4]
<i>D</i>	2	-0.111 65	7.5[-5]
<i>F</i>	3	-0.111 25	1.3[-5]

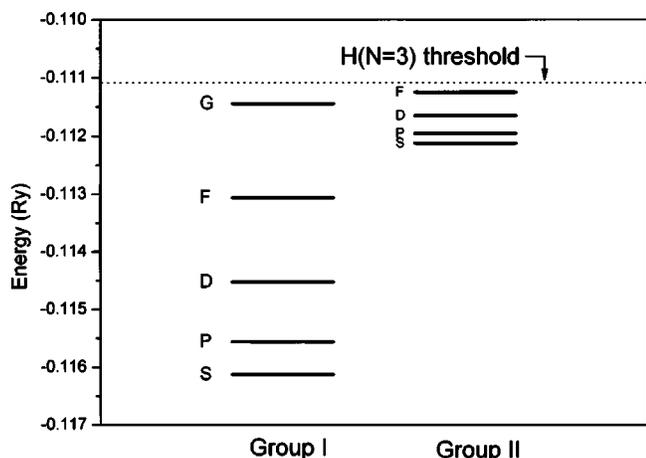


FIG. 3. Two groups of resonances for different angular momentum states lying below the H(N=3) threshold.

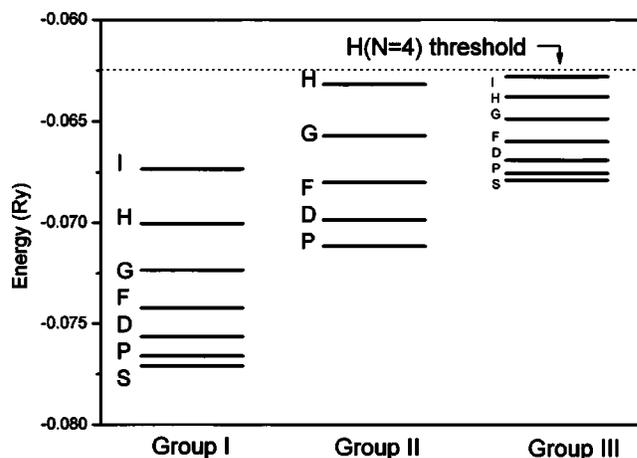


FIG. 4. Three groups of resonances for different angular momentum states lying below the H(N=4) threshold.

TABLE XI. Resonances in e^+ -H scattering below the H(N=4) threshold.

State	L	E_r (Ry)	$\Gamma/2$ (Ry)
Group I			
<i>S</i>	0	-0.077 087 6	4.74[-5]
<i>P</i>	1	-0.076 608 5	5.1[-5]
<i>D</i>	2	-0.075 650 4	6.05[-5]
<i>F</i>	3	-0.074 226 5	7.54[-5]
<i>G</i>	4	-0.072 351	7.4[-5]
<i>H</i>	5	-0.070 039	5.1[-5]
<i>I</i>	6	-0.067 337	1.67[-5]
Group II			
<i>P</i>	1	-0.071 155 8	5.96[-5]
<i>D</i>	2	-0.069 857 5	7.34[-5]
<i>F</i>	3	-0.067 999	8.8[-5]
<i>G</i>	4	-0.065 704 8	9.71[-5]
<i>H</i>	5	-0.063 182	4.1[-5]
Group III			
<i>S</i>	0	-0.067 893 5	4.75[-5]
<i>P</i>	1	-0.067 562 2	4.78[-5]
<i>D</i>	2	-0.066 912 8	4.88[-5]
<i>F</i>	3	-0.065 992	4.95[-5]
<i>G</i>	4	-0.064 872 7	2.85[-5]
<i>H</i>	5	-0.063 799	2.75[-5]
<i>I</i>	6	-0.062 823	2.12[-5]

literature. We next present our results for higher-angular-momentum resonances. Tables IV–VII show, respectively, the results for the $L=3$ (*F* states), 4 (*G* states), 5 (*H* states), and 6 (*I* states). Again, there are no published results in the literature for comparison.

