Electric-field effects on the N = 2 Feshbach resonances of H⁻

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Electric-field effects on the N=2 Feshbach resonances (both resonance positions and widths) of H⁻ are investigated theoretically using a method of complex-coordinate rotation. Products of Slater orbitals are used to represent the two-electron wave functions, with $l_{\max}=6$ employed for the individual electron. Block matrices with up to $L_{\max}=6$ (I states) are used. Convergence behavior for the resonance parameters (resonance energy and width) is examined by using different values of L_{\max} . Results for the electric-field effects on the nearly degenerate ${}^{1}P^{o}(1)$ and ${}^{1}S^{e}(2)$ states are given, as well as the effects on the nearby ${}^{1}D^{e}(1)$ state.

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I. INTRODUCTION

This work presents a theoretical investigation of electric-field effects on the N = 2 Feshbach resonances of H^- . The method of complex-coordinate rotation [1,2] is used. The field effects on the ${}^{1}P^{o}$ resonances in H⁻ have been subjected to continuous experimental studies. In a series of publications, the Stark effect on the lowest ${}^{1}P^{o}$ Feshbach resonance of H^- below the N=2 hydrogen threshold [3] and on the shape resonance above the N=2hydrogen threshold have been investigated [4]. In addition, the field effects on the $N = 3 {}^{1}P^{o}(1)$ state were observed [5], as well as on the ${}^{1}P^{o}$ states associated with other high excitation thresholds [6]. On the theoretical side, the field effects on the $N = 2^{-1}P^{\circ}$ shape resonance were studied by Wendoloski and Reinhardt [7], and by Du, Fabrikant, and Starace [8]. We have recently reported a theoretical investigation of field effects on the N=3 ${}^{1}P^{o}(1)$ resonance [9] by using a method of complexcoordinate rotation [1,2]. As for the N = 2 Feshbach resonances, since the ${}^{1}P^{o}(1)$ resonance lies at a position very close to the second member of the ${}^{1}S^{e}$ state, the ${}^{1}S^{e}(2)$ state, even a weak external electric field would cause a strong mixing of these two states and result in splitting the ${}^{1}P^{o}(1)$ state into two components. A third weak component, which was also observed in the experiment, is a result of the mixing of the ${}^{1}P^{o}(1)$ state with a nearby ${}^{1}D^{e}(1)$ state. A theoretical study [10] by using the stabilization method has found qualitative agreement with the experimental results for the resonance positions. However, in Ref. [10] the resonance widths were not investigated. In the present work we employ the method of complex-coordinate rotation such that the field effects on both the resonance positions and widths can be studied. Furthermore, we include higher angular-momentum states in our calculations to investigate the convergence behaviors for the resonance parameters. Our results are of experimental interest as the field effects on the resonance widths have been observed [3,4].

II. THEORY AND WAVE FUNCTIONS

The Stark effect of atoms or ions can be investigated by using a method of complex-coordinate rotation [1,2]. The Hamiltonian of an atom in an external field is

$$H = T + V + \bar{F} \cdot \bar{r} , \qquad (1)$$

where F is the external field, and T and V are the usual kinetic and potential operators, respectively. For the H^- system, T and V are given by

$$T = -\nabla_1^2 - \nabla_2^2 , \qquad (2)$$

and

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

where r_1 and r_2 are the coordinates of the electrons with respect to the nucleus and $r_{12} = |\overline{r_1} - \overline{r_2}|$. Atomic units are used in our work with energy in Rydberg units. The field strength is in Rydberg units and 1 Ry =2.57×10⁹ eV/cm.

Under the influence of the field, the bound states of the atoms or ions become quasibound states, and the electrons will tunnel through the potential barrier formed by the combined Coulomb and external electric fields. As a result, the energies of such states become complex. The real part of a complex energy represents the shifted resonance position and the imaginary part can be related to the lifetime of the quasibound state by the usual uncertainty principle.

