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Ritz variational calculation for two-electron–one-photon transitions in helium

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Variational calculations for the energy levels of doubly excited $3dnf$ $({}^{1,3}D^{\circ})$ states $(n=4-12)$ for helium have been performed using the extended Hylleraas basis set. No previous calculations for the energy eigenvalues for the $3dnf$ $({}^{1,3}D^{\circ})$ states for $(n=7-12)$ exist. Prediction of two-electron–one-photon peaks at 12.220, 12.649, 12.859, 12.978, 13.054, 13.110, 13.141, 13.168 and 13.213 eV corresponding to the transitions $2p^2$ $({}^3P^{\mathrm{e}})\rightarrow 3dnf$ $({}^3D^{\circ})$ $(n=4-12)$, respectively, is reported here. Highly precise energy eigenvalues of doubly excited $2pnd$ states $({}^{1,3}D^{\circ})$ $(n=3-8)$ for helium are also reported and the upper bound energies are the lowest yet obtained. The effective quantum numbers (n^*) of the above mentioned states are calculated using quantum defect theory.

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I. INTRODUCTION

Two-electron–one-photon transitions in atoms were predicted long ago by Heisenberg [1], Condon [2], and Goudsmit and Gropper [3]. After almost thirty years, Madden and Codling [4] first observed the two-electron–one-photon peaks while recording the photoabsorption spectra of helium placed in the field of synchrotron radiation. Since then, the study of doubly excited states of heliumlike systems has become a subject of interest of both theoreticians as well as experimentalists. A detailed list of references is given in a recent publication by Bhattacharyya *et al.* [5]. It is now well known that the origin of the three series of two-electron–one-photon peaks of heliumlike systems are due to the transitions between $1s^2$ $({}^1S^{\mathrm{e}})$ (lying below the $N=1$ ionization threshold of He$^+$) and three ${}^1P^{\circ}$ states $(sp,2n+)$, $(sp,2n-)$ and $(2pnd)$ (lying below the $N=2$ ionization threshold of He$^+$). With improved experimental technique due to Domke *et al.* [6] and Schulz *et al.* [7], the respective three series for helium have been observed within accuracy limits of 4 and 1 meV, respectively.

In a recent paper, the possibilities of observing another set of three series of two-electron–one-photon peaks due to the transitions from $2p^2$ $({}^3P^{\mathrm{e}})$ state (lying below the $N=2$ ionization threshold of He$^+$) to three ${}^3D^{\circ}$ states $(pd,3n+)$, $(pd,3n-)$, and $(3dnf)$ (lying below the $N=3$ ionization threshold of He$^+$) are given by Bhattacharyya *et al.* [5] and energy values were predicted for the first three members of the third $(3dnf)$ Rydberg series of helium originating from the lowest ${}^3P^{\mathrm{e}}\rightarrow 3dnf$ $({}^3D^{\circ})$ $(n=4,5,6)$ transitions. In this paper, we extend the doubly excited state wave function of Bhattacharyya *et al.* [5] to estimate the energy of $2pnd$ $({}^{1,3}D^{\circ})$ $(n=4-8)$ of helium and the energy of $3dnf$ $({}^{1,3}D^{\circ})$ $(n=7-12)$ states using elaborate trial basis functions.

II. METHOD

The ${}^{1,3}D$ state wave function of odd parity due to the (df) configuration of two electrons is given by

$$\psi = \sin\,\theta_{12}\Big[\Big\{(f\mp\tilde{f})\cos\tfrac{1}{2}\,\theta_{12}(5\cos\theta_{12}-1)\Big\}D_2^{1+} + \Big\{(f\pm\tilde{f})\sin\tfrac{1}{2}\theta_{12}(5\cos\theta_{12}+1)\Big\}D_2^{1-}\Big], \quad (1)$$

where the D's are the rotational harmonics depending on Eulerian angles θ, ϕ, ψ [8]. The upper sign in Eq. (1) corresponds to the singlet state and the lower sign to the triplet state.

The trial wave function $f(r_1,r_2,r_{12})$ is given by

$$f(r_1,r_2,r_{12}) = [b_1\eta_1(1)\eta_1(2) + b_2\eta_1(1)\eta_2(2) + b_3\eta_2(1)\eta_2(2)]g(1,2), \quad (2)$$

where

$$g(1,2) = r_1^3 r_2^2 \sum_{l\geq 0}\sum_{m\geq 0}\sum_{n\geq 0} C_{lmn} r_1^l r_2^m r_{12}^n, \quad (3)$$

$$\eta_i(j) = e^{-\rho_i r_j}, \quad (4)$$

and

$$\tilde{f} = f(r_2,r_1,r_{12}), \quad (5)$$

b_1, b_2, b_3 are linear parameters, and ρ is the nonlinear parameter. The symbols used are the same as in Bhattacharyya *et al.* [5]. The energy eigenvalues are determined by the matrix diagonalization method. We use atomic unit throughout. The nonlinear parameters ρ_1 and ρ_2 are optimized by the Nelder-Mead procedure [9]. We have carried out all calculations in quadruple precision.

