

Resonances in  $H^-$  associated with the  $N=4, 5,$  and  $6$  hydrogen thresholds

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In this work we report resonance parameters in electron-hydrogen scattering converging on the  $N=4, 5,$  and  $6$  hydrogenic thresholds. Results are calculated by a method of complex coordinate rotation. Hylleraas-type wave functions are used for  $L=0$  and  $L=1$  resonances, and products of Slater orbitals for states with  $L \geq 2$ . Both states with parities  $(-1)^L$  and  $(-1)^{L+1}$  are calculated. All the intrashell resonances (both electrons occupying the same shell) below the respective thresholds are included in this work with approximate quantum numbers  $K$  and  $T$  assigned to each state. Results are used to construct "supermultiplet" structures of the doubly excited resonances of hydrogen negative ions.

## I. INTRODUCTION

This paper reports resonance parameters for the doubly excited intrashell states in  $H^-$  associated with the  $N=4, 5,$  and  $6$  hydrogenic thresholds. This work is a part of continuing effort to carry out accurate calculations of resonance parameters for two-electron systems by using a method of complex coordinates.<sup>1-3</sup> Recently, there has been considerable interest in studying symmetries of two-electron Hamiltonians. These studies use a group-theoretical method,<sup>4</sup> and hyperspherical coordinates.<sup>5</sup> Accurate resonance parameters for both the resonance energy position and width are needed in such studies. Also, accurate resonance parameters would play an important role in the investigations of the grandparent model<sup>6,7</sup> for doubly excited states. In such a model, the two electrons are treated as a single entity under the influence of the bare nucleus (the grandparent). The energy levels of the doubly excited intrashell states can be fitted to a Rydberg-like sequence in a screened six-dimensional Coulomb potential in hyperspherical coordinates, converging to the two-electron breakup ionization limit. Because of the lack of experimental data for the highly excited states,<sup>8</sup> accurate results associated with high excitation thresholds would help to interpret such a model.

Because of the continuous interest in the doubly excited resonances in two-electron systems,<sup>9</sup> we now carry out an investigation of resonance states in  $H^-$  associated with the  $N=4, 5,$  and  $6$  hydrogenic thresholds. Furthermore, although there are a number of theoretical calculations of resonances in He atoms associated with the  $N=2$  and  $3$  thresholds,<sup>10</sup> there are very few accurate calculations of resonance parameters associated with high excitation thresholds in the literature.<sup>11</sup> A method that is able to calculate both resonance positions and total widths with accurate results is the method of complex coordinates.<sup>1-3</sup> The advantage of using this method is that resonance parameters can be obtained by using bound-state-type wave functions and no asymptotic wave functions are necessarily used. Such an advantage becomes apparent when we are calculating a resonance in which many channels are opened. Calculation of resonance position and total width

for a many-channel resonance is as straightforward as that for an elastic resonance.

## II. WAVE FUNCTIONS AND CALCULATIONS

The wave functions used in this work are of the Hylleraas type for  $L=0$  and  $1$  resonances,

$$\Psi = \sum C_{kmn} \exp[-\alpha(r_1+r_2)] r_{12}^k \times [r_1^n r_2^{m+L} Y_{00}(1) Y_{L0}(2) \pm r_2^n r_1^{m+L} Y_{00}(2) Y_{L0}(1)], \quad (1)$$

where  $(k+n+m) \leq \omega$ , with  $\omega$  a positive integer, and products of Slater orbitals for resonances with  $L \geq 2$ :

$$\Psi = A \sum_{la,lb} \sum_{i,j} C_{a_i,b_j} \eta_{a_i}(r_1) \eta_{b_j}(r_2) Y_{la,lb}^{LM}(1,2) S(\sigma_1, \sigma_2), \quad (2)$$

where

$$\eta_{a_i}(r) = r^{na_i} \exp(-\xi_{a_i} r).$$

In Eq. (2),  $A$  is the antisymmetrizing operator,  $S$  is a two-particle spin eigenfunction, and the  $\eta$  are individual Slater orbitals.  $Y$  is an eigenfunction of the total angular momentum  $L$ ,

