

Doubly excited $1,3P^e$ states in heliumlike systems

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Doubly excited or Feshbach-type resonant states in heliumlike systems, $Z=2-10$, have been calculated using the complex-rotation method. Using Hylleraas-type wave functions having up to 825 terms, we predict resonance parameters (both resonance positions and widths) below the $N=3, 4$, and 5 thresholds of the hydrogenic systems. The present results for $Z=7$ and 8 are compared with those of the close-coupling calculations and experimental results where available.

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Two-electron systems are the simplest quantum-mechanical systems which have been studied extensively for all kind of states: bound, excited, and resonant. Among these the parity-favored states $(-1)^L$ have been extensively studied compared to parity-unfavored states $(-1)^{L+1}$, where L is the angular momentum of the state. The $3P^e$ state in He below the $N=2$ threshold of He^+ has been known for a long time. Aashamar [1], Bhatia [2], and Drake [3] calculated the position of this state in H^- and Bhatia [2] has also calculated the position in He. Because of angular momentum and parity conversation, this state does not decay to the ground state but can make a radiative transition to the $3P^o$ autoionization state, which decays by emitting an electron. It can be produced in the presence of a photon.

$$h\nu + e + \text{He}^+ \rightarrow \text{He}(3P^e). \quad (1)$$

Such states must also be present below the higher thresholds as well and can be produced by the above-mentioned process or by

$$e + \text{He}^+(l=1) \rightarrow \text{He}(3P^e), \quad (2)$$

l can also be higher than 1. The final states can also be the $1P^e$ state. Therefore both $1,3P^e$ states must be present below the $N=3,4,5,\dots$ thresholds of hydrogenic systems. These states can decay by radiative transitions to $1,3P^o$ states or autoionize to

$$e + \text{He}^+. \quad (3)$$

He^+ can be in an excited state which could decay to a lower state by a photon emission.

A number of methods like close-coupling and Feshbach projection operator formalism have been used to calculate positions and widths of doubly excited states. In the latter method, resonance position and width are calculated separately and therefore need not be of the same accuracy. We have previously calculated resonance parameters for a number of states by the method of complex rotation, more recently for $3P^e$ resonant states in Ps^- [4]. In this paper we use the same method to calcu-

late resonance parameters of $1,3P^e$ states below $N=3, 4$, and 5 thresholds for $Z=2-10$. This method, as has been indicated in our previous papers, has the advantage of giving the resonance position and width at the same time. The coupling between various open channels can be taken into account by using only discrete or bound-state-

TABLE I. Convergence behavior for $N=3$ $3P^e$ resonances in He.

ω	N	E_r (Ry)	$\Gamma/2$ (Ry)
$3P^e(1)$ ($\alpha=\beta=0.6, \theta=0.3$)			
16	615	-0.672 175 672	0.004 488 78
17	715	-0.672 175 903	0.004 488 74
18	825	-0.672 175 775	0.004 488 75
$3P^e(2)$ ($\alpha=\beta=0.6, \theta=0.3$)			
16	615	-0.582 316 448	$7.400 51 \times 10^{-5}$
17	715	-0.582 316 447	$7.400 31 \times 10^{-5}$
18	825	-0.582 316 447	$7.400 44 \times 10^{-5}$
$3P^e(3)$ ($\alpha=\beta=0.6, \theta=0.3$)			
16	615	-0.543 114 289	0.001 788 65
17	715	-0.543 114 327	0.001 788 63
18	825	-0.543 114 288	0.001 788 64
$3P^e(4)$ ($\alpha=\beta=0.5, \theta=0.3$)			
16	615	-0.507 149 307	$2.352 31 \times 10^{-5}$
17	715	-0.507 149 303	$2.352 54 \times 10^{-5}$
18	825	-0.507 149 304	$2.352 30 \times 10^{-5}$
$3P^e(5)$ ($\alpha=\beta=0.5, \theta=0.3$)			
16	615	-0.501 863 612	0.000 855 440
17	715	-0.501 863 049	0.000 855 616
18	825	-0.501 863 050	0.000 855 304
$3P^e(6)$ ($\alpha=\beta=0.4, \theta=0.3$)			
16	615	-0.483 916 544	$1.441 39 \times 10^{-5}$
17	715	-0.483 916 560	$1.447 99 \times 10^{-5}$
18	825	-0.483 916 563	$1.444 38 \times 10^{-5}$
$3P^e(7)$ ($\alpha=\beta=0.4, \theta=0.3$)			
16	615	-0.481 918 711	0.000 453 925
17	715	-0.481 922 994	0.000 453 223
18	825	-0.481 919 231	0.000 455 822

