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On the existence of ^{1,3}P$^{\rm o}$ resonances in H$^-$ between n = 2 and 3 H thresholds

M.-K. Chen[a]

Department of Physics, National Chung-Hsing University, Taichung, Taiwan 40227

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Abstract. We examine the influence of relativistic and QED effects on the existence of the ^{1,3}P$^{\rm o}$ H$^-$ resonances between $n = 2$ and 3 hydrogen thresholds, the relativistic and QED corrections and the coupling effects between the high singlet and triplet states are considered as first-order perturbations. We firstly obtain accurate non-relativistic resonant energies and widths of fifteen ^{1}P$^{\rm o}$ resonances, and fifteen ^{3}P$^{\rm o}$ resonances. The fifteen ^{1}P$^{\rm o}$ resonances are classified to be $_3(2,0)^-_n$ $(4 \leq n \leq 12)$ and $_3(1,1)^+_n$ $(3 \leq n \leq 8)$. The fifteen ^{3}P$^{\rm o}$ resonances are classified to be $_3(2,0)^+_n$ $(3 \leq n \leq 12)$ and $_3(1,1)^-_n$ $(4 \leq n \leq 8)$. We found there exist six Feshbach resonances for $_3(2,0)^-_n(^1\mathrm{P^o})$ series, four Feshbach resonances for $_3(1,1)^+_n(^1\mathrm{P^o})$ series, seven Feshbach resonances for $_3(2,0)^+_n(^3\mathrm{P^o})$ series, and three Feshbach resonances for $_3(1,1)^-_n(^1\mathrm{P^o})$ series.

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1 Introduction

In H$^-$, an infinite series of Feshbach resonances convergering to the hydrogenic thresholds are expected, if the levels of the same principal quantum numbers, n, in hydrogen are regarded as degenerate. However, the hydrogenic levels with the same principal quantum number are not degenerate, if the relativistic and QED effects are considered. Therefore, the positions and possibility for resonances will be affected. In this paper, we study the resonant ^{1,3}P$^{\rm o}$ states in H$^-$ between the $n = 2$ and 3 hydrogen thresholds. The formation of highly excited resonant states of H$^-$ is very sensitive to electron-electron correlations and relativistic and QED effects. There are no reports about the terminating of the present resonant states to the author's knowledge.

These resonant states are the prototypes not only for the study of electron-electron correlations but also the dipole resonances. Experimentally, it is very difficult to observe these narrow resonant states. After the first observation [1] of the two ^{1}P$^{\rm o}$ resonances of H$^-$ between $n = 2$ and 3 hydrogen thresholds, there are only observations of the lowest ^{1}P$^{\rm o}$ resonances, which were reported by Cohen *et al.* [2], Halka *et al.* [3] and Williams [4] to the author's knowledge.

Recently, the observation of the narrow resonances of H$^-$ with high resolution is possible by the advanced techniques of the Doppler-tuned collinear laser spectroscopy. Balling *et al.* [5], and Andersen *et al.* [6], have observed the two lowest-lying members of the ^{1}P$^{\rm o}$ dipole series of autodetaching resonances in H$^-$ below the the $n = 2$ hydrogen threshold, by Doppler-tuned collinear laser spectroscopy with a resolution of 0.180 meV. Their results agree very well with the recent theoretical results [7–14]. By two-photon spectroscopy techniques, Stinz *et al.* [15] and Rislove *et al.* [16] measured the lowest ^{1}D$^{\rm e}$ of H$^-$ with high resolution. More recently, Balling *et al.* [17] and Raarup *et al.* [18] measured the lowest ^{1}P$^{\rm o}$ resonance below the H ($n = 2$) threshold by the momentum-spread reduction technique and electron cooling method. The most recent result is in better agreement with theoretical results. It may be expected that the observation of the narrow resonant states of H$^-$ will be available because of the advances in the improved accuracy of experiment.