$$Y_{la,lb}^{LM}(1,2) = \sum_{m_{la}} \sum_{m_{lb}} C(la, lb, L; m_{la}, m_{lb}, M) Y_{la, m_{la}}(1) Y_{lb, m_{lb}}(2) \quad (3)$$

with  $C$  the Clebsch-Gordan coefficients. It has been suggested<sup>7</sup> that the use of Slater orbitals to calculate resonances of high angular momenta and associated with higher excitation thresholds can produce accurate results. In a calculation of resonances in negative hydrogen ions, it was found that the use of Slater-orbital-type wave functions indeed produced results for some  $L \geq 2$  states that agree well with an extensive 18-state close-coupling calculation.

Quite extensive basis sets are used in this work. For example, for the  $1D^e$  resonances we use orbitals of nine  $s$ , eight  $p$ , seven  $d$ , six  $f$ , five  $g$ , four  $h$ , three  $i$ , two  $k$ , and  $l$ . These orbitals would couple to a total of 316 terms for

the  ${}^1D^e$  states. The actual numbers of terms for other resonant states differ slightly depending on different angular momenta and parities, as can be seen in Table I. But in any case, no less than 220 terms are used in the present calculation. Using such extensive basis sets, components of open channels below the  $N=6$  threshold are included in the wave functions either explicitly or impli-

citly. This is the reason why we are able to calculate the total widths for such highly excited resonances.

The method used to calculate resonance positions and widths is a method of complex coordinate rotation. The theoretical aspect of the complex rotation method was discussed in previous publications and will not be repeated here. Instead we only briefly describe the computational

TABLE I. Individual Slater-orbital-type wave functions used.

$l_i$	${}^1D^e$	${}^3D^e$	${}^1F^o$	${}^3F^o$	${}^1G^e$	${}^3G^e$	${}^1H^o$	${}^3H^o$
<i>s</i>	9	9	9	9	9	10	9	9
<i>p</i>	8	8	8	8	8	9	8	8
<i>d</i>	7	7	7	7	7	7	7	7
<i>f</i>	6	6	6	6	6	6	6	6
<i>g</i>	4	5	5	5	5	5	5	5
<i>h</i>	3	4	3	3	4	4	4	4
<i>i</i>	2	3	2	2	3	3	3	3
<i>k</i>	2	2	1	1	1	2	2	2
<i>l</i>	1				1	1	1	1
<i>m</i>							1	1
Total	281	277	283	283	320	319	301	301
$l_i$	${}^1J^e$	${}^3J^e$	${}^1K^o$	${}^3K^o$	${}^1L^e$	${}^3L^e$	${}^3M^o$	
<i>s</i>	10	10	10	10	10	10	11	
<i>p</i>	9	9	9	9	9	9	10	
<i>d</i>	8	8	8	8	8	8	9	
<i>f</i>	7	7	7	7	7	7	8	
<i>g</i>	6	6	6	6	6	6	7	
<i>h</i>	4	5	5	5	5	5	6	
<i>i</i>	3	3	3	3	4	4	5	
<i>k</i>	2	1	2	2		3	4	
<i>l</i>	1		1	1		2	3	
<i>m</i>			1	1		1	1	
Total	310	270	270	270	290	269	315	
$l_i$	${}^3P^e$	${}^1D^o$	${}^3D^o$	${}^1F^e$	${}^3F^e$	${}^1G^o$	${}^3G^o$	
<i>p</i>	10	10	10	9	9	9	9	
<i>d</i>	9	9	9	8	8	8	8	
<i>f</i>	8	8	8	7	7	7	7	
<i>g</i>	7	7	6	6	6	6	6	
<i>h</i>	6	6	5	5	5	5	5	
<i>i</i>	5	4	4	4	3	3	3	
<i>k</i>	4		3	3	2	2	2	
<i>l</i>	3		2	2	1	1	1	
<i>m</i>	2		1	1				
<i>n</i>	1							
Total	220	284	280	280	287	283	283	
$l_i$	${}^1H^e$	${}^3H^e$	${}^1J^o$	${}^3J^o$	${}^1K^e$	${}^3K^e$	${}^1L^o$	
<i>p</i>	9	9	9	9	10	9	10	
<i>d</i>	8	8	8	8	9	8	9	
<i>f</i>	7	7	7	7	8	7	8	
<i>g</i>	6	6	6	6	6	6	7	
<i>h</i>	5	5	5	5	5	5	6	
<i>i</i>	4	4	4	4	4	4	5	
<i>k</i>	3	3	3	3	3	3	4	
<i>l</i>	2	2	2	2	2	2	3	
<i>m</i>					1	1	2	
Total	296	323	280	280	258	261	328	