type functions and wave functions having the asymptotic forms are not needed. This is of particular advantage when there are a number of open channels, and the resonance parameters can be calculated in the same way as for the one-channel case. The method is capable of giving very accurate results. We continue these calculations for other two-electron systems. In this calculation we use Hylleraas-type wave functions [2,5]. The most general two-electron wave function for $1,3P^e$ is of the form

$$\begin{aligned} \Phi(r_1, r_2) = & \sin(\theta_{12}) r_1 r_2 \\ & \times \sum_{l,m,n \geq 0} C_{lmn} [r_1^l r_2^m \exp(-\alpha r_1 - \beta r_2) \\ & \pm (1 \rightarrow 2)] r_{12}^n \mathcal{D}_1^{0+}, \end{aligned} \quad (4)$$

where \mathcal{D}_1^{0+} is the rotational harmonic depending on Euler angles θ , ϕ , and ψ and $l + m + n \leq \omega$, with ω a positive integer or zero. Since

TABLE II. Doubly excited $3P^e$ states of helium. The threshold energies for $N=3, 4$, and 5 are -0.4444 , -0.25 , and -0.16 Ry.

	E_r (Ry)	$\Gamma/2$ (Ry)
$N=3$		
(1)	-0.672 175 8	0.004 488 7
(2)	-0.582 316 45	7.40×10^{-5}
(3)	-0.543 114 3	0.001 788 7
(4)	-0.507 149 30	2.3523×10^{-5}
(5)	-0.501 863 0	0.000 855
(6)	-0.483 916 6	1.44×10^{-5}
(7)	-0.481 92	0.00045
(8)	-0.471 787	8.0×10^{-6}
$N=4$		
(1)	-0.388 884	0.003 305
(2)	-0.356 514	0.004 807
(3)	-0.322 446	0.001 903
(4)	-0.310 353 6	0.000 258 5
(5)	-0.303 099	0.001 766
(6)	-0.296 063	0.001 05
(7)	-0.284 683	0.000 328 5
(8)	-0.284 682	0.000 837 9
(9)	-0.281 68	0.000 57
(10)	-0.274 59	0.000 612
(11)	-0.274 30	0.000 11
$N=5$		
(1)	-0.252 78	0.002 17
(2)	-0.238 60	0.003 54
(3)	-0.218 926	0.003 122
(4)	-0.214 53	0.001 53
(5)	-0.204 192	0.002 269
(6)	-0.197 204	0.000 906
(7)	-0.193 281	0.001 374
(8)	-0.190 507 7	8.85×10^{-5}
(9)	-0.190 268	0.001 48
(10)	-0.186 87	0.000 41
(11)	-0.183 02	0.000 94
(12)	-0.182 21	0.000 85
(13)	-0.181 449	4.2×10^{-5}

$$\mathcal{E}_{12} \mathcal{D}_1^{0+} = -\mathcal{D}_1^{0+}, \quad (5)$$

where \mathcal{E}_{12} is the exchange operator [5], the upper sign refers to triplet states and the lower sign refers to the singlet states.

$$\mathcal{P} \mathcal{D}_1^{0+} = +\mathcal{D}_1^{0+}, \quad (6)$$

where \mathcal{P} is the parity operator [5], indicates that the parity of the state represented by the wave function is even. The Hamiltonian is given by

$$\begin{aligned} H = & -\nabla_1^2 - \nabla_2^2 - 2Z/r_1 - 2Z/r_2 + 2/r_{12}, \\ = & T + V. \end{aligned} \quad (7)$$

