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Multichannel resonances in electron-hydrogen scattering

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Some lower-lying doubly excited resonances in electron-hydrogen scattering converging on the $N=3$, 4, and 5 hydrogenic thresholds, as well as some lower-lying P-wave resonances associated with the $N=6$ threshold, have been 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 $L \geq 2$. Results are compared with recent calculations. Furthermore, in addition to the usual resonances of parities $(-1)^L$, resonant states with parities $(-1)^{L+1}$ are also calculated. Results are used to construct the "supermultiplet" structures of the doubly excited resonances of two-electron atoms.

I. INTRODUCTION

There has been continuous interest in the studies of resonances in e^--H scattering as documented in literature.[1-4] For resonances associated with lower-lying hydrogenic thresholds quite accurate resonance parameters have been obtained by different methods. Recent interests are now concentrated on resonances associated with higher ($N=4$, 5, or higher) hydrogenic thresholds. In the experimental side, some P-wave doubly excited resonances converging on the $N=6$ hydrogenic threshold have been observed in a photoabsorption measurement of H^- in Los Alamos Meson Physics Facility[5] (LAMPF). On the theoretical side, some so-called doubly excited intrashell (both electrons occupy the same shell) resonances below the $N=4$ and 5 hydrogenic thresholds have been investigated by Kellman and Herrick,[6,7] who used a truncated diagonalization method (TDM) together with a group-theoretical approach. These doubly excited resonances revealed some quite symmetric "supermultiplet" structures of the two-electron Hamiltonian, in spite of the fact that the usual O(3) symmetry is broken by the presence of r_{12}, the term which represents the interactions of the two electrons. Furthermore, the supermultiplet structure of the doubly excited resonances is strikingly similar to the spectrum of a linear XYX triatomic molecule.[7] A simple picture to explain the molecularlike character of the doubly excited two-electron spectrum is the following: When the two electrons are both highly excited, say, to $N=4$ or 5 hydrogenic orbitals and with equal distances away from the nucleus (so-called intrashell), the two electrons are located, most of the time, on opposite sides of the nucleus by the strong angular correlation effects (or the Wannier effect). The two electron clouds, as usually interpreted from quantum-mechanical points of view, 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.

Because of this recent experimental and theoretical interest, an independent study of the doubly excited states is hence worthwhile. Furthermore, the numerical values calculated by Kellman and Herrick may not be very accurate due to the fact that the Feshbach shifts, the interacting between the open and closed channels, were not included in TDM, and the widths for most states associated with higher hydrogenic thresholds have not been calculated. All these facts contribute to the motivation for a new and accurate theoretical calculation.

A method which can provide resonance positions and widths with reasonable accuracy is the method of complex rotations (see Refs. 8–11 and references therein). Previous studies have indicated that quite accurate results could be obtained for $L=0$ and 1 resonances associated with the $N=3$ and 4 hydrogenic thresholds when Hylleraas-type wave functions were used.[8,10,11(a)] We now extend the calculations to resonances with higher angular momenta, i.e., $L \geq 2$, and associated with $N=3$, 4, and 5 hydrogenic thresholds. In addition, some P-wave $N=6$ resonances are also calculated.

II. WAVE FUNCTIONS AND CALCULATIONS

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

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

TABLE. I. Electron-hydrogen resonances below the $N=3$ hydrogenic threshold.

	Present complex rotation $-E_r$(Ry)	Present complex rotation Γ(Ry)	14-state[a] close coupling $-E_r$(Ry)	14-state[a] close coupling Γ(Ry)	18-state[b] close coupling $-E_r$(Ry)	18-state[b] close coupling Γ(Ry)
			$\pi=(-1)^L$			
$^1D^e(1)$	0.1319	0.0032	0.1318	0.00324	0.13191	0.00327
$^3D^e(1)$	0.11796	0.00075	0.11788	0.000755	0.11793	0.00075
$^3F^o(1)$	0.12302	0.00022	0.1228	0.00023	0.12303	0.000217
			$\pi=(-1)^{L+1}$			
$^3P^e(1)$	0.12552	0.00274				
$^1D^o(1)$	0.11886	0.00049				