procedures. First, we use the stabilization method to obtain optimized wave functions in which complex rotation calculations will then be carried out. The use of the stabilization method as a first step for the complex rotation method has been demonstrated in an electron-positronium resonance calculation.<sup>12</sup> Once the stabilized wave functions for a particular resonance are obtained, a straightforward complex rotation method is then applied, and the so-called "rotational paths" are examined. The final resonance parameters, both resonance positions and widths, are then deduced from conditions that the discretized complex eigenvalue is stabilized with respect to the nonlinear parameters in the wave functions [Eqs. (1) and (2)] and with respect to  $\theta$ , the so-called rotational angle of the complex transformation  $r \rightarrow r \exp(-i\theta)$ .

### III. RESULTS AND DISCUSSIONS

Tables II, III, and IV show results for all the doubly excited intrashell states associated with and below the  $N=4, 5$ , and  $6$  hydrogenic thresholds, respectively. Each state in these tables is classified by a set of quantum numbers  $(K, T, N, n, L, S, \pi)$ , where  $L$  and  $S$  are the total angular momentum and spin, respectively, and  $\pi$  the parity. The quantum number  $N$  denotes the  $N$ th threshold of the

hydrogen atom below which the resonances lie, and  $n$  has the usual meaning in a Rydberg series.<sup>13</sup> In this work only the lowest number for a given series is reported. In other words, all the resonant states reported here have values of  $n=N$ . Such states in which both electrons are occupying the same shell are called intrashell resonances. Quantum numbers  $K$  and  $T$  are the results of investigations by use of a group-theoretical method. In the absence of interactions between the two electrons, the energy spectrum of the two-electron Hamiltonian is simply the product of two  $O(3)$  groups. When the electron-electron interactions are turned on, the symmetry is broken. The individual angular momentum  $l$  for each electron is no longer a good quantum number although the total angular momentum  $L$  and total spin  $S$  are still constants of the motions. Approximately "good" quantum numbers have been obtained by Herrick and Sinanoglu<sup>4</sup> by diagonalizing the square of  $|\mathbf{A}_1 - \mathbf{A}_2|$ , where  $\mathbf{A}_1$  and  $\mathbf{A}_2$  are the Runge-Lenz vectors for electron 1 and 2, respectively. The rules that govern  $K$  and  $T$  are

$$T = 0, 1, 2, \dots, \min(L, n-1) \text{ for states with } \pi = (-1)^L,$$

$$T = 1, 2, 3, \dots, \min(L, n-1) \text{ for states with } \pi = (-1)^{L+1},$$

and

$$+K = N - T - 1, N - T - 3, \dots, 1 \text{ or } 0.$$

TABLE II. Resonances in  $e^-$ -H scattering converging on the  $N=4$  hydrogenic threshold.