In the method of complex-coordinate rotation, the radial coordinates are transformed by

$$r \rightarrow r e^{i\theta}$$
, (4)

and the Hamiltonian can be written as

$$H(\theta) = Te^{-2i\theta} + Ve^{-i\theta} + \overline{F} \cdot \overline{r}e^{i\theta} .$$
⁽⁵⁾

Complex eigenvalues are obtained by diagonalizing the

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transformed Hamiltonian,

$$E = \langle \Phi | H(\theta) | \Phi \rangle / \langle \Phi | \Phi \rangle \tag{6}$$

and the complex resonance energy is given by

$$E_{\rm res} = E_r - i\Gamma/2 , \qquad (7)$$

where E_r gives the shifted energy position, and Γ the resonance width with which the Stark broadening can be studied. The method is valid for isolated resonances and if the interaction with the background for such resonances is not too strong. This method was used by Reinhardt and co-workers to examine the Stark effect of hydrogen. They have examined the effect on the hydrogen ground state [11] and the N=2 excited states [12]. The field effects on the ${}^{1}P^{o}$ shape resonance in H⁻ lying above the N=2 hydrogen threshold were also studied [7]. Recently, we have carried out an investigation of electric-field effects on the $N=3 {}^{1}P^{o}(1)$ resonance of H⁻ by using a method of complex-coordinate rotation [9].

In the present work, we use products of Slater orbitals to represent the two-electron wave functions. The products of Slater orbitals are the following:

$$\Phi = A \sum_{la,lb} \sum_{ij} C_{a_i,b_j} \eta_{a_i}(r_1) \eta_{b_j}(r_2) Y_{la,lb}^{LM}(1,2) S(\sigma_1,\sigma_2)$$
(8)

where

$$\eta_{a_i}(r) = r^{na_i} \exp(-\xi_{a_i} r) .$$
⁽⁹⁾

In Eq. (8), A is the antisymmetrizing operator, S is a two-particle spin eigenfunction, and the η are individual Slater orbitals. Y is the eigenfunction of the total angular momentum L,

$$Y_{la,lb}^{LM}(1,2) = \sum_{m_{la}} \sum_{m_{lb}} C(la,lb,L;m_{la},m_{lb},M)Y_{la,m_{la}}(1) \\ \times Y_{la,m_{lb}}(2) , \qquad (10)$$

with C the Clebsch-Gordan coefficients.

III. CALCULATIONS AND RESULTS

For the M = 0 components of the Feshbach ${}^{1}P^{o}(1)$ and ${}^{1}S^{e}(2)$ states, block matrices with up to $L_{max} = 4$ are used to investigate the Stark mixing of such states. The block matrices of ${}^{1}S^{e}$, ${}^{1}P$, ${}^{1}D^{e}$, ${}^{1}F$, and ${}^{1}G^{e}$ are coupled together by the external dc fields. For the individual electron, we use Slater-type orbitals of 15 s-type, 15 p-type, 10 d-type, 5 f-type and 5 g-type. The highest l value for the individual electron is $l_{max} = 4$. The details of the wave function are shown in Table I. These orbitals would couple to form two-electron bases of 325 ${}^{1}S^{e}$ states, 450 ${}^{1}P^{o}$ states, 480 ${}^{1}D^{e}$ states, 375 ${}^{1}F^{o}$ states, and 285 ${}^{1}G^{e}$ states. A total of 1915 terms are used in the present investigation for the M = 0 components of the ${}^{1}P^{o}(1)$ and ${}^{1}S^{e}(2)$ resonances. For the field-free case, we need to use the basis functions that are capable of producing reasonably accurate resonance parameters of E_r and Γ . At the same time, we cannot afford to employ too extensive basis sets since the matrix sizes would increase rapidly when the individual angular-momentum states are coupled together by the external electric field. The use of the basis sets described in Table I represents a compromise. The resonance parameters for the ${}^{1}S^{e}(2)$ state obtained using such a basis set are $E_r = -0.2520393$ Ry and $\Gamma = 0.0001797$ Ry. These are compared with Callaway's algebraic closecoupling results of $E_r = -0.252034$ Ry and $\Gamma = 0.000182$ Ry (Ref. [13]). Our earlier complexrotation results using a more extensive term wave function gave resonance parameters of $E_r = -0.252042$ Ry and $\Gamma = 0.000176$ Ry (Ref. [14]). Resonance parameters for other calculations are shown in Table II. As for the ${}^{1}P^{o}(1)$ state our field-tree resonance parameters are $E_r = -0.252\,099\,9$ Ry and $\Gamma = 2.33 \times 10^{-6}$ Ry. They are compared with Callaway's results of $E_r = -0.2520992$ Ry and $\Gamma = 2.73 \times 10^{-6}$ Ry (Ref. [13]). Our earlier complex-rotation results gave resonance parameters of $E_r = -0.252\,099\,6\,\mathrm{Ry}$ and $\Gamma = 2.64 \times 10^{-6}\,\mathrm{Ry}$ (Ref. [14]).

