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# Quantification of entanglement entropies for doubly excited resonance states in two-electron atomic systems

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**Synopsis** In this work, we study the quantum entanglement for doubly excited resonance states in two-electron atomic systems such as the $H^-$ and $Ps^-$ ions and the He atom by using highly correlated Hylleraas type functions The resonance states are determined by calculation of density of resonance states with the stabilization method. The spatial (electron-electron orbital) entanglement entropies (linear and von Neumann) for the low-lying doubly excited states are quantified using the Schmidt-Slater decomposition method.

As quantum entanglement property plays a crucial role in areas such as quantum teleportation, quantum computation, and quantum cryptography [1], quantification of entanglement entropy in two interacting particles systems have attracted much attention (see [2-5], and references therein). In particular, considerable effort has been made on studies of entanglement for two-electron systems including model atoms, quantum dot systems, and natural two-electron atoms. In our recent works, we have studied the linear and von Neumann entropies of the ground and singly excited states in helium and the ground states of hydrogen negative ion and positronium ion [2-4], and have also quantified entanglement entropies for the doubly excited $2s^2$, $2s3s$ and $2p^2\ ^1S^e$ states in the helium atom [5]. Now we report results for the doubly excited $2s^2\ ^1S^e$ state in $H^-$ and $Ps^-$.

For *S*-states we use Hylleraas-type wave functions to describe the system, with

$$\Psi_{kmn}(\mathbf{r}_1,\mathbf{r}_2)=\sum_{kmn}C_{kmn}\left\{\exp\left[-\alpha\left(r_1+r_2\right)\right]r_1^k r_2^m r_{12}^n+\left(1\leftrightarrow 2\right)\right\},$$

where 1 and 2 denote the electron 1 and electron 2, respectively, and $r_{12}$ is the relative distance between the electron 1 and electron 2, and $k$, $m$, $n$ are positive integers or zero. First we employ the stabilization method (see Figure 1) to determine the resonance energy and width (see Figure 2) for a particular resonance state. Once the wave function is obtained, the linear entropy and von Neumann entropy for such a state are quantified using the Schmidt-Slater decomposition method [3]. By systematically examining the convergence behaviors of calculated entropies by using different wave functions (up to 252 terms), we are able to establish benchmark values of entropies for doubly excited states in the two-electron atomic systems.

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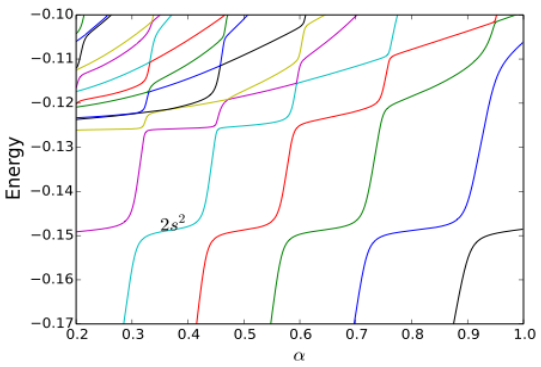


**Figure 1**. Stabilization plot for doubly excited states in $H^-$

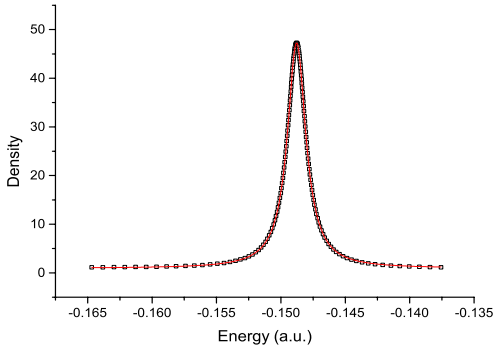


**Figure 2**. Fitting of density of resonance states for the $2s^2\ ^1S^e$ state in $H^-$

## References

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