Z is the nuclear charge, r_1 and r_2 are the coordinates of electrons with respect to the nucleus, and $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$. Energies are expressed in rydberg units. The method of complex rotation has been discussed by Ho [6]. Briefly, the Hamiltonian is analytically continued in the complex energy plane by making the dilatation transformation $r \rightarrow r \exp(i\theta)$ on the Hamiltonian, and for Coulomb potentials, we have

$$H(\theta) = T \exp(-2i\theta) + V \exp(-i\theta), \quad (8)$$

where θ is chosen between 0 and 45° . The eigenvalues are obtained by diagonalizing the analytically continued Hamiltonian

$$E = \langle \Phi H \Phi \rangle / \langle \Phi \Phi \rangle, \quad (9)$$

wherein eigenvalues and eigenvectors are complex while the basis functions continue to be real. Discrete complex eigenvalues have the form

$$E = E_r - i\Gamma/2, \quad (10)$$

where E_r gives the resonance position and Γ gives the resonance width. A resonance, if it exists on the second Riemann sheet, is "uncovered" by the cut once the "rotation angle" θ is greater than the absolute value of $\arg(E - E_{th})/2$, where E_{th} is the threshold energy below which resonances are being calculated. Its position then remains constant as θ increases, while the other roots follow the branch cut associated with that threshold. The cut makes an angle of $-\theta$ with the real axis at the lower threshold. In this method, resonance positions and widths are deduced from the conditions that a discrete complex eigenvalue is stabilized with respect to the non-linear parameters in the wave functions and with respect to θ , the rotation angle. Convergence behavior is examined by repeating the calculations for different expansion lengths. It should be pointed out that there are no variational bounds, like those obtained for bound states in variational methods, on the eigenvalues obtained in this method of complex rotation. However, the virial

TABLE III. Doubly excited $^3P^e$ states in helium sequence ($Z=3-6$).

	$Z=3$		$Z=4$		$Z=5$		$Z=6$	
	$-E_r$ (Ry)	$\Gamma/2$ (Ry)	$-E_r$ (Ry)	$\Gamma/2$ (Ry)	$-E_r$ (Ry)	$\Gamma/2$ (Ry)	$-E_r$ (Ry)	$\Gamma/2$ (Ry)
$N=3$	1.662 562 8	0.005 328 7	3.097 401	0.005 722 8	4.976 683	0.005 954	7.300 404	0.006 109 8
	1.511 577 6	7.0531×10^{-5}	2.885 086 04	7.2467×10^{-5}	4.702 915 83	7.3971×10^{-5}	6.965 1227 7	7.503×10^{-5}
	1.322 077 2	0.002 583 4	2.448 259	0.002 989 1	3.921 648	0.003 2355	5.742 244 9	0.003 401 4
	1.250 180 8	2.2094×10^{-5}	2.340 626 7	2.6379×10^{-5}	3.778 48	2.8846×10^{-5}	5.563 651 4	3.025×10^{-5}
	1.196 621	0.001 241	2.193 805	0.001 414 9	3.493 24	0.001 516 8	5.094 897 8	0.001 585
	1.159 262	1.19×10^{-5}	2.137 675	1.260×10^{-5}	3.418 646	1.221×10^{-5}	5.001 963	1.16×10^{-5}
	1.132 13	0.000 659	2.060 285	0.000 749 2	3.266 23	0.000 803	4.749 933 5	0.000 839
	1.110 658	6.990×10^{-6}	2.027 949	6.5×10^{-6}	3.223 20	5.74×10^{-6}	4.696 278 3	5.06×10^{-6}
$N=4$	0.952 438	0.004 239 8	1.766 005	0.004 706	2.829 63	0.004 98	4.143 29	0.005 16
	0.986 305	0.006 653	1.686 204	0.007 383	2.726 166	0.007 793	4.016 149	0.008 064
	0.818 279	0.000 103 4	1.576 142	8.710×10^{-5}	2.583 878	7.955×10^{-5}	3.841 542 6	7.490×10^{-5}
	0.784 869	0.002 722	1.452 262	0.003 152	2.324 658	0.003 419 5	3.402 056	0.003 602 7
	0.748 410 3	0.003 267	1.398 453	0.003 976	2.253 422	0.004 405	3.313 347 8	0.004 693 7
	0.710 290 3	0.001 461	1.340 157 5	3.621×10^{-5}	2.175 343	3.418×10^{-5}	3.215 604 7	3.250×10^{-5}
	0.710 085 0	4.2374×10^{-5}	1.305 095	0.001 664	2.080 447	0.001 792	3.036 338	0.001 881 3
	0.688 088	0.001 867	1.272 526	0.002 147	2.037 542	0.002 292	2.983 078	0.002 385
	0.667 440	0.000 783	1.238 674	2.214×10^{-5}	1.992 404	1.733×10^{-5}	2.926 806 3	1.38×10^{-5}
	0.665 879	2.803×10^{-5}	1.219 03	0.000 88	1.936 409	0.000 953	2.819 564	0.000 998
	0.653 429	0.001 072	1.198 53	0.001 154	1.909 438	0.001 19	2.786 081	0.001 220
					1.881 02	8.0×10^{-6}	2.750 736 4	4.94×10^{-6}