Using the wave functions described in Table I, we calculate the field effects on the ${}^{1}S^{e}(2)$ and ${}^{1}P^{o}(1)$ states as

	l=0		l = 1		l=2		<i>l</i> =3		<i>l</i> =4	
n _j	ξj	n _j	ξj	n _j	ξj	n _j	ξj	n _j	ξj	
0	1.0	1	1.0	2	1.0	3	1.0	4	1.0	
1	1.0	2	1.0	3	1.0	3	0.5	4	0.5	
2	1.0	3	1.0	2	0.5	3	0.25	4	0.25	
0	0.5	1	0.5	3	0.5	3	0.125	4	0.125	
1	0.5	2	0.5	2	0.25	3	0.063	4	0.063	
2	0.5	3	0.5	3	0.25					
0	0.25	1	0.25	2	0.125					
1	0.25	2	0.25	3	0.125					
2	0.25	3	0.25	2	0.063					
0	0.125	1 .	0.125	3	0.063					
1	0.125	2	0.125							
2	0.125	3	0.125							
0	0.063	1	0.063							
1	0.063	2	0.063							
2	0.063	3	0.063							

TABLE I. Parameters used in the Slater-orbital basis.

TABLE II. Doubly excited Feshbach resonances of H^- below the N = 2 hydrogen threshold.

Ref.	$2s3s {}^{1}S^{e}(2)$	$2s 3p {}^{1}P^{o}(1)$	$2p^{2} D^{e}(1)$
		$E_r(\mathbf{Ry})$	
а	-0.2520393	-0.2520999	-0.2558835
b	-0.252034	-0.2520992	
с	-0.252042	-0.252 099 6	
d	-0.252035	-0.252099	
e	-0.252036	-0.252097	
f			-0.2558737
		Γ (R y)	
a	1.797×10^{-4}	2.33×10^{-6}	6.325×10^{-4}
b	1.82×10^{-4}	2.73×10^{-6}	
с	1.76×10^{-4}	2.64×10^{-6}	
d	1.87×10^{-4}	3.44×10^{-6}	
e	1.95×10^{-4}		
f			6.334×10^{-4}

^aPresent calculation.

^bCallaway; algebraic close coupling [13].

^cHo: complex-rotation, configuration-interaction functions [14]. ^dChang and Tang: nonvariational configuration interaction with finite *B*-spline basis [15].

^ePathak *et al.*: *R* matrix [16].

^fBhatia and Ho: complex-rotation, Hylleraas functions [17].

the field strength is increased from zero. Table III shows our results. For the entries under the headings of ${}^{1}P^{o}(1)$ and ${}^{1}S^{e}(2)$, it should be understood that the headings are meant for the field-free case. When the field is nonzero, the total angular momentum L is no longer a good quantum number; the ${}^{1}P^{o}(1)$ and ${}^{1}S^{e}(2)$ are hence mixtures of different angular-momentum states due to the coupling of the external field. Table IV shows results for the ${}^{1}P^{o}(1)$ state with $M = \pm 1$. In this case, the ${}^{1}S^{e}$ states are no longer relevant. We add 170 ${}^{1}P^{e}$ states and 150 ${}^{1}H^{o}$ states. The total number of terms in the basis is 1910 for $M = \pm 1$.