In order to shed light on the understanding of the resonances in the e^+ -H system, we separate the various angular momentum states into different groups according to their order of appearance. Table VIII and Fig. 1 show a group of resonances lying below the H ($N=2$) threshold with the threshold energy of $E_t=-0.25$ Ry. The *D*-wave results are taken from Ref. [10]. Table IX and Fig. 2 show two groups of resonances lying below the Ps ($N=2$) threshold with the threshold energy of $E_t=-0.125$ Ry. From Fig. 2 it is seen that the resonances in each group follow a regular pattern, and that they seem to belong to a “family” of resonances. Similarly, Table X and Fig. 3 show two groups of resonances lying below the H ($N=3$) threshold with threshold energy of $E_t=-0.11111$ Ry. As for the resonances lying below the H ($N=4$) threshold with the threshold energy of $E_t=-0.0625$ Ry, we show three groups of resonances in Table XI and Fig. 4. It is interesting to point out that the lowest-angular-momentum state for the second group of resonances is an $L=1$ state. As we go to the higher-energy region, we have found one group of resonances lying between the H ($N=4$) threshold and the Ps ($N=3$) threshold (the threshold energy $E_t=-0.0555555$ Ry), and they are shown here in Table XII and Fig. 5. For this group of resonances, the lowest-angular-momentum state is a *P* state. In Table XIII

TABLE XII. Resonances in e^+ -H scattering below the Ps ($N=3$) threshold.

State	L	E_r (Ry)	$\Gamma/2$ (Ry)
<i>P</i>	1	-0.059 804	4.3[-4]
<i>D</i>	2	-0.059 11	2.7[-4]
<i>F</i>	3	-0.058 055	1.98[-4]
<i>G</i>	4	-0.056 963	2.68[-4]
<i>H</i>	5	-0.055 95	3.35[-4]

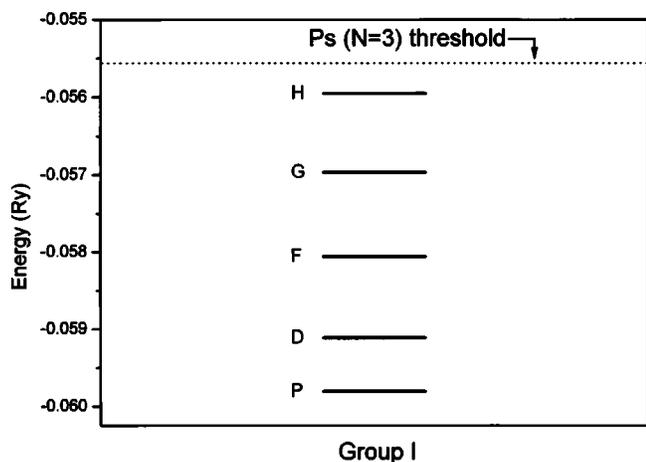


FIG. 5. A groups of resonances for different angular momentum states lying between the H ($N=4$) threshold and the Ps ($N=3$) threshold.

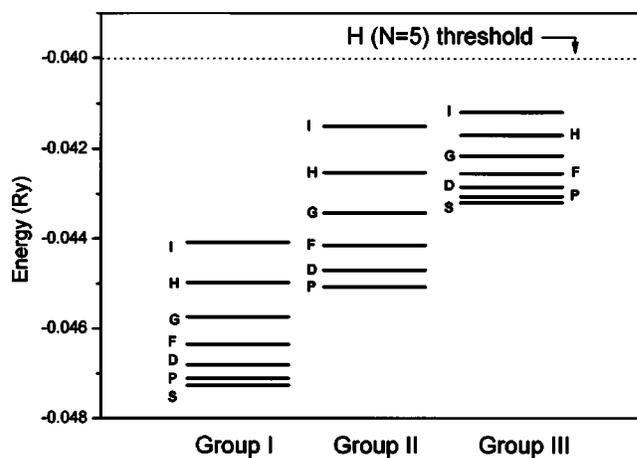


FIG. 6. Three groups of resonances for different angular momentum states lying below the H ($N=5$) threshold.

and Fig. 6 we show two groups of resonances lying below and approaching the H ($N=5$) threshold with the threshold energy of $E_t = -0.04$ Ry. Again, for the second group of resonances in this region, the lowest-angular-momentum state is a P state. Finally, in Table XIV and Fig. 7 we show four groups of resonances lying below the Ps ($N=4$) threshold with threshold energy of $E_t = -0.03125$ Ry. It is seen that, in the first and third groups of resonances, the lowest member starts from $L=1$ and the second group starts from $L=2$. At present, it is not fully understood why for some groups of resonances the S state or the S and P states are lacking. While we have not examined the qualitative aspect of the resonances reported here, it is worthwhile to make a con-

TABLE XIII. Resonances in e^+ -H scattering below the H ($N=5$) threshold.

State	L	E_r (Ry)	$\Gamma/2$ (Ry)
Group I			
S	0	-0.047 268	8.6[-6]
P	1	-0.047 115 5	8.2[-6]
D	2	-0.046 811 3	7.0[-6]
F	3	-0.046 352 3	5.1[-6]
G	4	-0.045 738 2	6.2[-6]
H	5	-0.044 975	1.3[-5]
I	6	-0.044 078	2.8[-5]
Group II			
P	1	-0.045 074 2	5.62[-5]
D	2	-0.044 701 5	6.55[-5]
F	3	-0.044 149 5	6.98[-5]
G	4	-0.043 423 4	6.05[-5]
H	5	-0.042 527	4.3[-5]
I	6	-0.041 504	3.45[-5]

TABLE XIV. Resonances in e^+ -H scattering below the Ps ($N=4$) threshold.