[a]Reference 12.
[b]Reference 13.

and products of Slater orbitals for resonances with $L \geq 2$;

$$\Psi = A \sum_{l_a,l_b} \sum_{i,j} C_{ai,bj} \eta_{ai}(r_1) \eta_{bj}(r_2) \times Y^M_{Ll_al_b}(1,2) S(\sigma_1,\sigma_2), \tag{2}$$

where

$$\eta_{ai}(r) = r^{\eta_{ai}} e^{-\xi_{ai} r}. \tag{3}$$

In Eq. (1) values for the integers k,m,n, are governed by $k+m+n \geq \omega$ with ω a positive integer. In Eq. (2) A is the antisymmetrizing operator, S is a two-particle spin eigenfunction, Y is a two-particle spherical harmonic, and the η are individual Slater orbitals. The use of the product of Slater orbitals for resonances with high angular momenta is suggested by the following: It is believed that the explicit r_{12} terms, which play an important role in regions where r_{12} is small, are less important for states associated with higher hydrogenic thresholds and with large angular momenta. As a result the use of separable Slater orbital wave functions would give reasonable values for such highly excited resonances.

The theoretical aspect of the complex-coordinate

TABLE II. Electron-hydrogen resonances converging on the $N=4$ hydrogenic threshold.

	$-E_r$ (Ry)	Γ (Ry)	$-E_r$ (Ry)	Γ (Ry)
	(1)		(2)	
		$\pi=(-1)^L$		
$^1D^e$	0.077475	0.0019	0.06898	0.00152
$^3D^e$	0.07315	0.0021		
$^1F^o$	0.07025	0.00130		
$^3F^o$	0.0756	0.0029	0.0653	0.00065
$^1G^e$	0.07275	0.00140		
$^3G^e$	0.0657	0.00032		
$^3H^o$	0.06781	0.00013		
		$\pi=(-1)^{L+1}$		
$^3P^e$	0.07445	0.00208		
$^1D^o$	0.07304	0.0024		
$^3D^o$	0.06905	0.0015		
$^1F^e$	0.06525	0.00055		
$^3F^e$	0.07054	0.00168		
$^1G^o$	0.06622	0.00018		

TABLE III. Electron-hydrogen resonances converging on the $N=5$ hydrogenic threshold.

	$\pi=(-1)^L$					
	(1)		(2)		(3)	
	$-E_r$ (Ry)	Γ (Ry)	$-E_r$ (Ry)	Γ (Ry)	$-E_r$ (Ry)	Γ (Ry)
$^1S^e$	0.051 55	0.001 1	0.047 0	0.001 3		
$^1P^o$	0.049 10	0.001 6	0.043 75	0.001 1		
$^3P^o$	0.051 35	0.001 2	0.046 55	0.001 3		
$^1D^e$	0.050 75	0.001 3	0.046 5	0.001 4	0.045 6	0.001 4
$^3D^e$	0.048 5	0.001 3	0.042 64	0.000 6		
$^1F^o$	0.047 537	0.001 44	0.043 7	0.001 0		
$^3F^o$	0.050 08	0.001 2	0.044 65	0.000 76		
$^1G^e$	0.048 85	0.001 5	0.043 74	0.000 9		
$^3G^e$	0.046 55	0.001 25	0.041 5	0.000 8		
$^1H^o$	0.044 4	0.000 64				
$^3H^o$	0.047 8	0.001 8	0.041 45	0.000 4		
$^1I^e$	0.045 58	0.000 54				
$^3I^e$	0.041 7	0.000 26				
$^3K^o$	0.042 8	0.000 2				
	$\pi=(-1)^{L+1}$					
$^3P^e$	0.049 15	0.001 6	0.0436 4	0.001 1		
$^1D^o$	0.048 54	0.001 4	0.0428 5	0.000 59		
$^3D^o$	0.046 46	0.001 4				
$^1F^e$	0.045 55	0.001 3				
$^3F^e$	0.047 7	0.001 4	0.0437	0.001 0		
$^1G^o$	0.046 66	0.001 68	0.0414 5	0.000 6		
$^3G^o$	0.043 68	0.000 88				
$^3H^e$	0.044 8	0.001 4				
$^1I^o$	0.042 02	0.000 16				