On the theoretical side, the negative ions represent a significant challenge. For negative ions because the potentials are weaker and the wave functions are much more diffuse, it is difficult to obtain accurate wave functions. In our previous calculations [13,19] for the H$^-$ resonances, the size of the highly excited states extend up to $r = 30\,000$ a.u. and $55\,000$ a.u. Another difficulty is to calculate the rapidly decreasing widths accurately. The theoretical accuracy for ^{1}P$^{\rm o}$ resonances has been improved recently. Sadeghpour *et al.* [20] studied three ^{1}P$^{\rm o}$ resonances by the R-matrix method, Tang *et al.* [7] two ^{1}P$^{\rm o}$ resonances by the hyperspherical coordinate close-coupling method, Cortes and Martin [21] four ^{1}P$^{\rm o}$ resonances by the L^2 basis method, Lindroth [8] six ^{1}P$^{\rm o}$ resonances by the discrete basis complex-rotation method, Bürgers and

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[a] e-mail: `mkc1@phys.nchu.edu.tw`

Lindroth [14] six $^1\mathrm{P}^\mathrm{o}$ resonances by a complex-rotation method using a Sturmian-type basis in perimetric coordinates, Ho [22] four $^1\mathrm{P}^\mathrm{o}$ resonances by the complex-rotation method, and Kuan *et al.* [23] six $^1\mathrm{P}^\mathrm{o}$ resonances by the saddle-point complex-rotation method. Pathak *et al.* [24] and Odgers *et al.* [25] employed the *R*-matrix method without and with continuum channels to calculate $^{1,3}\mathrm{P}^\mathrm{o}$ resonances. Venuti and Decleva [27] studied $^1\mathrm{P}^\mathrm{o}$ with multichannel continuum states in a set of *B*-spline basis functions. Bylicki and Nicolaides [28,29] studied $^{1,3}\mathrm{P}^\mathrm{o}$ with diffuse Slater-type orbitals.

2 Theory

The saddle-point complex rotation method with *B*-spine functions [30] will be briefly described [9,31] here.

We constructed the wave functions in terms of B splines of order k and total number N, defined between two end points, $r_{\min} = 0$ and $r_{\max} = R$, and build vacancies into the wave functions, in a configuration interaction scheme, we have the trial wave function for a two-electron system with an exponential sequence

$$\begin{aligned}\Psi &= A(1 - P(\mathbf{r}_1)(1 - P(\mathbf{r}_2)) \\ &\quad\times \sum_{i,j,l_1,l_2} C_{i,j,l_1,l_2} \Phi_{i,j}(\mathbf{r}_1, \mathbf{r}_2) Y^{LM}_{l_1,l_2} \chi(1,2), \qquad (1)\end{aligned}$$

with

$$\Phi_{i,j}(\mathbf{r}_1, \mathbf{r}_2) = \frac{B_{i,k}(r_1)}{r_1} \frac{B_{j,k}(r_2)}{r_2}, \qquad (2)$$

$$Y^{LM}_{l_1,l_2} = \sum_{m_1,m_2} \langle l_1 l_2 m_1 m_2 | LM \rangle Y_{l_1,m_1}(\hat{r_1}) Y_{l_2,m_2}(\hat{r_2}), \qquad (3)$$

and

$$i \geq j - jm, \qquad (4)$$

where L is the total angular momentum and the numbers i and j are positive integers, which are not larger than N [32], and jm is some selected integer [33]. A is the antisymmetrization operator, $\chi(1,2)$ is the spin wave function, and $P(\mathbf{r})$ is a projection operator

$$P(\mathbf{r}) = P_{1s}(\mathbf{r}) + P_{2s}(\mathbf{r}) + P_{2p}(\mathbf{r}). \qquad (5)$$

For the present, the $1s$, $2s$ and $2p$ orbitals are the vacancy orbitals. We assume it to be hydrogenic with effective nuclear charge, q. The saddle-point variation is carried out by first minimizing the energy with respect to C_{i,j,l_1,l_2} and the set of *B*-spine basis functions, and then maximizing the energy with respect to the effective nuclear charge, q, to obtain the saddle-point energy and wave function. The *B*-spline basis functions with an exponential knot sequence [32,34] are employed in the present calculations. We then calculate the resonance energy and width by a complex-rotation method. We choose the open-channel components [35] to be:

$$\Psi_{\text{open}} = A \sum_i \psi_i(\mathbf{r}_1) \sum_{l_2} \sum_{ki=l_2}^{KI} C_{ki} u_{ki}(\mathbf{r}_2) Y^{L,M}_{l_1,l_2} \chi(1,2), \qquad (6)$$