$(2s+1)L\pi$	$K$	$T$	$N$	$n$	$-E_r$ (Ry)	$\Gamma$ (Ry)
$^1S^e$	3	0	4	4	0.079 275	0.0019
$^1S^e$	1	0	4	4	0.069 45	0.001 76
$^1P^o$	2	1	4	4	0.074 33	0.002 02
$^1P^o$	0	1	4	4	0.062 61	0.000 32
$^3P^o$	3	0	4	4	0.078 72	0.002 04
$^3P^o$	1	0	4	4	0.068 535	0.001 17
$^3P^e$	2	1	4	4	0.074 45	0.002 08
$^3P^e$	0	1	4	4	0.062 96	0.0003
$^1D^e$	3	0	4	4	0.077 50	0.0019
$^1D^e$	1	2	4	4	0.068 98	0.001 52
$^1D^e$	1	0	4	4	0.066 25	0.000 48
$^3D^e$	2	1	4	4	0.073 15	0.0021
$^1D^o$	2	1	4	4	0.073 04	0.0024
$^3D^o$	1	2	4	4	0.069 03	0.001 52
$^1F^o$	2	1	4	4	0.070 25	0.0013
$^1F^o$	0	3	4	4	0.062 94	0.0010
$^3F^o$	3	0	4	4	0.075 6	0.0029
$^3F^o$	1	2	4	4	0.065 28	0.0006
$^1F^e$	1	2	4	4	0.065 26	0.000 58
$^3F^e$	2	1	4	4	0.070 54	0.001 68
$^3F^e$	0	3	4	4	0.062 94	0.001 04
$^1G^e$	3	0	4	4	0.072 75	0.0014
$^3G^e$	2	1	4	4	0.065 7	0.0004
$^1G^o$	2	1	4	4	0.066 22	0.0002
$^3H^o$	3	0	4	4	0.067 81	0.000 13

TABLE III. Resonances in  $e^-$ -H scattering converging on the  $N=5$  hydrogenic threshold.

$(2s+1)L^\pi$	$K$	$T$	$N$	$n$	$-E_r$ (Ry)	$\Gamma$ (Ry)
$^1S^e$	4	0	5	5	0.0514	0.0014
$^1S^e$	2	0	5	5	0.046 65	0.0013
$^1S^e$	0	0	5	5	0.040 42	0.000 28
$^1P^o$	3	1	5	5	0.049 10	0.0015
$^1P^o$	1	1	5	5	0.043 75	0.0012
$^3P^o$	4	0	5	5	0.0512	0.0014
$^3P^o$	2	0	5	5	0.046 55	0.0013
$^3P^e$	3	1	5	5	0.049 15	0.0016
$^3P^e$	1	1	5	5	0.0437	0.0011
$^1D^e$	4	0	5	5	0.050 75	0.0013
$^1D^e$	2	2	5	5	0.0465	0.0014
$^1D^e$	2	0	5	5	0.0456	0.0014
$^1D^e$	0	2	5	5	0.040 34	0.0006
$^3D^e$	3	1	5	5	0.0485	0.0013
$^3D^e$	1	1	5	5	0.042 64	0.0006
$^1D^o$	3	1	5	5	0.048 54	0.0014
$^1D^o$	1	1	5	5	0.042 86	0.0006
$^3D^o$	2	2	5	5	0.046 46	0.0014
$^3D^o$	0	2	5	5	0.0403	0.000 44
$^1F^o$	3	1	5	5	0.047 54	0.001 45
$^1F^o$	1	3	5	5	0.043 72	0.0010
$^1F^o$	1	1	5	5	0.0412	0.0006
$^3F^o$	4	0	5	5	0.050 08	0.0013
$^3F^o$	2	2	5	5	0.045 57	0.001 24
$^3F^o$	2	0	5	5	0.044 65	0.000 75
$^1F^e$	2	2	5	5	0.045 55	0.001 25
$^3F^e$	3	1	5	5	0.0477	0.0014
$^3F^e$	1	3	5	5	0.0437	0.0010
$^3F^e$	1	1	5	5	0.041 44	0.0005
$^1G^e$	4	0	5	5	0.048 85	0.0015
$^1G^e$	2	2	5	5	0.043 74	0.0010
$^1G^e$	2	0	5	5	0.042 70	0.0004
$^1G^e$	0	4	5	5	0.040 50	0.0009
$^3G^e$	3	1	5	5	0.046 55	0.001 25
$^3G^e$	1	3	5	5	0.0415	0.0009
$^1G^o$	3	1	5	5	0.046 66	0.001 68
$^1G^o$	1	3	5	5	0.041 45	0.0006
$^3G^o$	2	2	5	5	0.043 68	0.0009
$^3G^o$	0	4	5	5	0.040 58	0.0008
$^1H^o$	3	1	5	5	0.0444	0.000 64
$^3H^o$	4	0	5	5	0.047 85	0.0018
$^3H^o$	2	2	5	5	0.041 45	0.0004
$^1H^e$	2	2	5	5	0.041 38	0.000 48
$^3H^e$	3	1	5	5	0.044 65	0.0009
$^1I^e$	4	0	5	5	0.045 58	0.000 54
$^3I^e$	3	1	5	5	0.0417	0.0003
$^1I^o$	3	1	5	5	0.042 02	0.000 18
$^3K^o$	4	0	5	5	0.0428	0.0002

TABLE IV. Resonances in  $e^-$ -H scattering converging on the  $N=6$  hydrogenic threshold.