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TABLE I. Nonrelativistic energy eigenvalues $-E$ (a.u.) and effective quantum numbers (n^*) for $3dnf$ (n=4–12) $^3D^o$ states of helium. ρ_1, ρ_2 are the nonlinear parameters.

M	$3d4f^{a}$ $\rho_1=0.3233$ $\rho_2=0.6777$	$3d5f^{a}$ $\rho_1=0.2581$ $\rho_2=0.6590$	$3d6f^{a}$ $\rho_1=0.1113$ $\rho_2=0.6451$	$3d7f$ $\rho_1=0.1402$ $\rho_2=0.6825$	$3d8f$ $\rho_1=0.1135$ $\rho_2=0.6664$	$3d9f$ $\rho_1=0.0781$ $\rho_2=0.4371$	$3d10f$ $\rho_1=0.1171$ $\rho_2=0.6096$	$3d11f$ $\rho_1=0.1223$ $\rho_2=0.6548$	$3d12f$ $\rho_1=0.1285$ $\rho_2=0.6797$
12	0.25888	0.24366	0.23506	0.20255	0.18024	0.16615	0.14715	0.13706	0.13102
27	0.25949	0.24487	0.23712	0.23280	0.21651	0.18863	0.19106	0.18040	0.15592
51	0.25994	0.24509	0.23757	0.23330	0.23047	0.20371	0.20465	0.19665	0.19141
84	0.26049	0.24528	0.23773	0.23345	0.23063	0.22230	0.21085	0.20522	0.19933
129	0.26061	0.24537	0.23782	0.23349	0.23072	0.22463	0.22513	0.20993	0.20347
186	0.26088	0.24545	0.23786	0.23351	0.23075	0.22750	0.22717	0.22285	0.21126
258	0.26105	0.24553	0.23790	0.23353	0.23076	0.22842	0.22754	0.22579	0.21904
345	0.26125	0.24560	0.23792	0.23354	0.23077	0.22867	0.22758	0.22643	0.22342
450	0.26142	0.24566	0.23795	0.23357	0.23078	0.22872	0.22759	0.22659	0.22493
	0.2501[b]	0.2402[b]							
	0.251106[c]	0.240946[c]	0.235351[c]						
	0.2512[d]	0.2403[d]							
	0.25118595[e]								
n^*	3.5715298	4.6187748	5.6383408	6.6378830	7.6437152	8.7720798	9.6513427	10.699284	13.588718

[a] Reference [5].
[b] Reference [20].
[c] Reference [14].
[d] Reference [21].
[e] Reference [12].

Transforming the rotational harmonics D_2^{1+} (θ,ϕ,ψ) and D_2^{1-} (θ,ϕ,ψ) in polar angles of two electrons (θ_1, ϕ_1; θ_2, ϕ_2), it can easily be shown that the wave function ψ given by Eq. (1) corresponds to the configuration (df) for two electrons with angular momentum equal to 2. Similarly it can be shown [5] that the wave function ψ given in Eq. (1) with a replacement in the θ_{12} dependent part associated with D_2^{1+} and D_2^{1-} by $\sin\theta_{12}\cos\frac{1}{2}\theta_{12}$ and $\sin\theta_{12}\sin\frac{1}{2}\theta_{12}$, respectively, represents the $^{1,3}D^{\circ}$ state wave function due to (pd) configuration. The separability of odd parity D states into (pd) and (df) configurations is remarkable. It is interesting to note that the $^{1,3}D^{\circ}$ state wave functions due to the (pd) and (df) configurations are orthogonal to each other. This can be demonstrated easily by performing integrals over the θ_{12} part of the respective wave functions. The above physical interpretation of Eq. (1) enables us to apply the Hylleraas-Undheim theorem [10] successfully to obtain the energy values of the first nine $^{1,3}D^{\circ}$ states of helium due to (df) configuration.