with

$$u_{ki}(\mathbf{r}_2) = r_2^{ki} \mathrm{e}^{-\beta_i r_2}, \qquad (7)$$

where ψ_i is the the $1s$, $2s$ and $2p$ radial wave function of hydrogen. The non-negative integer, KI, is chosen to be large enough to ensure the accuracy of the resonance energy and width in the calculation by the complex-rotation method. The trial wave functions are composed of the saddle-point wave functions (the closed-channel components) and the open-channel components, Ψ_{open}, in which each radial coordinate r_i in $u_{kc}(\mathbf{r}_i)$ takes the form $r_i \mathrm{e}^{\mathrm{i}\theta}$.

In practice, in using the saddle-point wave functions as the closed-channel components to carry out the complex-rotation calculation, we only varied these coefficients of the partial waves which make major contributions to the saddle-point energies. We found that we can combine a few terms of the saddle-point wave functions (Eq. (1)) to a single term to reduce the working space required for the complex-rotation. calculations. The accuracy was deemed sufficient for our calculations. The closed-channel components for our calculation is constructed from the saddle-point wave function similarly as our previous works.

Gailitis and Damburg [36] pointed out that the position and possibility for H^- resonances will be affected, if the relativistic and QED effects are considered so that the hydrogenic levels with the same principal quantum number are not degenerate. In this paper, we included the Breit-Pauli relativistic and mass-polarization corrections as first-order perturbations by using the saddle-point wave functions as zero-order perturbation wave functions. Our previous results [13] with the first-order perturbation relativistic and mass-polarization corrections are in good agreement with other results [10,11] in a jj coupling scheme. The relativistic and mass-polarization operators are

$$H_1 = -\frac{1}{8c^2} \sum_{i=1}^{2} p_i^4, \qquad (8)$$

$$H_2 = \frac{\pi}{2c^2} \sum_{i=1}^{2} \delta(\mathbf{r}_i), \qquad (9)$$

$$H_3 = -\frac{\pi}{2c^2} \sum_{i,j=1,i\neq j}^{2} [1 + \frac{8}{3} \mathbf{s}_i \cdot \mathbf{s}_j] \delta(\mathbf{r}_{ij}), \qquad (10)$$

$$H_4 = -\frac{1}{M} \sum_{i<j}^{2} \nabla_i \cdot \nabla_j. \qquad (11)$$

As the states are closer to the threshold, the spin-orbit interactions and the mixing between the singlet and triplet

Table 1. Energies ($-E_r$) and widths for doubly excited ${}_3(2,0)_n^-({}^1\mathrm{P}^{\mathrm{o}})$ between the $n = 2$ and 3 thresholds (in a.u.). $A[-n]$ means $A \times 10^{-n}$. The number in parentheses is the uncertainty in the last digit quoted.

	state	$-E_r$	width	state	$-E_r$	width
present	$n = 4$	0.0585718	0.900[−5]	$n = 5$	0.0561168	0.212[−5]
[23]		0.0585708	0.8979[−5]		0.0561144	0.201[−5]
[22]		0.0585718	0.8986[−5]		0.0561167	0.21[−5]
[14]		0.05857181141	0.899726[−5]		0.05611640047	0.225904[−5]
[21]		0.0585697	0.7115[−5]		0.0560759	0.2378[−5]
[7]		0.05859	0.960[−5]		0.05614	
[20]		0.058866	0.148[−4]			
[24]		0.058572			0.056145	
[25]		0.05869			0.05610	
[27]		0.0585697	0.8968[−5]		0.05611661	0.2136[−5]
[28]		0.0585718096	0.89874[−5]		0.056116399	0.22578[−5]
present	$n = 6$	0.0556630	0.408[−6]	$n = 7$	0.05557632	0.191[−6]
[23]		0.0556628	0.415[−6]			
[14]		0.055663057	0.396[−6]			
[27]		0.05566923	0.4611[−6]		0.055577632	0.1188[−6]
[28]		0.0556630559	0.39548[−6]		0.0555763099	0.20030[−6]
[21]		0.0556290	0.297[−6]			
present	$n = 8$	0.05555957	0.154[−7]	$n = 9$	0.05555631	0.30[−8]
[27]		0.055559828	0.1760[−7]			
[28]		0.055559575918	0.15172[−7]		0.055556333474	0.2901[−8]
present	$n = 10$	0.055555703	0.63[−9]	$n = 11$	0.055555587	0.12[−9]
[28]		0.05555570632	0.588[−9]		0.055555583	0.11[−9]
present	$n = 12$	0.055555565	0.36[−10]			