method was discussed in previous publications and will not be repeated here. Instead, we only briefly describe the computational procedures. First, we use the stabilization method to obtain optimized wave functions in which complex-coordinate-rotation calculations will then be carried out. The use of the stabilization method as a first step for the complex-coordinate-rotation method has been demonstrated in an electron-positronium resonance calculation.[9] Once the stabilized wave functions for a particular resonance are obtained, a straightforward complex-coordinate-rotation method was 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 discrete complex eigenvalue was stabilized with respect to the nonlinear parameters in the wave functions [Eqs. (1) and (2)] and with respect to θ, the so-called rotational angle of the complex transformation $r \rightarrow re^{i\theta}$. Up to a total of 286 terms are used in the expansions [Eqs. (1) and (2)]. The actual number of terms for each resonance will differ slightly depending on different angular momenta and parities. But in any case, no less than 220 terms are used in the present investigation.

TABLE IV. Lower-lying P-wave resonances in e^--H scattering converging on the $N=6$ hydrogenic threshold.

	$-E_r$ (Ry)	Γ (Ry)
$^1P^o(1)$	0.034 75	0.001 0
$^1P^o(2)$	0.031 80	0.000 9
$^3P^o(1)$	0.035 922	0.001 0
$^3P^o(2)$	0.033 22	0.001 12

III. RESULTS AND DISCUSSIONS

In Table I, results for resonances below the $N=3$ threshold are shown and compared with other calculations. It is seen that the present calculations agree

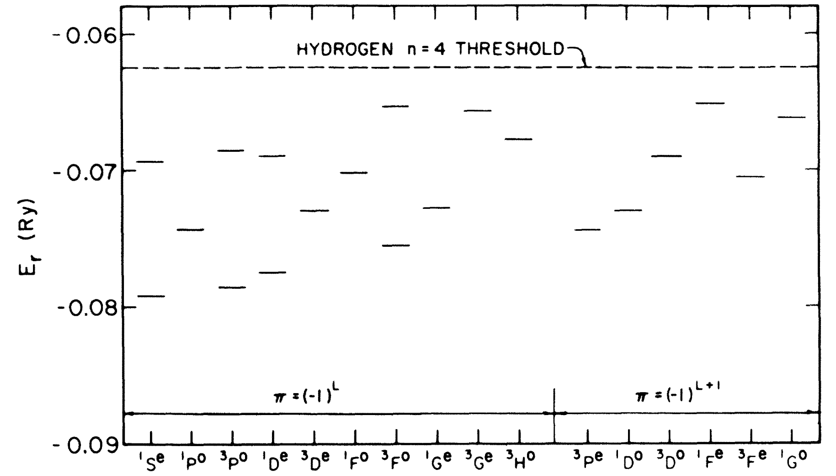

FIG 1. Doubly excited resonances in H^- converging on the $N=4$ hydrogenic threshold.

very well with close-coupling calculations[12,13] for resonances converging on the $N=3$ threshold. This indicates the use of the products of Slater orbitals is indeed able to produce quite accurate results for resonances with higher angular momenta and converging on higher hydrogenic thresholds. Next, some lower-lying resonances associated with the $N=4$ and 5 hydrogenic thresholds are similarly calculated, and our results are reported in Tables II and III, respectively. It should be mentioned that many of the widths reported for the $N=4$ and 5 resonances are calculated for the first time.[14,15]

In this work we have also located some P-wave resonances associated with $N=6$ hydrogenic threshold. The results are shown in Table IV, and they should be helpful for experimental references.