$(2s+1)L^\pi$	$K$	$T$	$N$	$n$	$-E_r$ (Ry)	$\Gamma$ (Ry)
$^1S^e$	5	0	6	6	0.035 99	0.000 92
$^1S^e$	3	0	6	6	0.033 35	0.0010
$^1S^e$	1	0	6	6	0.030 15	0.0008
$^1P^o$	4	1	6	6	0.034 75	0.0010
$^1P^o$	2	1	6	6	0.031 78	0.0009
$^1P^o$	0	1	6	6	0.028 05	0.0006
$^3P^o$	5	0	6	6	0.035 922	0.0010
$^3P^o$	3	0	6	6	0.033 22	0.0011
$^3P^o$	1	0	6	6	0.029 96	0.0007
$^3P^e$	4	1	6	6	0.034 75	0.0010
$^3P^e$	2	1	6	6	0.031 7	0.0009
$^3P^e$	0	1	6	6	0.028 1	0.0003
$^1D^e$	5	0	6	6	0.035 8	0.0010
$^1D^e$	3	2	6	6	0.033 3	0.0010
$^1D^e$	3	0	6	6	0.032 95	0.0010
$^1D^e$	1	2	6	6	0.030 05	0.000 75
$^1D^e$	1	0	6	6	0.029 53	0.0006
$^3D^e$	4	1	6	6	0.034 45	0.001 05
$^3D^e$	2	1	6	6	0.031 42	0.0010
$^1D^o$	4	1	6	6	0.034 45	0.001 05
$^1D^o$	2	1	6	6	0.031 4	0.0010
$^3D^o$	3	2	6	6	0.033 3	0.0011
$^3D^o$	1	2	6	6	0.030 05	0.0007
$^1F^o$	4	1	6	6	0.034 05	0.0010
$^1F^o$	2	3	6	6	0.031 75	0.0010
$^1F^o$	2	1	6	6	0.030 88	0.0009
$^1F^o$	0	3	6	6	0.028 1	0.0008
$^3F^o$	5	0	6	6	0.035 35	0.0009
$^3F^o$	3	2	6	6	0.032 8	0.0009
$^3F^o$	3	0	6	6	0.032 45	0.0010
$^3F^o$	1	2	6	6	0.029 35	0.0005
$^3F^o$	1	0	6	6	0.028 65	0.0005
$^1F^e$	3	2	6	6	0.032 8	0.000 95
$^1F^e$	1	2	6	6	0.029 3	0.0004
$^3F^e$	4	1	6	6	0.034 08	0.001 08
$^3F^e$	2	3	6	6	0.031 78	0.0010
$^3F^e$	2	1	6	6	0.030 9	0.000 88
$^3F^e$	0	3	6	6	0.028 1	0.0006
$^1G^e$	5	0	6	6	0.034 95	0.0010
$^1G^e$	3	2	6	6	0.032 3	0.0010
$^1G^e$	3	0	6	6	0.031 95	0.0005
$^1G^e$	1	4	6	6	0.030 15	0.000 75
$^1G^e$	1	2	6	6	0.028 35	0.0007
$^3G^e$	4	1	6	6	0.033 45	0.0009
$^3G^e$	2	3	6	6	0.031 1	0.000 75
$^3G^e$	2	1	6	6	0.029 95	0.0004
$^1G^o$	4	1	6	6	0.033 55	0.0009
$^1G^o$	2	3	6	6	0.031 12	0.0007
$^1G^o$	2	1	6	6	0.030 2	0.0004
$^3G^o$	3	2	6	6	0.032 3	0.0010
$^3G^o$	1	2	6	6	0.028 35	0.0007
$^1H^o$	4	1	6	6	0.032 85	0.0010
$^1H^o$	2	3	6	6	0.029 90	0.0006
$^1H^o$	2	1	6	6	0.028 8	0.0007
$^1H^o$	0	5	6	6	0.028 35	0.0009

TABLE IV. (Continued).