theorem

$$2\langle \Phi | T | \Phi \rangle = -\langle \Phi | V | \Phi \rangle, \quad (11)$$

is satisfied [6] when $\partial E / \partial \theta = 0$.

We now present results of our calculation, first for the $^3P^e$ states. In Table I, the convergence behavior of the

first seven states in He below the $N=3$ threshold of He^+ is shown. It can be seen that, except for the seventh state, eigenvalues have converged to at least six decimal places when the number of terms in the wave function is increased from 615 to 825. The angle θ is kept fixed at 0.3 and the $\alpha=\beta$ range from 0.6 to 0.4 from the lowest state to the highest one. In Table II, positions and widths

TABLE IV. Doubly excited $^3P^e$ states in helium sequence ($Z=7-10$).

	$Z=7$		$Z=8$		$Z=9$		$Z=10$	
	$-E_r$ (Ry)	$\Gamma/2$ (Ry)	$-E_r$ (Ry)	$\Gamma/2$ (Ry)	$-E_r$ (Ry)	$\Gamma/2$ (Ry)	$-E_r$ (Ry)	$\Gamma/2$ (Ry)
$N=3$	10.068 566	0.006 220 0	13.281 169	0.006 302 7	16.938 214	0.006 367 1	21.039 702	0.006 418 6
	9.671 734 2	7.578×10^{-5}	12.822 764 8	7.643×10^{-5}	16.418 222 8	7.677×10^{-5}	20.458 113 4	7.7103×10^{-5}
	7.910 052 7	0.003 520 7	10.425 073 9	0.003 610 9	13.287 310 5	0.003 681 3	16.497 641	0.003 738 0
	7.696 104	3.108×10^{-5}	10.175 813 0	3.160×10^{-5}	13.002 766 0	3.193×10^{-5}	16.176 955 9	3.2143×10^{-5}
	6.998 766	0.001 634	9.204 847	0.001 671	11.713 143	0.001 701	14.523 654	0.001 724
	6.887 554 4	1.10×10^{-5}	9.075 389 1	1.05×10^{-5}	11.565 456	9.999×10^{-6}	14.357 749 0	9.613×10^{-6}
	6.511 403	0.000 867	8.550 635	0.000 888	10.867 63	0.000 904	13.462 401	0.000 917
	6.447 136	4.54×10^{-6}	8.475 765 0	4.10×10^{-6}	10.782 163	3.79×10^{-6}	13.366 329 2	3.612×10^{-6}
$N=4$	5.7069 9	0.005 267	7.5206	0.005 33	9.584 29	0.005 37	11.897 95	0.005 40
	5.556 141	0.008 261	7.346 142	0.008 413	9.386 151	0.008 532	11.676 165	0.008 625
	5.349 164 3	7.169×10^{-5}	7.106 759 1	6.932×10^{-5}	9.114 335 8	6.7502×10^{-5}	11.371 899 9	6.608×10^{-5}
	4.684 456	0.003 736	6.171 856	0.003 839	7.864 258	0.003 920	9.761 658 6	0.003 986
	4.578 244	0.004 901 3	6.048 11 91	0.005 057 9	7.772 979	0.005 180 4	9.602 827	0.005 278 8
	4.460 909 8	3.105×10^{-5}	5.911 240 3	2.980×10^{-5}	7.566 586 5	2.8739×10^{-5}	9.426 942 9	2.7846×10^{-5}
	4.171 772	0.001 948	5.489 752 8	0.002 001	6.987 281 0	0.002 042	8.665 359 5	0.002 077
	4.109 130	0.002 453	5.415 702	0.002 504	6.902 802	0.002 545	8.570 435	0.002 579
	4.041 795 4	1.130×10^{-5}	5.337 343 4	9.5×10^{-6}	6.813 441 0	8.3×10^{-6}	8.470 086 0	7.4×10^{-6}
	3.868 51	0.001 04	5.083 24	0.001 077	6.4637 6	0.001 109	8.010 088	0.001 144
	3.828 467	0.001 248	5.036 606	0.001 274	6.4105 10	0.001 297	7.950 188	0.001 318
	3.786 231	3.43×10^{-6}	4.987 509	2.49×10^{-6}	6.3545 69	2.01×10^{-6}	7.887 415	1.80×10^{-6}