states become more important, while the Coulomb interaction between the two electrons becomes less important. It may have an influence on the formation of the resonances. Therefore, we considered the spin-orbit interactions and the mixing between the singlet and triplet states for the highly excited states.

3 Results and discussion

We study the ${}^{1,3}\mathrm{P}^{\mathrm{o}}$ resonances of H^- between the $n = 2$ and 3 hydrogen thresholds. R, the end points, are extended to 40 000 a.u. in order to get well-converged energies and widths. We calculated $\langle\theta_{12}\rangle$, and classified the resonances by the set of quantum numbers, ${}_N(K,T)_n^A$, with the help of Lin's results [37,38]. We calculated fifteen ${}^1\mathrm{P}^{\mathrm{o}}$ and fifteen ${}^3\mathrm{P}^{\mathrm{o}}$ resonances to examine to possibility of the resonances including the relativistic and QED effects. The nonrelativistic results are tabulated in Tables 1, 2 and 3. The fifteen ${}^1\mathrm{P}^{\mathrm{o}}$ resonances are classified to be ${}_3(2,0)_n^-$ ($4 \le n \le 12$) and ${}_3(1,1)_n^+$ ($3 \le n \le 8$). The fifteen ${}^3\mathrm{P}^{\mathrm{o}}$ resonances are classified to be ${}_3(2,0)_n^+$ ($3 \le n \le 12$) and ${}_3(1,1)_n^-$ ($4 \le n \le 8$). To author's knowledge, these two ${}^1\mathrm{P}^{\mathrm{o}}$ resonances, ${}_3(2,0)_{12}^-$ and ${}_3(1,1)_8^+$, and ten ${}^3\mathrm{P}^{\mathrm{o}}$ resonances, ${}_3(2,0)_n^+$ ($7 \le n \le 12$) and ${}_3(1,1)_n^-$ ($5 \le n \le 8$) have not been studied until now and before 2002 respectively. We included 4–7 partial waves to ensure the energies and widths converged well as shown in Tables 1, 2 and 3. In Tables 1 and 2, we compared our present resonant energies of widths of ${}^1\mathrm{P}^{\mathrm{o}}$ resonances with the other theoretical results. Our energy of the ${}_3(1,1)_3^+$ is in good agreement with those of Kuan *et al.* [23], Lindroth [8], Ho [22], Venuti and Decleva [27] and Bylicki and Nicolaides [28]. However, the experimental results [1–3] are larger than our result and others [7,8,20–23]. All the theoretical widths of the lowest ${}^1\mathrm{P}^{\mathrm{o}}$ resonance agree well with the experimental results [3]. Our results for the energies of higher ${}^1\mathrm{P}^{\mathrm{o}}$ resonances, ${}_3(2,0)_n^-$ ($4 \le n \le 6$) and ${}_3(1,1)_n^+$ ($4 \le n \le 5$), also agree well with the available theoretical results [8,22,23,27,28]. Up to ${}_3(2,0)_6^-$ and ${}_3(1,1)_4^+$ resonances, our widths agree well with those of Kuan *et al.* [23] and Lindroth [8]. Kuan *et al.* [23] did not calculate the ${}_3(2,0)_7^-$ (sixth) resonance. They regarded the ${}_3(1,1)_5^+$ resonance as the sixth resonance. The ${}_3(2,0)_7^-$ and ${}_3(1,1)_5^+$ resonances are nearly degenerate. The results of the R-matrix methods [20,24,25] are less accurate.