The aim of the present paper is to raise the question of whether or not the mixing of (pd) and (df) configurations in $^{1,3}D^{\circ}$ state is inherent in nature. Bhatia [11] included both the configurations and obtained the energy values of $2pnd$ ($^{1,3}D^{\circ}$) states by using the Ritz variational method. According to Bhatia [11] this mixing of (pd) and (df) configurations is necessary to facilitate only the convergence of energy eigenvalues. In the previous paper [5] we have calculated only the energy of the $2p3d$ ($^{1,3}D^{\circ}$) state of helium by excluding the (df) configuration and obtained the lower energy values than that of Bhatia [11] without loss of convergence. The present calculation for the energy eigenvalues of the $2pnd$ ($^{1,3}D^{\circ}$) state with n=4–8 also confirms the fact that better energy eigenvalues without loss of convergence can be achieved by excluding (df) configuration. Besides excluding (pd) and (df) configuration mixing our basis set differs from that of Bhatia [11] in the sense that we used the triple exponential basis set as is evident from expression (2) whereas Bhatia [11] adopted the single exponential basis set. The effect of (pd) on (df) configuration cannot be studied within the purview of the Ritz variational method. Complex rotation [12] or stabilization methods [13] may be useful for this purpose.

We have calculated the effective quantum number n^* for $3dnf$ ($^{1,3}D^{\circ}$) (n=4–12) and $2pnd$ ($^{1,3}D^{\circ}$) (n=3–8) states of helium by using the formula [14] given by

$$E=-\frac{1}{2}\left[\left(\frac{Z}{N}\right)^2+\left(\frac{Z-1}{n^*}\right)^2\right], \tag{6}$$

Where E is the energy of the state below total ionization, N is the inner electron quantum number, and Z is the atomic number.

III. RESULTS AND DISCUSSION

The energy eigenvalues of different $3dnf$ ($^3D^{\circ}$) (n=4–12) states of helium are given in Table I. In the first column of Table I the total number of terms (M) in the wavefunction is given. In other columns, the energy values of different states are shown in accordance with increasing M. A similar presentation of the energy eigenvalues for $3dnf$ ($^1D^{\circ}$) (n=4–12) states of helium is given in Table II. Avail-

TABLE II. Nonrelativistic energy eigenvalues $-E$ (a.u.) and effective quantum numbers (n^*) for $3dnf$ ($n=4-12$) $^1D^{\text{o}}$ states of helium. ρ_1, ρ_2 are the nonlinear parameters.

M	$3d4f$[a] $\rho_1=0.3663$ $\rho_2=0.7268$	$3d5f$[a] $\rho_1=0.2655$ $\rho_2=0.6354$	$3d6f$[a] $\rho_1=0.1211$ $\rho_2=0.6351$	$3d7f$ $\rho_1=0.1401$ $\rho_2=0.6977$	$3d8f$ $\rho_1=0.1072$ $\rho_2=0.6647$	$3d9f$ $\rho_1=0.1297$ $\rho_2=0.5235$	$3d10f$ $\rho_1=0.1153$ $\rho_2=0.6125$	$3d11f$ $\rho_1=0.1128$ $\rho_2=0.6310$	$3d12f$ $\rho_1=0.1240$ $\rho_2=0.6630$
12	0.26018	0.24438	0.23592	0.20236	0.17992	0.17371	0.15529	0.14653	0.13825
27	0.26114	0.24556	0.23758	0.23312	0.20696	0.20071	0.19196	0.18483	0.17808
51	0.26130	0.24563	0.23788	0.23341	0.23054	0.20908	0.20572	0.19752	0.19179
84	0.26183	0.24576	0.23801	0.23359	0.23075	0.22361	0.21230	0.20871	0.20069
129	0.26213	0.24587	0.23807	0.23364	0.23081	0.22754	0.22562	0.21321	0.20724
186	0.26244	0.24600	0.23811	0.23367	0.23084	0.22843	0.22734	0.22451	0.21386
258	0.26261	0.24606	0.23815	0.23369	0.23086	0.22888	0.22760	0.22624	0.22063
345	0.26284	0.24612	0.23819	0.23371	0.23087	0.22896	0.22763	0.22660	0.22418
450	0.26299	0.24617	0.23822	0.23373	0.23088	0.22897	0.22764	0.22661	0.22530
	0.2513[b]	0.2410[b]							
	0.252640[c]	0.241913[c]	0.235935[c]						
	0.2528[d]	0.2416[d]							
	0.252743435[e]								
n^*	3.5020834	4.5693286	5.5905582	6.5915761	7.5994434	8.6080467	9.6067040	10.674872	12.725123

[a] Reference [5].
[b] Reference [20].
[c] Reference [14].
[d] Reference [21].
[e] Reference [12].

able other theoretical energy values of $3dnf\,(^{1,3}D^{\circ})$ ($n=4-6$) states of helium are included in Tables I and II for a comparison with the present results. The energy of the $2p^2\,(^3P^{\text{e}})$ state of helium is taken as $-0.710\,50$ a.u. [15].