Throughout this work for the investigation of Stark mixing of the ${}^{1}P^{o}(1)$ and ${}^{1}S^{e}(2)$ states, block matrices with up to G states are used for the M = 0 components. In order to examine the convergence behaviors for the resonance parameters, we have performed calculations with different L_{max} values. In general, when the field strength is increased, states with higher angular momentum would become more important since more channels are open by the external field. For the strongest field strength (F=0.0001 Ry) we have considered here, we also carried out a calculation for $L_{\text{max}} = 3$, and for $L_{\text{max}} = 4$ and $l_{\text{max}} = 3$. Results are shown in Table V. From such a test we estimate that the uncertainty in width for the ${}^{1}S^{e}(2)$ state is within 25%, and 7% for the ${}^{1}P^{o}(1)$ state. The uncertainties in widths for weaker field strengths are less than these estimates. For practical purposes we have not extended beyond $L_{\text{max}} = 4$ when the wave function described in Table I is used. As compared to the earlier work reported in the literature, using the notation of $[L_{max}, l_{max}]$, terms] the basis sets used in Ref. [10] were [2,2,96]. In comparison, we use [4,4,1915] for the M=0 components of the ${}^{1}S^{e}(2)$ and ${}^{1}P^{o}(1)$ states. As for the $M=\pm 1$ components of the ${}^{1}P^{o}$ state, we use basis sets of [4,4,1910], compared to [2,2,74] used in Ref. [10].

The field effects on the resonance positions for the ${}^{1}P^{o}(1)$ and ${}^{1}S^{e}(2)$ states are also shown in Fig. 1. Due to the accidental near degeneracy for these two states, the M=0 states exhibit a linear Stark effect, while the $M = \pm 1$ states decrease slowly as the external field strengths are increased. Such effects were observed in the laboratory by Gram et al. [3]. A theoretical investigation was carried out by Callaway and Rau [10] using a stabilization method. Qualitative agreements were found between theoretical resonance positions and those of experimental observations. In Ref. [10], however, the resonance widths were not investigated. Furthermore, to our knowledge, the electric-field effects on the resonance widths of the ${}^{1}S^{e}(2)$ and ${}^{1}P^{o}(1)$ states have not been successfully investigated using other ab initio theoretical methods. The results reported in our present work provide a quantitative perspective for the field effects on the N=2 Feshbach resonances for both resonance positions and widths. Also in Fig. 1, our results indicate that the ${}^{1}P^{o}(1)$ resonance would lie lower than the ${}^{1}S^{e}(2)$ state. As such, the $M = \pm 1$ components would start out from the lower state. Our finding is consistent with the experimental observations [3,4].

The electric-field effects on the widths for the ${}^{1}S^{e}(2)$ and ${}^{1}P^{o}(1)$ states are shown in Table III and in Fig. 2. It is seen that when the field is turned on, the width for the ${}^{1}P^{o}(1)$ state starts to increase while that for the ${}^{1}S^{e}(2)$ state starts to decrease. Our finding of the initial decrease in width for the ${}^{1}S^{e}(2)$ state is consistent with the experimental observations [3,4]. Furthermore, the increase and decrease in widths for the ${}^{1}P^{o}(1)$ and ${}^{1}S^{e}(2)$

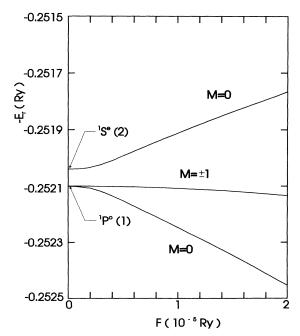


FIG. 1. Electric-field effects on the resonance energies of the ${}^{1}P^{o}(1)$ and ${}^{1}S^{e}(2)$ states.

states, respectively, are nearly the same. In other words, the widths for these two states are about to average each other out even though in the field-free case the width for the ${}^{1}S^{e}(2)$ state is about 80 times larger than that for the ${}^{1}P^{o}(1)$ state. When the external field reaches 8×10^{-6} Ry approximately, the two widths seem to stay constant and roughly equal to each other until the field reaches about 2×10^{-5} Ry. After that the width for the ${}^{1}P^{o}(1)$ state increases more rapidly than that for the ${}^{1}S^{e}(2)$ state, and overtakes the latter state when the field reaches about $F=2.5 \times 10^{-5}$ Ry. The width for the ${}^{1}S^{e}(2)$ state stays nearly constant until $F=3 \times 10^{-5}$ Ry. After that, the width increases more rapidly for increasing field strengths. Our finding of the "average intensity" for the widths when the external field is turned on is consistent with the study done by Bryant *et al.* [4], who considered a model problem with two nearly degenerate resonance states. Using the perturbation treatment, they also found that the two widths start to average each other out when the field is turned on from zero, and eventually the state with the narrower field-free width would overtake the other state in width when the field strength is further increased. Our present work is an *ab initio* treatment of a real atomic two-electron system that verifies the experimental finding [3,4] and their analyses in Ref. [4].