In addition to the resonances of parities $(-1)^L$, we have also calculated resonances parameters for

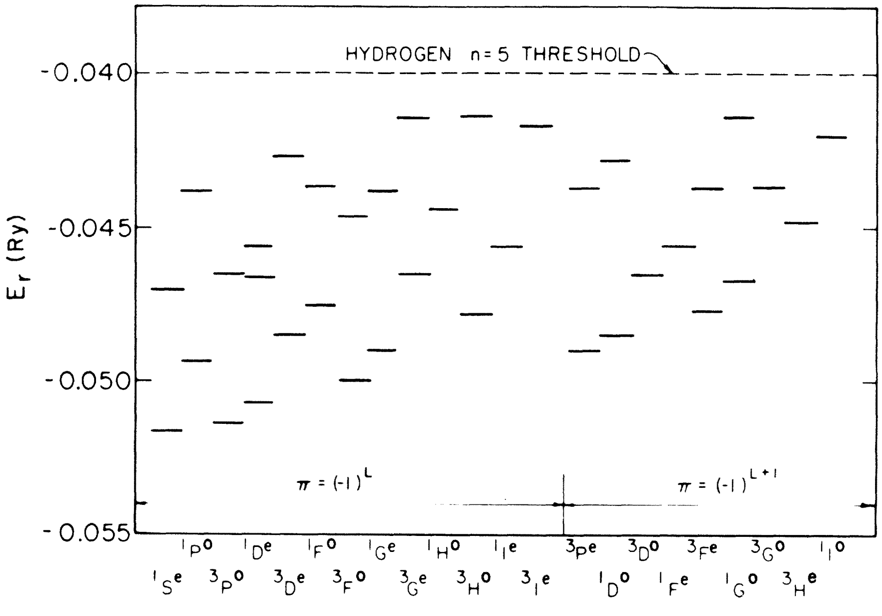

FIG. 2. Doubly excited resonances in H^- converging on the $N=5$ hydrogenic threshold.

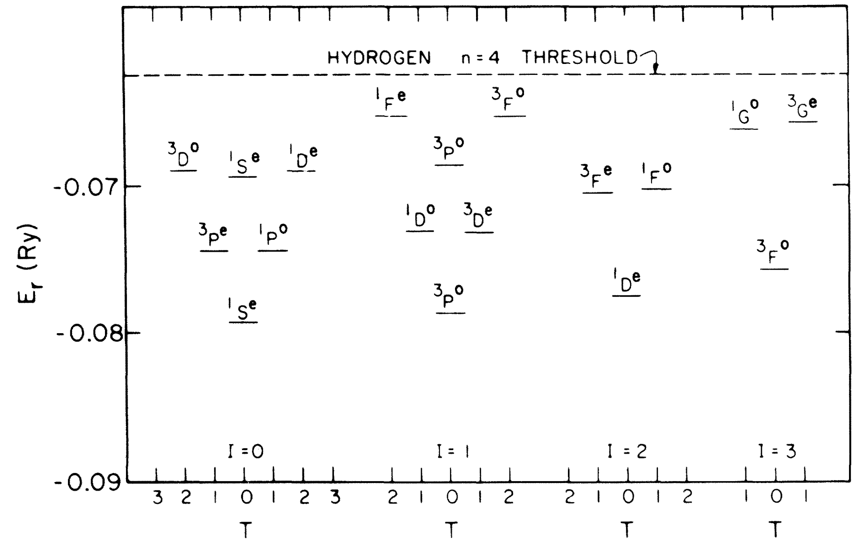

FIG. 3. Doubly excited $N=4$ resonances of H^- plotted according to the I supermultiplet structure of Ref. 7. The relation between I and T is $I=L-T$.

states with parities of $(-1)^{L+1}$. These resonances, of course, cannot be formed by electron impact on the ground state of hydrogen atoms due to conservations of parity and angular momentum. They can, however, be formed by electron impact on excited states of hydrogen atoms, although this may be difficult experimentally. Similarly, these resonant states with $(-1)^{L+1}$ parities will be autoionized to the excited states of hydrogen atoms. One of the reasons to calculate the doubly excited states with parities of $(-1)^{L+1}$ is to construct the supermultiplet structures of the doubly excited resonances in the two-electron atoms as discussed recently by Herrick and Kellman.[6] Our results for these states are shown in Table III.