$(2x+1)L^\pi$	$K$	$T$	$N$	$n$	$-E_r$ (Ry)	$\Gamma$ (Ry)
${}^3H^o$	5	0	6	6	0.0343	0.0008
${}^3H^o$	3	2	6	6	0.0315	0.0009
${}^3H^o$	3	0	6	6	0.031 05	0.0004
${}^3H^o$	1	4	6	6	0.028 75	0.0008
${}^1H^e$	3	2	6	6	0.0315	0.0008
${}^1H^e$	1	4	6	6	0.028 75	0.0006
${}^3H^e$	4	1	6	6	0.0328	0.0011
${}^3H^e$	2	3	6	6	0.029 85	0.0007
${}^3H^e$	2	1	6	6	0.028 95	0.0004
${}^3H^e$	0	5	6	6	0.028 35	0.0008
${}^1I^e$	5	0	6	6	0.033 45	0.0012
${}^1I^e$	3	2	6	6	0.030 12	0.0008
${}^1I^e$	3	0	6	6	0.029 55	0.000 35
${}^3I^e$	4	1	6	6	0.0320	0.0007
${}^3I^e$	2	3	6	6	0.0286	0.0006
${}^1I^o$	4	1	6	6	0.0321	0.0009
${}^1I^o$	2	3	6	6	0.0286	0.0006
${}^3I^o$	3	2	6	6	0.030 08	0.0006
${}^1K^o$	4	1	6	6	0.030 39	0.0004
${}^3K^o$	5	0	6	6	0.032 75	0.0009
${}^3K^o$	3	2	6	6	0.028 60	0.0004
${}^3K^o$	3	0	6	6	0.028 00	0.0006
${}^1K^e$	3	2	6	6	0.028 50	0.0004
${}^3K^e$	4	1	6	6	0.030 65	0.0004
${}^1L^e$	5	0	6	6	0.031 07	0.000 22
${}^3L^e$	4	1	6	6	0.028 80	0.000 32
${}^1L^o$	4	1	6	6	0.028 98	0.000 26
${}^3M^o$	5	0	6	6	0.029 40	0.000 28

The physical meanings for  $K$  and  $T$  can be described briefly as follows.  $K$  is related to  $-\langle \cos\theta_{12} \rangle$ , where  $\theta_{12}$  represents the angle between the two electron vectors. The larger the positive  $K$ , the closer the value of  $-\langle \cos\theta_{12} \rangle$  is to unity. The two electrons in this situation are located near the opposite sides of the nucleus. The quantum number  $T$  describes the orientations between the orbitals of the two electrons. For example, a state with  $T=0$  implies that the two electrons are moving on the same plane. The quantum numbers  $K$  and  $T$  hence describe the angular correlations between the two doubly excited electrons.

Lin,<sup>5</sup> by use of hyperspherical coordinates,<sup>14</sup> has also investigated classifications of doubly excited resonances in two-electron systems. The physical meanings of the quantum numbers  $K$  and  $T$  are similar to those in Ref. 4, although in Ref. 5 the quantum numbers of  $K$  and  $T$  were assigned by examining the asymptotic ( $R \rightarrow \infty$ ) behaviors of the potential curves in hyperspherical coordinates. In addition, a quantum number  $A$  is used in Ref. 5 to describe radial correlations. The quantum number  $A$  is denoted by  $+1$ ,  $-1$ , or  $0$ . A state with  $A = +1$  would have an antinode for  $\alpha$  at about  $\alpha = \pi/4$ , and a state with  $A = -1$  would have a node. States that do not have a

clear node or antinode at  $\alpha = \pi/4$  would have a value of  $A = 0$ , and their characters are similar to those of singly excited states. Also, states with  $L > 2(N-1)$  must have  $A = 0$ . In the present work all the states reported here would have  $A = +1$  characters.