Table VII. Doubly excited $1P^e$ states in helium sequence ($Z=7-10$).

	$Z=7$		$Z=8$		$Z=9$		$Z=10$	
	$-E_r$ (Ry)	$\Gamma/2$ (Ry)	$-E_r$ (Ry)	$\Gamma/2$ (Ry)	$-E_r$ (Ry)	$\Gamma/2$ (Ry)	$-E_r$ (Ry)	$\Gamma/2$ (Ry)
$N=3$	7.997 305	9.421×10^{-5}	10.526 844	9.697×10^{-5}	13.403 605	9.929×10^{-5}	16.627 585 8	0.000 101 0
	7.805 601 9	2.777×10^{-6}	10.304 859	2.896×10^{-6}	13.151 344	2.993×10^{-6}	16.345 055 7	3.070×10^{-6}
	7.030 271	7.557×10^{-5}	9.241 579	7.880×10^{-5}	11.755 110	8.120×10^{-5}	14.570 863	8.33×10^{-5}
	6.925 567	1.960×10^{-6}	9.119 632 7	2.054×10^{-6}	11.615 925	2.128×10^{-6}	14.414 441 6	2.188×10^{-6}
	6.526 450	5.14×10^{-5}	8.568 23	5.37×10^{-5}	10.887 79	5.58×10^{-5}	13.485 13	5.72×10^{-5}
	6.464 82	1.26×10^{-6}	8.496 26	1.31×10^{-6}	10.805 48	1.35×10^{-6}	13.392 49	1.39×10^{-6}
$N=4$	4.731 653	0.000 127 1	6.226 776	0.000 130 6	7.926 898	0.000 133 1	9.832 020	0.000 135 6
	4.650 585	0.000 252 8	6.133 095	0.000 262 8	7.820 598	0.000 271	9.713 097	0.000 276 8
	4.530 735	4.790×10^{-6}	5.993 994	4.89×10^{-6}	7.662 256	4.97×10^{-6}	9.535 519 4	5.04×10^{-6}
	4.190 874	0.000 122 9	5.510 869	0.000 127 4	7.011 419 8	0.000 131 1	8.692 526 6	0.000 134 1
	4.136 345	0.000 223	5.447 531	0.000 234	6.939 267	0.000 243	8.611 554	0.000 250 7
	4.066 840	3.51×10^{-6}	5.366 413	3.55×10^{-6}	6.846 543	3.58×10^{-6}	8.507 230	3.61×10^{-6}
	3.876 93	9.4×10^{-5}	5.093 16	9.7×10^{-5}	6.475 213	1.0×10^{-4}	8.023 08	1.04×10^4
	3.840 38	0.000 164	5.050 58	0.000 173	6.426 599	0.000 180	7.968 43	0.000 186
$N=5$	3.133 630	0.000 119	4.123 051	0.000 122	5.248 030	0.000 123	6.508 564	0.000 126
	3.093 133	0.000 303	4.076 330	0.000 314	5.195 084	0.000 322	6.449 389	0.000 330
	3.036 136	0.000 374	4.010 298	0.000 390	5.120 009	0.000 408	6.365 266	0.000 418
	2.955 164	4.54×10^{-6}	3.916 134	4.48×10^{-6}	5.012 660	4.42×10^{-6}	6.244 741	4.34×10^{-6}