As for the rapid increase for the autoionization widths at high fields, such a phenomenon is similar to the oneelectron cases. When the field is increased to a certain critical value, the effective potential barrier formed by the combined electric-field potential and the Coulomb poten-

TABLE III. Electric-field effects on the ${}^{1}P^{o}(1)$ and ${}^{1}S^{e}(2)$ Feshbach resonances below the H(N=2) threshold. The number in square brackets indicates the power of 10 by which the preceding quantity is to be multiplied.

	¹ <i>P</i> ^o	(1)	${}^{1}S^{e}(2)$		
$F (10^{-6} \text{ Ry})$	E_r (R y)	Г (Ry)	E_r (R y)	Γ (Ry)	
0	-0.252 099 9	2.3314[-6]	-0.2520393	1.7973[-4]	
1	-0.252 101 2	6.6873[-6]	-0.2520386	1.7535[-4]	
2	-0.252 107 0	1.8978[-5]	-0.2520333	1.6301[-4]	
3	-0.2521184	3.4884[-5]	-0.2520229	1.4702[-4]	
4	-0.2521342	4.7843[-5]	-0.2520083	1.3394[-4]	
5	-0.2521520	5.6342[-5]	-0.251 992 1	1.2530[-4]	
6	-0.252 170 3	6.1852[-5]	-0.2519757	1.1960[-4]	
7	-0.252 189 0	6.5582[-5]	-0.251 959 5	1.1566[-4]	
8	-0.2522078	6.8212[-5]	-0.251 943 4	1.1280[-4]	
9	-0.252 226 8	7.0127[-5]	-0.251 927 5	1.1061[-4]	
10	-0.2522460	7.1561[-5]	-0.251 911 8	1.0893[-4]	
11	-0.2522654	7.2659[-5]	-0.251 896 4	1.0752[-4]	
13	-0.252 305 1	7.4262[-5]	-0.251 866 1	1.0539[-4]	
15	-0.252 345 3	7.5360[-5]	-0.2518361	1.0371[-4]	
17	-0.2523882	7.7234[-5]	-0.2518077	1.0249[-4]	
19	-0.2524321	7.9988[-5]	-0.251 779 8	1.0157[-4]	
20	-0.2524546	8.2005 -5	-0.251 766 2	1.0126[-4]	
21	-0.2524776	8.4626[-5]	-0.251 752 9	1.0111[-4]	
22	-0.2525009	8.7976 -5	-0.251 739 7	1.0113[-4]	
23	-0.2525246	9.2179[-5]	-0.251 726 7	1.0135[-4]	
24	-0.2525486	9.7340[-5]	-0.2517139	1.0176[-4]	
25	-0.2525728	1.0356[-4]	-0.251 701 3	1.0239[-4]	
26	-0.252 597 2	1.1090[-4]	-0.2516889	1.0323[-4]	
27	-0.2526217	1.1940[-4]	-0.251 676 7	1.0430[-4]	
28	-0.252 646 1	1.2899[-4]	-0.2516646	1.0560[-4]	
29	-0.252 670 6	1.3970[-4]	-0.2516527	1.0715[-4]	
30	-0.252 694 9	1.5142[-4]	-0.251 640 9	1.0897[-4]	
32.5	-0.2527547	1.8448[-4]	-0.251 612 3	1.1484[-4]	
35	-0.2528131	2.2136[-4]	-0.2515844	1.2281[-4]	
37.5	-0.2528700	2.6047[-4]	-0.2515570	1.3330[-4]	
40	-0.252 926 1	3.0096[-4]	-0.251 529 8	1.4523[-4]	
45	-0.2530369	3.8629[-4]	-0.2514757	1.7443[-4]	
50	-0.253 146 9	4.8007[-4]	-0.251 421 7	2.0809[-4]	
60	-0.2533583	6.9984[-4]	-0.251 314 4	2.8653[-4]	
70	-0.2535462	9.4956[-4]	-0.2512060	3.7535[-4]	
80	-0.2537077	1.1893[-3]	-0.251 097 1	4.6527[-4]	
90	-0.2538587	1.3940[-3]	-0.250 991 7	5.5318[-4]	
100	-0.2540132	1.5753[-3]	-0.2508926	6.4350[-4]	

TABLE IV. Electric-field effects on the $M = \pm 1$ components of the N = 2 Feshbach ${}^{1}P^{o}(1)$ resonance of H⁻. The number in square brackets indicates the power of 10 by which the preceding quantity is to be multiplied.