State	L	E_r (Ry)	$\Gamma/2$ (Ry)
Group I			
P	1	-0.037 11	2.34[-4]
D	2	-0.036 862	2.33[-4]
F	3	-0.036 52	2.3[-4]
G	4	-0.036 025	1.85[-4]
H	5	-0.035 4	1.35[-4]
I	6	-0.034 65	1.75[-4]
Group II			
D	2	-0.034 935	8.9[-5]
F	3	-0.034 435	8.0[-5]
G	4	-0.033 795	1.05[-4]
H	5	-0.033 1	1.0[-4]
Group III			
S	0	-0.034 96	9.6[-5]
P	1	-0.034 808	8.8[-5]
D	2	-0.034 493	7.5[-5]
F	3	-0.034 03	8.7[-5]
G	4	-0.033 53	1.0[-4]
H	5	-0.032 83	5.8[-5]
Group VI			
P	1	-0.034 26	1.8[-4]
D	2	-0.034 05	1.7[-4]
F	3	-0.033 75	1.8[-4]
G	4	-0.033 278	9.0[-5]
H	5	-0.032 58	9.5[-5]

ture that for each group (family) of resonances, all the members seem to have similar potential curves, if plotted in hyperspherical coordinates. The difference between them is that each state has a different angular momentum barrier.

It should also be mentioned that in the course of our present investigation we have observed that there are more resonances lying below and close to a given hydrogen or positronium threshold than the ones we have reported here. Basically, they are the higher members of the dipole series, a result of an attractive induced dipole potential created between a positron and an excited hydrogen atom, or between an excited positronium atom and the hydrogen nucleus. Such an attractive dipole potential behaves like r^{-2} in the asymptotic region, and it is expected to be able to support quasibound states since an excited positronium atom (or an excited hydrogen atom) is a highly polarizable system. A quasibound state lying in a scattering continuum would manifest itself as a resonance in positron-atom scattering. The resonance width for a higher member of the dipole series decreases rapidly, and the calculation for such a higher-lying resonance is not an easy task, since it is difficult to reach convergence for a resonance with an extremely narrow width. Presumably, if more extensive basis sets for the wave functions were used, resonance parameters could be determined to a desirable accuracy. But for practical reasons the most extensive wave functions used in the present investigation are limited to those given in Table I. Nevertheless, to the best of our knowledge, there are no results available in the literature for the high-partial-wave resonances reported here. It is our hope that our findings will stimulate further investigation of the resonances in the e^+ -H system.

IV. SUMMARY AND DISCUSSION

In this work, we have presented a theoretical calculation of high-partial-wave resonances in e^+ -H scattering using the method of complex-coordinate rotation together with the use of highly correlated Hylleraas functions. Angular momentum

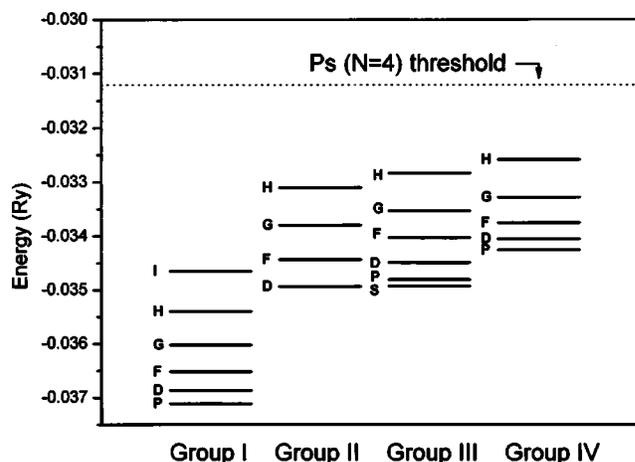


FIG. 7. Four groups of resonances for different angular momentum states lying below the Ps ($N=4$) threshold.

states of $L=3$ to 6 lying below the H ($N=5$) threshold have been reported. Our results can provide a useful reference for future studies. There have been ongoing experimental activities searching for atomic resonances in positron-atom and positron-molecule scattering [21]. The resonances predicted in the present work and in the earlier investigations are of narrow widths. The verification of such resonances in laboratories will be a great challenge for experimentalists for some years to come. Nevertheless, with the recent development in producing high-intensity positron beams with resolution of about a few meV [22], it is hoped that observation of the narrow resonances e^+ -H scattering may soon become a reality.

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