Figure 1 shows the  $N=6$  doubly excited states in the so-called  $I$  supermultiplet. (The quantum number  $I$  is defined as  $I = L - T$ , and has the same meaning as the ro-vibration quantum number  $R$  used in triatomic molecules.<sup>15</sup>) For example, states with  $I=0$  are the ground states for various rotor series. Figure 1(a) shows resonant states with quantum number  $I=0$ . Figure 1(b) shows  $I=1$  and  $2$ , etc. These figures show the vibrational characters for the  $N=n=6$  states. Similar figures for the  $N=n=5$  and  $N=n=4$  states were shown in a previous calculation.<sup>16</sup> Rotational characters of these doubly excited states can be constructed from the results given in Tables II–IV. It is now evident that the spectra of the doubly excited states of  $H^-$  are very similar to those of a linear triatomic  $XYX$  molecule. Such molecularlike characters (see Fig. 2) are now understood as follows: when the two electrons are both highly excited and with equal distances away from the nucleus (so-called intrashell), the two electrons are located on opposite sides of the nucleus

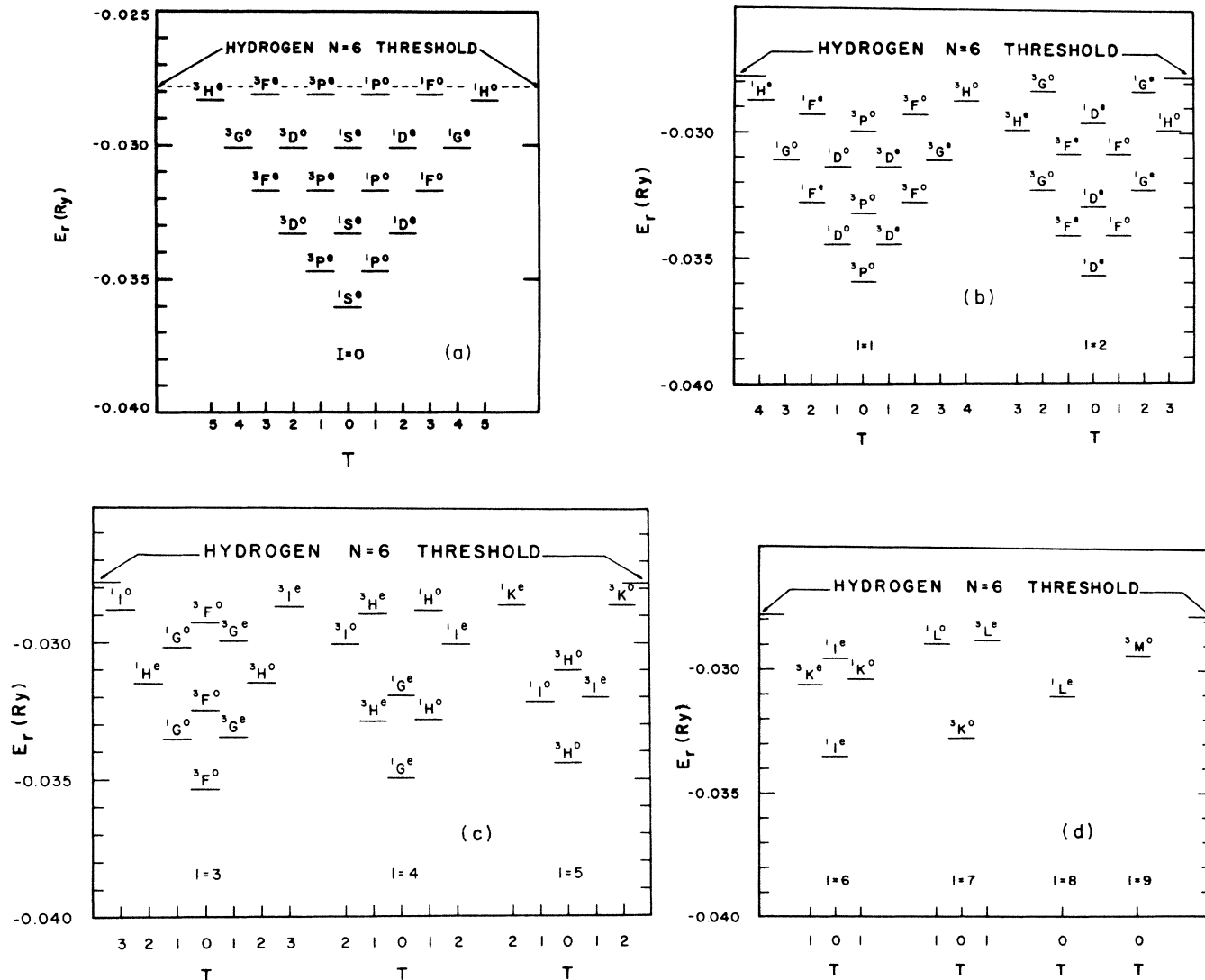


FIG. 1. Doubly excited  $N=6$  resonances of  $H^-$  plotted according to the  $I$  supermultiplet structure of Ref. 7: (a)  $I=0$ ; (b)  $I=1$  and 2; (c)  $I=3, 4$ , and 5; (d)  $I=6, 7, 8$ , and 9.

by strong angular correlation effects. The two electron clouds now behave very much like two condensed fluid drops, and undergo collective rotational, vibrational, and bending motions, in a manner similar to a linear  $XYX$  triatomic molecule.

In summary, we have calculated some lower-lying dou-

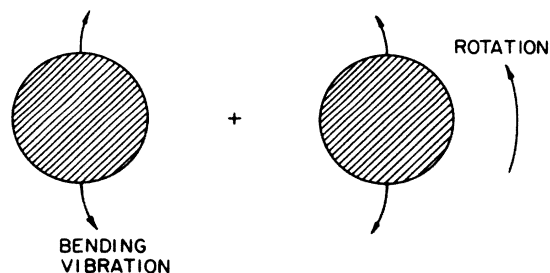


FIG. 2. Triatomic-molecular-like characters of doubly excited intrashell resonant states in  $H^-$ .

