

Metastable-bound and Resonance energies of doubly excited $1,3F^e$ states of two-electron atoms

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Synopsis Precise energy eigenvalues of doubly excited $1,3F^e$ states originating from $2pnf$ ($n \geq 4$) configuration of *He* atom have been calculated by using Ritz variational method in Hylleraas coordinates. 20 metastable-bound states below $n = 2$ ionization threshold are obtained. Resonance states below $n = 3$ and $n = 4$ are also obtained.

Precise theoretical estimation of energies of doubly excited states (DES) of two electron atoms are of great importance for astrophysical data analysis, solar coronal line identification, plasma diagnostics etc. On the basis of coupling scheme of angular momentum and parity conservation rule the DES can be divided into two categories, bound and resonance/autoionizing states [1]. Among such non-autoionizing DES, $2p4f$ ($1,3F^e$) state is the lowest lying F state of even parity. In the autoionization process the electronic repulsion is responsible to push one electron into the continuum leaving the two electron atom in an ionized configuration, so electronic correlation effect plays very important role for such theoretical studies. The energy eigenvalues of $2pnf$ $1,3F^e$ states of helium for $n = 4 - 19$ have been reported by Eiglsperger *et al.* [2]. There are few studies, where the resonance states of $1,3F^e$ states of helium [3] have been carried out below $n = 3$ ionization threshold. We here present the precise energy eigenvalues of $2pnf$ $1,3F^e$ states of helium for $n = 4 - 23$ and new resonance states of $1,3F^e$ symmetry above $n = 3$ ionization threshold.

The non-relativistic Hamiltonian for a two electron atom is expressed as

$$H = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}} \quad (1)$$

where Z is the atomic number. The $1,3F^e$ state wave function is given by

$$\Psi = f_3^0 D_3^0 + f_3^{2+} D_3^{2+} + f_3^{2-} D_3^{2-} \quad (2)$$

where, $f_3^0 = -(f \mp \tilde{f}) \sin \theta_{12}$, $f_3^{2+} = \frac{\sqrt{15}}{6} (f \mp \tilde{f}) \sin 2\theta_{12}$ and $f_3^{2-} = \frac{\sqrt{15}}{6} (f \pm \tilde{f}) (1 - \cos 2\theta_{12})$. The upper sign corresponds to the singlet state and the lower sign to the triplet state. D 's are the rotational harmonics depending upon the Eulerian angles θ , ϕ , ψ [4], the explicit forms of which are given by $D_3^0 = \frac{5\cos^3\theta - 3\cos\theta}{2}$, $D_3^{2+} = \frac{\sqrt{15}}{2} \cos 2\psi \sin^2 \theta \cos \theta$

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and $D_3^{2+} = \frac{\sqrt{15}}{2} \sin 2\psi \sin^2 \theta \cos \theta$. The trial radial wave function $f(r_1; r_2; r_{12})$ can be written as

$$f(r_1, r_2, r_{12}) = \left[\sum_{i=1}^9 \sum_{j=1}^9 \eta_i(1) \eta_j(2) \right] g(1, 2) \quad (3)$$

where $i \geq j$ and

$$g(1, 2) = r_1^3 r_2 \sum_{l \geq 0} \sum_{m \geq 0} \sum_{n \geq 0} C_{lmn} r_1^l r_2^m r_3^n \quad (4)$$

with $\eta_i(j) = e^{-\rho_i r_j}$ and $\tilde{f} = f(r_2, r_1, r_{12})$.

$b_1, b_2; b_3$ are linear parameters and ρ 's are the non-linear parameters.

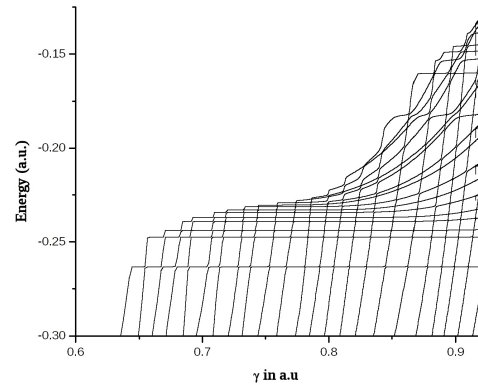


Figure 1. Enlarged view of a portion of the stabilization plot for the $1F^e$ states of helium between the energy interval of -0.30 to -0.125 a.u.

References

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