There are few results of ${}_3(1,1)_n^+$ ($n \ge 6$) and ${}_3(2,0)_m^-$ ($m \ge 5$) resonances. The present energies still agree very well with those of Venuti and Decleva [27], and Bylicki and Nicolaides [28] for the higher states. The agreement is about within first six or seven digits. Our widths also agree well with those of Venuti and Decleva [27], and Bylicki and Nicolaides [28]. Our energies and widths of ${}^1\mathrm{P}^{\mathrm{o}}$ resonances agree well with those of Bylicki and Nicolaides [28] up to ${}_3(2,0)_n^-$ ($n = 11$) and ${}_3(1,1)_m^-$ ($m = 7$) resonances.

In Table 3, we compared our present energies and widths of ${}^3\mathrm{P}^{\mathrm{o}}$ resonances with other theoretical results [24–26]. The ${}_3(2,0)_n^+$ ($n \ge 7$) and ${}_3(1,1)_n^-$ ($n \ge 5$) resonances have not been studied before 2002. Our energies of the three lowest ${}_3(2,0)_n^+$ resonances agree with the theoretical results [24–26,29] within the first three or four digits. The widths of the different theories agree with each other within no more than the first two digits. The agreement of the width of ${}_3(2,0)_5^+$ amongst the tabulated

Table 2. Energies ($-E_r$) and widths for doubly excited $_3(1,1)^+_n(^1\mathrm{P^o})$ between the $n = 2$ and 3 thresholds (in a.u.). $A[-n]$ means $A \times 10^{-n}$. The number in parentheses is the uncertainty in the last digit quoted.

	state	$-E_r$	width	state	$-E_r$	width
present	$n = 3$	0.0627170	0.116[−2]	$n = 4$	0.0559065	0.696[−4]
[23]		0.06271668	0.1190[−2]		0.0558981	0.7045[−4]
[22]		0.06271675	0.1191[−2]		0.055907	0.70[−4]
[14]		0.0627167721	0.11914806[−2]		0.0559062460	0.710292[−4]
[21]		0.0626468	0.1013[−2]		0.0558367	0.6582[−4]
[7]		0.06272	0.120[−2]		0.05591	0.570[−4]
[20]		0.062695	0.123[−2]		0.055832	0.427[−4]
[24]		0.062713	0.126[−2]		0.055903	0.67[−4]
[25]		0.06272	0.106[−2]		0.05589	0.70[−4]
[27]		0.06271651	0.11916[−2]		0.0559045	0.7061[−4]
[28]		0.06271692	0.119006[−2]		0.05590626	0.70948[−4]
[1]		0.06261(15)	0.101(3)[−2]		0.05573(15)	0.588(111)[−4]
[2]		0.062605(37)	0.14(1)[−2]			
[3]		0.06253(11)	0.11(1)[−2]			
present	$n = 5$	0.05557598	0.396[−5]	$n = 6$	0.055556757	0.245[−6]
[23]		0.0555745	0.3650[−5]			
[14]		0.0555764	0.52[−5]			
[27]		0.05557517	0.4067[−5]		0.055556725	0.2444[−6]
[28]		0.0555763612	0.41854[−5]		0.05555679529	0.25698[−6]
present	$n = 7$	0.0555556090	0.13[−7]	$n = 8$	0.0555555577	0.5[−9]
[28]		0.05555562951	0.15280[−7]			

Table 3. Energies ($-E_r$) and widths for doubly excited $^3\mathrm{P^o}$ between the $n = 2$ and 3 thresholds (in a.u.). $A[-n]$ means $A \times 10^{-n}$. The number in the parentheses is the uncertainty in the last digit quoted.