$F (10^{-6} \text{ Ry})$	E_{γ} (Ry)	Γ (R y)
0	-0.252 099 9	2.3314[-6]
2	-0.2521002	2.3338[-6]
4	-0.252 100 7	2.3638[-6]
6	-0.252 102 3	2.4174[-6]
8	-0.252 104 4	2.5012[-6]
10	-0.2521073	2.6277[-6]
12	-0.252 110 8	2.8200[-6]
14	-0.2521151	3.1206[-6]
16	-0.2521202	3.6057[-6]
18	-0.2521262	4.4084[-6]
20	-0.2521331	5.7478[-6]
30	-0.2521820	3.3389[-5]
40	-0.252 240 3	1.1040[-4]
50	-0.2522945	2.2998[-4]
60	-0.252 339 9	3.6821[-4]
70	-0.252 381 0	5.1575[-4]
80	-0.2524206	6.7874[-4]
90	-0.2524550	8.6149[-4]
100	-0.252 478 5	1.0597[-3]

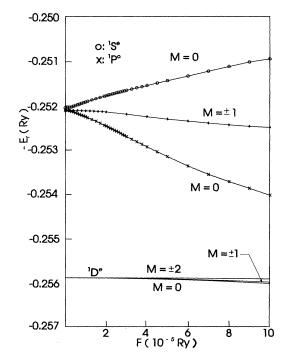


FIG. 3. Electric-field effects on the resonance energies of ${}^{1}P^{o}(1), {}^{1}S^{e}(2)$, and the nearby ${}^{1}D^{e}(1)$ states.

TABLE V. Resonance parameters obtained using different L_{max} for F = 0.0001 Ry.

			${}^{1}P^{o}(1)$		${}^{1}S^{e}(2)$		
$L_{\rm max}$	l _{max}	Terms	E_r (Ry)	Γ (R y)	E_r (R y)	$\Gamma(\mathbf{R}\mathbf{y})$	
3	4	1630	-0.254 000	0.001 674	-0.350 813	0.000 818	
4	3	1570	-0.254028	0.001 661	-0.250845	0.000 728	
4	4	1915	-0.254013	0.001 575	-0.250 893	0.000 644	

tial is dominated by the former potential. As a result, the thickness of the effective potential barrier is decreased for increasing field strengths. The required time for the electron to tunnel out is subsequently shorter, and the autoionization width hence becomes larger. At low fields, the two-electron correlation effect is still the dominating factor, and the autoionization of the electron would follow mostly the route through Coulomb interactions, just like the field-free cases. The widths are therefore nearly constant until the field strength reaches a critical value at which the two-electron correlation bonding is "broken up" by the external field. After that, the one-electron autoionization process becomes more important for increas-

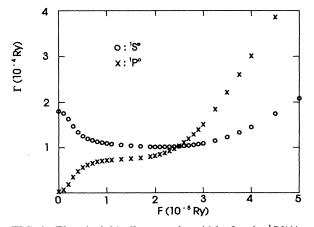


FIG. 2. Electric-field effects on the widths for the ${}^{1}P^{o}(1)$ and ${}^{1}S^{e}(2)$ states.

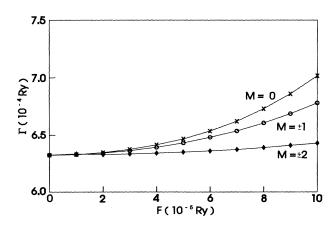


FIG. 4. Electric-field effects on the widths of the ${}^{1}D^{e}(1)$ state with $M = 0, \pm 1$, and ± 2 components.