In Figs. 1 and 2, the resonance positions are plotted according to the usual O(3) scheme for resonances converging on $N=4$ and 5 hydrogenic thresholds, respectively. It is seen that the symmetry of the Hamiltonian is not easily recognized.

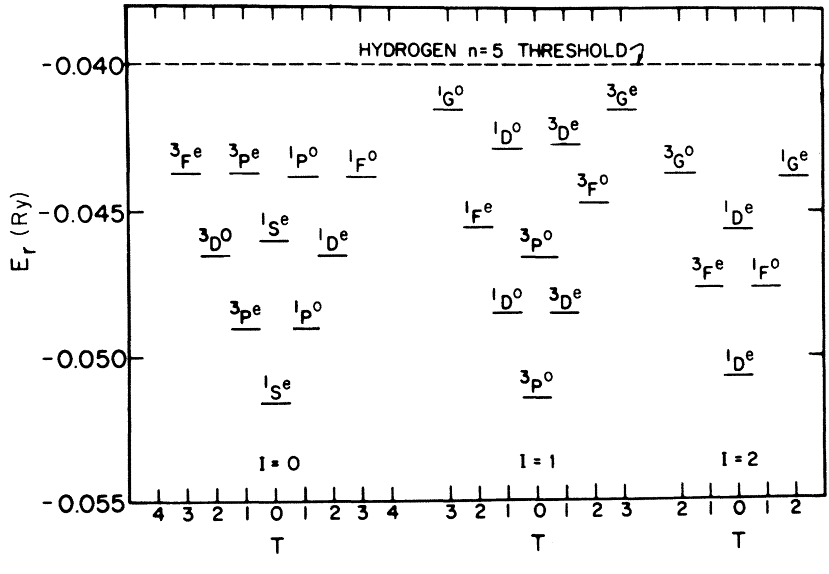

FIG. 4. Doubly excited $N=5$ resonances of H^- plotted according to the I supermultiplet structure of Ref. 7. The relation between I and T is $I=L-T$.

Next, we plot our results in the so-called I supermultiplet according to Ref. 6; the symmetry of the Hamiltonian is now evident as can be seen in Figs. 3. It should be mentioned that for the $N=4$ resonances previous complex-coordinate-rotation results for $L=0$ and 1 states are used to construct Figs. 1 and 2 [Ref. 11(a)].

One interesting aspect of the present results is the near identical resonance parameters for states with the same quantum number K and with low values of I.[16] For example, in the supermultiplet $I=0$ and $N=5$, the resonant parameters (both resonance position and width) for states $^1F^o(2)$,$^1P^o(2)$,$^3P^e(2)$, and $^3F^e(2)$ are nearly the same. Their resonance positions have values from $-0.043\,64$ to $-0.043\,75$ Ry and widths from 0.0010 to 0.0011 Ry. This indicates that not only do these resonances have nearly the same closed-channel part wave functions (since their resonance positions are nearly the same), but their open-channel wave functions are also nearly identical (since they have the same widths).

In summary, we have carried out an extensive calculation of several lower-lying resonances associated with the $N=3$, 4, and 5 hydrogenic thresholds, as well as some lower-lying P-wave resonances associated with the $N=6$ hydrogenic threshold. It is believed that the results reported in this work are quite accurate and should be useful references for future theoretical and experimental work.

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[15] Some preliminary results were reported by Y. K. Ho and J. Callaway, in *Abstracts of the XII International Conference of the Physics of Electronic and Atomic Collisions, Gatlinburg, Tennessee, 1981*, edited by S. Datz (North-Holland, Amsterdam, 1981), pp. 209, 210.

[16] The rules governing the approximately "good" quantum numbers K and T are $T=0,1,2,\ldots,L$, for states of $\pi=(-1)^L$ and $T>0$ for states of $\pi=(-1)^{L+1}$; $\pm K=N-T-1,N-T-3,\ldots,0$ or 1, where N is the hydrogenic threshold below which resonances lie. For more discussion about the group theoretical approach to the doubly excited state of two-electron systems, readers are referred to Refs. 6 and 7, and references therein.