	state	$-E_r$	width	state	$-E_r$	width
			$_3(2,0)^+_n$			
present	$n = 3$	0.0679169	0.162[−2]	$n = 4$	0.0574345	0.314[−3]
[24]		0.067914	0.172[−2]		0.057418	0.304[−3]
[25]		0.06792	0.150[−2]		0.05742	0.249[−3]
[26]		0.06792	0.165[−2]		0.05742	0.306[−3]
[4]					0.05735(25)	0.37(15)[−3]
[29]		0.0679079	0.16460[−2]		0.0574266	0.3096[−3]
present	$n = 5$	0.0558891	0.492[−4]	$n = 6$	0.0556223	0.934[−5]
[24]		0.055908	0.564[−4]		0.055624	0.120[−4]
[25]		0.05590	0.435[−4]		0.05578	
[26]		0.05591	0.61[−4]			
[29]		0.05591071	0.6350[−4]		0.055624008	0.12472[−4]
present	$n = 7$	0.0555692	0.24[−5]	$n = 8$	0.05555820	0.50[−6]
[29]		0.0555687942	0.2420[−5]		0.0555581183	0.4678[−6]
present	$n = 9$	0.05555607	0.10[−6]	$n = 10$	0.055555656	0.18[−7]
[29]		0.05555605184	0.9078[−7]		0.05555565165	0.1758[−7]
present	$n = 11$	0.055555579	0.35[−8]	$n = 12$	0.055555559	0.21[−9]
[29]		0.0555555727	0.70[−8]			
			$_3(1,1)^-_n$			
present	$n = 4$	0.0563804	0.434[−5]	$n = 5$	0.0556044	0.28[−6]
[24]		0.056380	0.400[−5]			
[25]		0.056345				
[26]		0.05638	0.418[−5]			
[29]		0.05638066	0.4246[−5]		0.05560440463	0.28952[−6]
present	$n = 6$	0.05555839	0.28[−7]	$n = 7$	0.055555690	0.36[−8]
[29]		0.05555846646	0.1856[−7]		0.055555729276	0.1058[−8]
present	$n = 8$	0.055555561	0.13[−9]			
[29]		0.05555556586	0.17[−8]			

Table 4. Contribution of ^{1}P$^{\text{o}}$ resonant energies between the $n = 2$ and 3 H thresholds in H$^-$ (in a.u.). The H($3p_{1/2}$) threshold, -0.055556296 a.u. E_r means the nonrelativistic resonant energy. E_{tot} is the sum of columns 3-6. $A[b]$ means $A \times 10^b$.

n	$-E_{\text{tot}}$	$-E_r$	$\langle H_1 \rangle$	$\langle H_2 \rangle$	$\langle H_4 \rangle$
$_3(2,0)_n^-$					
4	0.0585717	0.0585718	−9.1[−7]	4.0[−7]	6.3[−7]
5	0.0561172	0.0561168	−8.4[−7]	3.6[−7]	1.2[−7]
6	0.0556635	0.0556630	−8.3[−7]	3.5[−7]	2.5[−8]
7	0.05557682	0.05557632	−8.7[−7]	3.7[−7]	4.8[−9]
8	0.05556006	0.05555957	−8.4[−7]	3.5[−7]	9.0[−10]
9	0.05555681	0.05555631	−8.5[−7]	3.5[−7]	2.5[−10]
10	0.055556189	0.055555703	−8.26[−7]	3.40[−7]	-
11	0.055556083	0.055555587	−8.48[−7]	3.52[−7]	-
12	0.055556064	0.055555565	−8.52[−7]	3.53[−7]	-
$_3(1,1)_n^+$					
3	0.0627171	0.0627170	−6.4[−7]	2.0[−7]	3.2[−7]
4	0.0559068	0.0559065	−4.9[−7]	1.3[−7]	1.2[−7]
5	0.05557631	0.05557598	−4.1[−7]	7.6[−8]	8.0[−9]
6	0.05555709	0.055556757	−4.3[−7]	9.3[−8]	4.7[−10]
7	0.0555559991	0.0555556090	−5.8[−7]	1.9[−7]	-
8	0.0555559477	0.0555555577	−6.8[−7]	2.9[−7]	-

Table 5. Contribution of ^{3}P$^{\text{o}}$ resonant energies between the $n = 2$ and 3 H thresholds in H$^-$ (in a.u.). The H($3p_{1/2}$) threshold, -0.055556296 a.u. E_r means the nonrelativistic resonant energy. E_{tot} is the sum of columns 3-6. $A[b]$ means $A \times 10^b$.