[7] has been carried out for $Z=7$ for states below the $N=3$ threshold. A comparison of their results with the present resonance parameters for the six $3P^e$ and five $1P^e$ states is given in Table VIII. The positions in this table, as also in Ref. [7], are given with respect to the $N=2$ state of N^{6+} . Three to four significant figures have been retained as has been done in Ref. [7]. The agreement between the two calculations is very good. The experimental results given in Ref. [7] have been obtained by double-electron capture by N^{7+} using He, H_2 , and Ar as targets. The experimental values are 29.9, 73.6, and 58.2 eV for $3P(1)$, $3P(6)$, and $1P(1)$, which agree fairly well

TABLE VIII. Comparison of present and close-coupling results for N^{5+} . Units: eV

State	Present		Close-coupling ^a	
	Position	Width	Position	Width
$3P(1)$	29.68	0.17	29.9	0.17
$3P(2)$	35.08	0.0021	35.4	0.0021
$3P(3)$	59.05	0.095	59.2	0.095
$3P(4)$	61.96	0.0008	62.2	0.001
$3P(5)$	71.45	0.044	71.6	0.044
$3P(6)$	72.96	0.0003	73.1	0.0004
$3P(7)$	78.08	0.024	78.2	0.024
$1P(1)$	57.86	0.0026	58.0	0.0026
$1P(2)$	60.47	0.000 08	60.6	0.000 08
$1P(3)$	71.02	0.0021	71.1	0.0020
$1P(4)$	72.44	0.000 05	72.6	0.000 05
$1P(5)$	77.87	0.0014	78.0	0.0016

^aReference [7].

with the calculated values 29.68, 72.96, and 57.86 eV. The present value of 72.96 is close to the close-coupling value 73.10, indicating that the experimentally determined position 73.6 eV is not very accurate.

A similar close-coupling calculation [8] has been carried out for $Z=8$ for states below the $N=3$ threshold of O^{7+} . A comparison of their results with the present results for four $3P^e$ and four $1P^e$ states is given in Table IX. The positions are given with respect to the $N=2$ threshold of O^{7+} . The agreement between the two calculations is very good. The only experimental position for $1P^e$ is 77.49 eV which agrees very well with our calculated value 77.49 eV. The experimental position was determined by double capture by O^{8+} using He or H_2 .

In summary, we have carried out a calculation for $1,3P^e$

TABLE IX. Comparison of present and close-coupling results for O^{6+} . Units: eV

State	Present		Close-coupling ^a	
	Position	Width	Position	Width
$3P(1)$	36.99	0.171	37.13	0.13
$3P(2)$	43.23	0.0021	43.46	0.0021
$3P(3)$	75.85	0.098	76.01	0.098
$3P(4)$	79.24	0.000 86		
$3P(5)$	92.45	0.045	92.60	0.046
$1P(1)$	74.47	0.0026	74.61	0.0025
$1P(2)$	77.49	0.000 079	77.66	0.000 079
$1P(3)$	91.95	0.0021	92.09	0.0021
$1P(4)$	93.61	0.000 056	93.76	0.000 049

^aReference [8].

states using the method of complex rotation. We find a large number of resonances below the $N=3$, 4, and 5 hydrogenic thresholds. At present, there are theoretical and experimental results for $Z=7$ and 8 to compare with. We hope this paper will encourage further experi-

ments and calculations.

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