Energy eigenvalues of different $2pnd\,(^{1,3}D^{\circ})$ ($n=3-8$) states are displayed in Tables III and IV, respectively. The energy eigenvalues for $2pnd(^{1,3}D^{\circ})$ ($n=3-6$) states as obtained by Bhatia [11] are included in Tables III and IV for comparison with the present results. It is remarkable that for a given number of terms (M) the results of the present basis set are better than those of Bhatia [11], e.g., our results of the $2p4d\,(^3D^{\circ})$ state for the 69-parameter calculation is better than that of the 112-parameter calculation of Bhatia [11]; again, our 51-parameter result for $2p5d\,(^1D^{\circ})$ is better than that of the 112-parameter result of Bhatia [11] as is evident from the data presented in Tables III and IV, respectively. Substantial reduction of the number of terms i.e., the basis set size, is a clear advantage of the present method for a particular energy value. To the best of our knowledge, the nonrelativistic energy eigenvalue obtained by us for each of the $2pnd\,(^{1,3}D^{\circ})$ ($n=3-8$) states is the lowest yet obtained and is in good agreement with the experimental value obtained by Berry *et al.* [16]. Recently Coreno *et al.* [17] observed $2p7d$ and $2p8d(^3D^{\circ})$ states of helium by photon induced fluorescence spectroscopy. Present results of 65.126 and 65.194 eV for $2p7d$ and $2p8d$, states, respectively, are in reasonably good agreement with those observed by Coreno *et al.* [17]. The latest calculation of energies of $2pnd\,(^3D^{\circ})$ ($n=3-8$) states is due to Zitnik *et al.* [18]. They added a spin-orbit mixing term to the nonrelativistic Hamiltonian and expanded the wave functions in a basis set which contains 272 configuration state functions of symmetry $^3D^{\circ}$ and 393 functions for each symmetry $^1P^{\circ}$ and $^3P^{\circ}$. Although it was noted that energy of the $2pnd\,(^3D^{\circ})$ states is lowered for a fraction of meV due to the spin-orbit interaction with the neighboring $n+{}^1P^{\circ}$ state, present results show that nonrelativistic (correlation) effects are still more important to accurately determine the energy states with low n. For example, for the $2p4d(^3D^{\circ})$ state we obtained energy $-0.532\,678$ a.u. compared to $-0.532\,541$ a.u., the value obtained by Zitnik *et al.* [18]. This confirms the well known fact that the Hylleraas basis set is much more effective in describing correlations than expansion in terms of single configurations in the central field of hydrogenlike helium. The calculated effective quantum numbers for $3dnf\,(^{1,3}D^{\circ})$ ($n=4-12$) and $2pnd\,(^{1,3}D^{\circ})$ ($n=3-8$) states of helium are displayed in the last line of each Table I–IV. From a closer look on the effective quantum number values, we observe loss of accuracy for higher n values. This is possibly due to the finite size of the basis set. For higher n values like $3d11f$ and $3d12f\,(^3D^{\circ})$, more accurate energy values can be achieved by increasing the number of parameters in the basis set. As there were no prior results for these states, the present results may serve as a future reference.

Different theoretical methods have been applied to incorporate electron correlation effects in the doubly excited states of two electron atoms. Calculations involving the group theoretical approach by Herrick and Sinanoglu [19] (compiled by Shearer-Izumi [20]), truncated diagonalization method by Lipsky *et al.* [14], pseudopotential Feshbach formalism by Bachau *et al.* [21], a complex rotation method by Ho and Bhatia [12], were performed to estimate energy values of

TABLE III. Nonrelativistic energy eigenvalues $-E$ (a.u.) and effective quantum numbers (n^*) for $2pnd$ ($n=3-8$) $^3D^o$ states of helium. ρ_1, ρ_2 are the nonlinear parameters.