n	$-E_{\text{tot}}$	$-E_r$	$\langle H_1 \rangle$	$\langle H_2 \rangle$	$\langle H_4 \rangle$
$_3(2,0)_n^+$					
3	0.0679175	0.0679169	−1.13[−6]	5.4[−7]	−2.7[−8]
4	0.0574350	0.0574345	−9.0[−7]	3.9[−7]	−2.6[−8]
5	0.0558896	0.0558891	−8.5[−7]	3.6[−7]	5.5[−9]
6	0.0556228	0.0556223	−8.4[−7]	3.5[−7]	3.2[−9]
7	0.0555699	0.0555692	−8.4[−7]	3.5[−7]	0.7[−9]
8	0.0555825	0.0555820	−8.5[−7]	3.5[−7]	0.3[−9]
9	0.05555656	0.05555607	−8.4[−7]	3.5[−7]	
10	0.055556151	0.055555656	−8.60[−7]	3.65[−7]	
11	0.055556073	0.055555579	−8.92[−7]	3.98[−7]	
12	0.055556068	0.055555559	−8.36[−7]	3.27[−7]	
$_3(1,1)_n^-$					
4	0.0563802	0.0563804	−4.9[−7]	1.3[−7]	5.2[−7]
5	0.0556047	0.0556044	−4.5[−7]	1.1[−7]	3.7[−8]
6	0.0555843	0.0555839	−5.0[−7]	1.3[−7]	2.1[−9]
7	0.05555605	0.055555690	−4.9[−7]	1.3[−7]	
8	0.05555593	0.055555561	−4.9[−7]	1.2[−7]	

results shows spread. Our energy of the $_3(2,0)_6^+$ resonance agree with that of Pathak *et al.* [24] and Bylicki and Nicolaides [29] better than that of Odgers *et al.* [25]. For higher resonances, more discrepancies appear among the theories. However, our energies of $_3(2,0)_n^+$ $(7 \le n \le 11)$ and $_3(1,1)_n^+$ $(4 \le n \le 8)$ resonances and widths of $_3(2,0)_n^+$ $(7 \le n \le 10)$ and $_3(1,1)_n^+$ $(n = 4, 5)$ resonances agree with those of Bylicki and Nicolaides [29] better than those of other states. The only experimental results [4] for the $_3(2,0)_n^+$ $(n = 4)$ resonance are in agreement with our present results and others [24–26]. However, the accuracy of the experimental results [4] is not good enough. It demands more experimental and theoretical studies on these states.

For the highly excited states of H$^-$, the outer electron can be well regarded to be bound in a dipole potential which decays as $1/r^2$ far from the nucleus. However, if the relativistic and QED effects are considered, the dipole potential will decay faster than $1/r^2$ at large distances because the levels with the same n quantum number in hydrogen are not perfectly degenerate. The dipole potential will not be deep enough to support infinite dipole states. As the state of H$^-$ is very close to the H threshold, the energy of the state is comparable to the fine-structure splitting of the $3p$ state of hydrogen, for the present case. The positions and possibility for resonances will be affected, if the relativistic and QED effects are considered. In Tables 4 and 5, we calculated the

Table 6. Energies of ${}^3\mathrm{P}^\mathrm{o}$ resonances including $\langle H_\mathrm{so} + H_\mathrm{soo}\rangle$. E means the energy without the corrections of spin-orbit interactions. E_tot is the sum of columns 3-4. $A[b]$ means $A \times 10^b$.

n	$-E_\mathrm{tot}$	$-E$	$\langle H_\mathrm{so} + H_\mathrm{soo}\rangle$
		${}_3(2,0)_n^+$	
10	0.055556212	0.055556151	−6.10[−8]
11	0.05555614	0.055556073	−6.86[−8]
12	0.05555614	0.055556068	−7.63[−8]
		${}_3(1,1)_n^-$	
7	0.05555610	0.05555605	−4.69[−8]
8	0.0555598	0.05555593	−4.85[−8]