	M = 0		$M = \pm 1$		$M = \pm 2$	
$F (10^{-5} \text{ Ry})$	E_r (R y)	Γ (R y)	E_r (R y)	Γ (R y)	E_r (R y)	Γ (R y)
0	-0.2558835	0.000 632 5	-0.2558835	0.000 632 5	-0.2558835	0.000 632 5
1	-0.2558848	0.000 633 0	-0.2558846	0.000 632 9	-0.2558839	0.000 633 4
2	-0.2558886	0.000 634 6	-0.2558875	0.000 634 2	-0.2558845	0.000 632 9
3	-0.2558949	0.000 637 4	-0.255 892 4	0.000 636 3	-0.2558857	0.000 633 4
4	-0.255 903 8	0.000 641 3	-0.2558993	0.000 639 2	-0.2558873	0.000 634 1
5	-0.2559152	0.000 646 7	-0.255 908 1	0.000 643 1	-0.2558893	0.000 635 0
6	-0.255 929 1	0.000 653 6	-0.2559189	0.000 648 0	-0.255 891 9	0.000 636 1
7	-0.255 945 5	0.000 662 3	-0.2559317	0.000 653 8	-0.255 894 9	0.000 637 5
8	-0.2559644	0.000 673 0	-0.2559463	0.000 660 8	-0.255 898 3	0.000 639 0
9	-0.2559858	0.000 686 0	-0.255 962 9	0.000 668 9	-0.2559022	0.000 640 9
10	-0.256 009 6	0.000 701 7	-0.2559814	0.000 678 2	-0.2559066	0.000 642 9

TABLE VI. Electric-field effects on the ${}^{1}D^{e}(1)$ resonance of H⁻

ing field strengths as was described above. From our calculations, such critical field strength is about $F=2.5 \times 10^{-5}$ Ry for the ${}^{1}P^{o}(1)$ state, and $F=3.0\times 10^{-5}$ Ry for the ${}^{1}S^{e}(2)$ state.

In the present work, we also carry out an investigation of the field effects on the doubly excited $2p^{21}D^{e}(1)$ state. First we construct the wave function for the field-free case that could produce resonance parameters comparable to the other accurate results in the literature. We employ orbitals with 9 s-type, 8 p-type, 7 d-type, 6 f-type, 5 g-type, 4 h-type, and 3 *i*-type to construct the twoelectron wave functions. These orbitals form a basis of 301 terms for the ${}^{1}D^{e}$ state. We obtain $E_{r} = -0.255\,835$ Ry and $\Gamma = 6.325 \times 10^{-4}$ Ry. They are compared with the other complex-coordinate rotation calculation using extensive Hylleraas functions of $E_{r} = -0.255\,8737$ Ry and $\Gamma = 6.334 \times 10^{-4}$ Ry.

When the external electric field is turned on, we employ wave functions with total angular-momentum states with up to $L_{\rm max} = 6$ for the M = 0 component. The angular-momentum states constructed using the aforementioned orbitals consist of 161 ${}^{1}S^{e}$ states, 232 ${}^{1}P^{o}$ states, 301 ${}^{1}D^{e}$ states, 300 ${}^{1}F^{o}$ states, 300 ${}^{1}G^{e}$ states, 250 ${}^{1}H^{o}$ states, and 206 ${}^{1}I^{e}$ states. They are all coupled together to form a total expansion set of 1750 terms when the field is nonzero. After examining the convergence behavior for the resonance parameters by using different $L_{\rm max}$ values, we have obtained converged results for field strengths up to 1×10^{-4} Ry, and they are shown here in Table V and in Fig. 3. In Fig. 3, we also show the Stark mixing on the nearby ${}^{1}S^{e}(2)$ and ${}^{1}P^{o}(1)$ states.