	$2p3d$[a]		$2p4d$		$2p5d$		$2p6d$		$2p7d$	$2p8d$
M	Bhatia[b]	Present $\rho_1=0.390\,205\,72$ $\rho_2=0.989\,089\,83$	Bhatia[b]	Present $\rho_1=0.264\,085\,22$ $\rho_2=1.005\,384\,78$	Bhatia[b]	Present $\rho_1=0.203\,105\,91$ $\rho_2=0.996\,510\,74$	Bhatia[b]	Present $\rho_1=0.172\,479\,28$ $\rho_2=1.002\,961\,38$	Present $\rho_1=0.172\,479\,30$ $\rho_2=1.002\,962\,40$	Present $\rho_1=0.160\,000\,00$ $\rho_2=0.990\,000\,00$
8	0.558858 81		0.531554825							
12		0.559233 91		0.532491 37		0.510118 05				
20	0.559294 75		0.532542790		0.517015550					
27		0.559324 23		0.532654 25		0.520674 22				
40	0.559325785		0.532669585		0.520590355		0.508968105			
51		0.559328 07		0.532676 73		0.520700 51		0.514282 88		
69		0.559328 23		0.532678 49		0.520703 18		0.514287 86		
70	0.559328 16		0.532674725		0.520682045		0.513684750			
84		0.559328 24		0.532678 51		0.520703 20		0.514287 88	0.509617 98	
111		0.559328 25		0.532678 59		0.520703 42		0.514288 26	0.510378 84	
112	0.559328 25		0.532678075		0.520693865		0.514235780			
129		0.559328 26		0.532678 59		0.520703 43		0.5142882 66	0.510378 85	
186		0.559328 26		0.532678 60		0.520703 45		0.5142882 97	0.510448 40	
258		0.559328 26		0.532678 60		0.520703 45		0.5142883 03	0.510452 67	0.507945 30
n^*		2.9030053		3.9115058		4.9147319		5.9151926	6.9171446	7.9355083

[a] Reference [5].
[b] Reference [11].

TABLE IV. Nonrelativistic energy eigenvalues $-E$ (a.u.) and effective quantum numbers (n^*) for $2pnd$ ($n=3-8$) $^1D^o$ states of helium. ρ_1, ρ_2 are the nonlinear parameters.

	$2p3d$[a]		$2p4d$		$2p5d$		$2p6d$		$2p7d$	$2p8d$
M	Bhatia[b]	Present $\rho_1=0.396\,016\,60$ $\rho_2=0.975\,740\,14$	Bhatia[b]	Present $\rho_1=0.263\,635\,30$ $\rho_2=0.959\,997\,94$	Bhatia[b]	Present $\rho_1=0.206\,658\,23$ $\rho_2=0.993\,129\,72$	Bhatia[b]	Present $\rho_1=0.172\,479\,28$ $\rho_2=1.002\,961\,38$	Present $\rho_1=0.102\,777\,00$ $\rho_2=0.950\,412\,84$	Present $\rho_1=0.127\,603\,85$ $\rho_2=1.438\,851\,27$
8	0.562662 06		0.529565525							
12		0.563676 20		0.534372 24		0.515562 81				
20	0.563733795		0.533483235		0.519026430					
27		0.563795 27		0.534556 23		0.521587 79				
40	0.563796245		0.534505525		0.521244140		0.504391695			
51		0.563799 81		0.534575 24		0.521655 64		0.514815 61		
69		0.563800 29		0.534576 23		0.521658 74		0.514832 53		
70	0.563800235		0.534562695		0.521602520		0.512079175			
84		0.563800 37		0.534576 25		0.521658 75		0.514832 55	0.510436 32	
111		0.563800 41		0.534576 35		0.521658 98		0.514833 52	0.510725 47	
112	0.563800405		0.534576015		0.521642770		0.51426906			
129		0.563800 41		0.534576 36		0.521658 99		0.514833 52	0.510725 49	
186		0.563800 42		0.534576 38		0.521659 01		0.514833 58	0.510772 83	
258		0.563800 42		0.534576 38		0.521659 01		0.514833 59	0.510787 23	0.508014 58
n^*		2.7994626		3.8025288		4.8045838		5.8065000	6.8072904	7.9007577

[a] Reference [5].

[b] Reference [11].

various doubly excited states of helium. However, as far as $^{1,3}D^{\circ}$ states are concerned, the calculations are limited to $(3dnf,\ n \leqslant 6)$ of helium. This is clearly reflected in Table I and II. As no previous calculations for energy values of $3dnf\ (^{1,3}D^{\circ})\ (n=7-12)$ states of helium exist, no comparison with the present results is possible.

Doubly excited states could also be detected in electron impact excitation experiments [22,23] where both dipole allowed and forbidden transitions are possible. The energy levels above the ground state of helium can be observed in electron energy loss spectra. We predict the peak positions at 71.902, 72.331, 72.541, 72.660, 72.736, 72.792, 72.823, 72.850, and 72.895 eV in the electron energy loss spectra corresponding to the transitions $1s^2 \rightarrow 3dnf(^3D^{\circ})\ (n=4-12)$, respectively. The ground state energy of helium is taken as −2.903 784 1 a.u. [24]. Conversion factor 1 a.u. =27.211 383 86 eV [25] is used.

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