first-order perturbation relativistic and mass-polarization corrections and to examine the possibility of the Feshbach ${}^{1,3}\mathrm{P}^\mathrm{o}$ resonances formed below the $3\mathrm{P}_{1/2}$ hydrogenic threshold. We calculated $\langle H_2\rangle$ and $\langle H_3\rangle$ by using the global expressions of $\delta(\mathbf{r}_i)$ and $\delta(\mathbf{r}_{ij})$ for smaller uncertainties. $\langle H_3\rangle$ is very small for the present ${}^1\mathrm{P}^\mathrm{o}$ states and vanishes for the present triplet sates. We showed $\langle H_1\rangle$, $\langle H_2\rangle$ and $\langle H_4\rangle$ in Tables 4 and 5. In comparing the energies, E_tot, with the $\mathrm{H}(3p_{1/2})$ threshold [39], −0.055556296 a.u., we found six lowest members of ${}_3(2,0)_n^-({}^1\mathrm{P}^\mathrm{o})$ series, four lowest members of ${}_3(1,1)_n^+({}^1\mathrm{P}^\mathrm{o})$ series, seven lowest members of ${}_3(2,0)_n^+({}^3\mathrm{P}^\mathrm{o})$ series, and three lowest members of ${}_3(1,1)_n^-({}^1\mathrm{P}^\mathrm{o})$ series exist as Feshbach resonances. However, we calculated the effects of spin-orbit and spin-other-orbit interactions, H_so and H_soo, as first-order perturbation corrections for the highest five ${}^3\mathrm{P}^\mathrm{o}$ states, ${}_3(2,0)_m^+$ $(10 \leq m \leq 12)$ and ${}_3(1,1)_n^-$ $(7 \leq n \leq 8)$. They are shown in Table 6. Including the corrections, $\langle \mathrm{H}_\mathrm{so}\rangle$ and $\langle \mathrm{H}_\mathrm{soo}\rangle$, the energies of the highest five ${}^3\mathrm{P}^\mathrm{o}$ states, ${}_3(2,0)_m^+$ $(10 \leq m \leq 12)$ and ${}_3(1,1)_n^-$ $(7 \leq n \leq 8)$, are still larger than the $\mathrm{H}(3p_{1/2})$ threshold. We therefore consider the coupling of the highest five ${}^3\mathrm{P}^\mathrm{o}$ states with $J = 1$ and the near-degenerate ${}^1\mathrm{P}_1^\mathrm{o}$ states by near-degenerate perturbation theory [13]. However, it is found the coupling between the singlet and triplet states has no influence on the existence of Feshbach resonances. The admixture of the $(3p\epsilon d){}^3\mathrm{D}^\mathrm{o}$ continuum with the ${}^{1,3}\mathrm{P}^\mathrm{o}$ resonances has negligible influence as we found in our previous work [13]. For example, the ${}^3\mathrm{P}^\mathrm{o}$ state, ${}_3(2,0)_{10}^+$, is very close to the $\mathrm{H}(3p_{1/2})$ threshold. We calculated the coupling between this state and the ${}^1\mathrm{P}^\mathrm{o}$ states, ${}_3(2,0)_n^-$ $(9 \leq n \leq 11)$ and ${}_3(1,1)_n^+$ $(6 \leq n \leq 8)$. The energy of ${}_3(2,0)_{10}^+({}^3\mathrm{P}^\mathrm{o})$ is shifted to be −0.05556285 a.u., which is larger than the $\mathrm{H}(3p_{1/2})$ threshold.

In summary, we obtained accurate energies and widths of ten ${}^1\mathrm{P}^\mathrm{o}$ and ten ${}^3\mathrm{P}^\mathrm{o}$ by constructing wave functions with B-spline functions variationally without extra parameters. The B-spline functions are flexible, and do not decay exponentially as Slater-type functions. Therefore, the long-rang part of wave functions can be represented efficiently by B-spline functions. There are two highly ${}^1\mathrm{P}^\mathrm{o}$ resonances, which have not been studied until now, and ten highly ${}^3\mathrm{P}^\mathrm{o}$ resonances, which have not been studied before 2002. Including the relativistic and QED effects, we found there exist six Feshbach resonances for ${}_3(2,0)_n^-({}^1\mathrm{P}^\mathrm{o})$ series, four Feshbach resonances for ${}_3(1,1)_n^+({}^1\mathrm{P}^\mathrm{o})$ series, seven Feshbach resonances for ${}_3(2,0)_n^+({}^3\mathrm{P}^\mathrm{o})$ series, and three Feshbach resonances for ${}_3(1,1)_n^-({}^1\mathrm{P}^\mathrm{o})$ series. Unlike the ${}^3\mathrm{P}^\mathrm{o}$ resonances [13] below $n = 2$ H threshold, the existence of the present ${}^3\mathrm{P}^\mathrm{o}$ resonances is not affected by the spin-orbit and spin-other-orbit interactions.

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