bly excited resonances in  $H^-$  associated with and below the  $N=4, 5$ , and 6 hydrogenic thresholds. Both resonance positions and total widths are calculated by use of a complex coordinate rotation method. All the doubly excited intrashell resonant states below the respective hydrogenic thresholds are now included in this work.<sup>17</sup> The present results lend support to the view that the triatomic molecularlike characters of the doubly excited intrashell states do exist in highly excited resonances. This work also provides parameters for total widths for such resonances. Since the widths are related to the inverse of the autoionization lifetimes, the present results would be useful for future investigations of the underlying mechanism of autoionization. With respect to the grandparent model<sup>6,7</sup> of doubly excited states, autoionizing states associated with higher excitation thresholds are needed to interpret such a model. Investigations of resonance states (higher than  $N=6$ ) are of interest and are continuing. Also under current investigation are the possible shape resonances above respective thresholds, as calculated by

Herrick *et al.*<sup>15</sup> who used somewhat simpler wave functions. They concluded that more elaborate calculations are needed to shed light on the supermultiplet structures that include resonance states both above and below the respective excitation thresholds.

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<sup>17</sup>Some of the  $N=4$  and  $5$  resonances have been reported in Ref. 16. For completeness we include them here such that all the doubly excited intrashell resonances below the  $N=4$  and  $5$  thresholds are now included in this work. The  $N=5$  states with  $K=0$  and  $I=0$  are reported for the first time. According to the present calculation, these states [ $^1S^o(0,0)$ ,  $^1D^o(0,2)$ ,  $^1G^o(0,4)$ ,  $^3D^o(0,2)$ , and  $^3G^o(0,4)$ ] now lie below the  $N=5$  threshold, while they are shown to lie above the threshold according to the calculation in Ref. 15. Similarly for the  $N=4$  resonances the present results indicate that resonances with  $I=0$  and  $K=0$  [the  $^1P^o(0,1)$ ,  $^1F^o(0,3)$ ,  $^3P^o(0,1)$ , and  $^3F^o(0,3)$  states] are located below the  $N=4$  threshold, and the results in Ref. 15 indicated that they lie above.