For completeness, we also investigate the field effects on the $M \neq 0$ component of the ${}^{1}D^{e}$ state. For $M = \pm 1$, states with $L \ge 1$ are coupled together by an external field. In this case, we add 83 ${}^{1}P^{e}$ terms and 160 ${}^{1}D^{o}$ terms (the ${}^{1}S^{e}$ states are no longer relevant) to form a total of 1832 terms in the basis sets. As for the $M = \pm 2$ components, only states with $L \ge 2$ are relevant. In this case, we include 160 ${}^{1}D^{o}$, and 177 ${}^{1}F^{e}$ terms to form a total basis of 1694 terms. Again, after examining the convergence behaviors for the resonance parameters, we have obtained converged results for the field strengths up to $F = 1 \times 10^{-4}$ Ry. The results are shown in Table VI. Figure 3 shows the field effects on the resonance positions, and Fig. 4 shows the field effects on the resonance widths. In general, the electric-field effects on the ${}^{1}D^{e}$ states are quite weak. Among the M components the external field has a somewhat more pronounced effect on the M = 0 and $M = \pm 1$ states than on the $M = \pm 2$ states for both the resonance positions and widths.

In summary, we have presented an investigation of field effects on the Feshbach resonances of H^- below the H(N=2) threshold. Our results are useful references for other theoretical investigations and experimental measurements for such interesting phenomena.

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- E. Balslev and J. M. Combs, Commun. Math. Phys. 22, 296 (1971); B. Simon, *ibid.* 27, 1 (1972).
- [2] Y. K. Ho, Phys. Rep. 99, 1 (1983); W. P. Reinhardt, Annu. Rev. Phys. Chem. 33, 223 (1982); B. R. Junker, Adv. At. Mol. Phys. 18, 208 (1982).
- [3] P. A. M. Gram, J. C. Pratt, M. A. Yates-Williams, H. C. Bryant, J. B. Donahue, H. Sharifian, and H. Tooloonchi,

Phys. Rev. Lett. 40, 107 (1978).

[4] H. C. Bryant, David A. Clark, Kenneth B. Butterfield, C. A. Frost, H. Sharifian, H. Tootoonchi, J. B. Donahue, P. A. M. Gram, M. E. Hamm, R. W. Hamm, J. C. Pratt, M. A. Yates, and W. W. Smith, Phys. Rev. A 27, 2889 (1983); G. Comtet, C. J. Harvey, J. E. Stewart, H. C. Bryant, K. B. Butterfield, D. A. Clark, J. B. Donahue, P. A. M.

Gram, D. W. MacArthur, V. Yuan, W. W. Smith, and Stanley Cohen, *ibid.* 35, 1547 (1987).

- [5] S. Cohen, H. C. Bryant, C. J. Harvey, J. E. Steward, K. B. Butterfield, D. A. Clark, J. B. Donahue, D. W. MacArthur, G. Comtet, and W. W. Smith, Phys. Rev. A 36, 4728 (1987).
- [6] M. Halka, H. C. Bryant, C. Johnstone, B. Marchini, W. Miller, A. H. Mohagheghi, C. Y. Tang, K. B. Butterfield, D. A. Clark, S. Cohen, J. B. Donahue, P. A. M. Gram, R. W. Hamm, A. Hsu, D. W. MacArther, E. P. MacKerrow, C. R. Quick, J. Tiee, and K. Rozsa, Phys. Rev. A 46, 6942 (1992).
- [7] John J. Wendoloski and W. P. Reinhardt, Phys. Rev. A 17, 195 (1978).
- [8] N. Y. Du, I. I. Fabrikant, and A. F. Starace, Phys. Rev. A

48, 2968 (1993).

- [9] Y. K. Ho and J. Callaway, Phys. Rev. A 50, 4941 (1994).
- [10] J. Callaway and A. R. P. Rau, J. Phys. B 11, L289 (1978).
- [11] A. Maquet, S. I. Chu, and W. P. Reinhardt, Phys. Rev. A 27, 2946 (1983).
- [12] C. Cerjan, R. Hedges, C. Holt, W. P. Reinhardt, K. Scheibner, and J. J. Wendoloski, Int. J. Quantum Chem. 14, 393 (1978).
- [13] J. Callaway, Phys. Rev. Lett. 68A, 313 (1978), and unpublished.
- [14] Y. K. Ho, Chin. J. Phys. 29, 327 (1991).
- [15] T. N. Chang and X. Tang, Phys. Rev. A 44, 232 (1992).
- [16] A. Pathak, A. E. Kingston, and K. A. Berrington, J. Phys. B 21, 2939 (1988).
- [17] A. K. Bhatia and Y. K. Ho, Phys. Rev. A 41, 504 (1990).