An analysis of Helium resonant states in terms of entropy, information, complexity and entanglement measures

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An analysis of Helium resonant states in terms of entropy, information, complexity and entanglement measures

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Synopsis Shannon entropies and Fisher information calculated from one-particle density distributions and von Neumann and linear entropies (the latter two as a measure of entanglement) computed from the reduced one-particle density matrix are analyzed for the $^{1,3}S^e$,$^{1,3}P^o$ and $^{1,3}D^e$ Rydberg series of He doubly excited states below the second ionization threshold. We find that both Fisher information and entanglement measures are able to discriminate resonances pertaining to different $(K,T)^A$ series.

The electronic density $\rho(\mathbf{r})$ in atoms, molecules and solids is, in general, a distribution that can be observed experimentally, containing spatial information projected from the total wave function. These density distributions can be thought as probability distributions subject to the scrutiny of the analytical methods of information theory, namely, entropy measures, quantifiers for the complexity, or entanglement measures. Resonant states in atoms have special properties in their wave functions, since although they pertain to the scattering continuum spectrum, they show a strong localization of the density in regions close to the nuclei. Although the classification of resonant doubly excited states of He-like atoms in terms of labels of approximate quantum numbers has not been exempt from controversies, a well known proposal follows after the works by Herrick and Sinanoğlu and Lin [1], with a labeling based on K, T, and A numbers in the form $_{n_1}(K,T)^A_{n_2}$ for the Rydberg series of increasing n_2 and for a given ionization threshold He$^+$ (N=n_1). In this work we intend to justify this kind of classification from the topological analysis of the one-particle $\rho(r)$ and two-particle $\rho(r_1,r_2)$ density distributions of the localized part of the resonances (computed with a Feshbach projection formalism and CI wave functions in terms of B-splines bases), using global quantifiers (Shannon, Tsallis or Rényi entropies) as well as local ones (Fisher information) [2]. For instance, the Shannon entropy is obtained after global integration of the density $S^{Shannon}[\rho]= -\int\rho(\mathbf{r})log\rho(\mathbf{r})d\mathbf{r}$ and the Fisher information contains local information on the gradient of the distribution $I^{Fisher}[\rho]=\int|\nabla log\rho(\mathbf{r})|^2d\mathbf{r}$. In addition, we also study measures for the entanglement using the von Neumann and linear entropies [3], computed from the reduced one-particle density matrix $\rho(\mathbf{r}_1,\mathbf{r}'_1)$=$\int d\mathbf{r}_2\Psi(\mathbf{r}_1,\mathbf{r}_2)\Psi^*(\mathbf{r}'_1,\mathbf{r}_2)$ within our correlated CI approach.

We find in this study that measures like the Shannon entropy hardly distinguishes among resonances in the whole Rydberg series. On the contrary, the Fisher information and measures of entanglement via von Neumann and linear entropies are able to qualitatively discriminate the resonances according to their $(K,T)^A$ labels (see Figure 1).

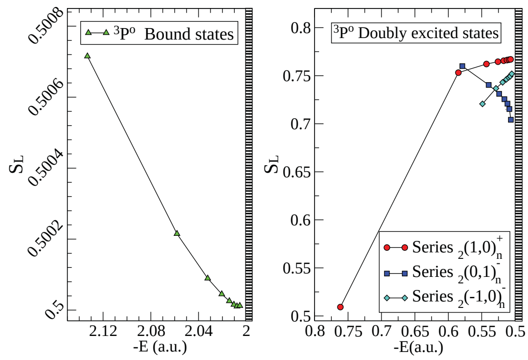

Figure 1. Linear entropy S_L as a measure of entanglement for $^3P^o$ bound and resonant states in Helium. Whereas for the Rydberg series of singly excited states S_L takes a monotonically decreasing value until the first ionization threshold He$^+$(N=1) is reached, the three $(K,T)^A$ Rydberg resonant series split off, converging to different limits at the second ionization threshold He$^+$(N=2).

References

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