The Limits of Stability in Three-Body Coulomb Systems

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Negative atomic ions owe their existence to electron correlation. Exploring the correlated motion of electrons at low nuclear charge and capturing this behaviour in future theoretical method developments, such as correlation functionals, is an important step forward in ensuring new methods can address increasingly exotic and complex systems.
A number of proofs exist regarding the stability of a system with respect to the number of electrons, nuclei and charge [1]. In this talk, we explore the limits of stability for a three-body system interacting via Coulomb forces. Exploiting the series solution method with a Laguerre basis, we calculate high accuracy fully-correlated and Hartree-Fock energies and wavefunctions [2], before extending this fully-correlated ground state methodology to excited S states.
Additionally, we report a variational method for calculating the critical nuclear charge for binding two electrons in the ground state and excited S states of fully-correlated systems, explore the effects of nuclear motion, determine the critical nuclear charge for binding within the Hartree-Fock approximation, and calculate accurate electron correlation data at low nuclear charge Z (Figure 1) [3]; these data are available to download for benchmarking and new developments.
It will be shown that the nuclear charge required to prevent electron detachment increases as the nuclear mass decreases, that the outer electron remains localized at a finite distance from the nucleus as the binding energy of the outer electron approaches zero, the condition for the emergence of a secondary Coulomb hole, and that a minimum in the correlation energy occurs at $Z \approx Z_C^{HF}$.

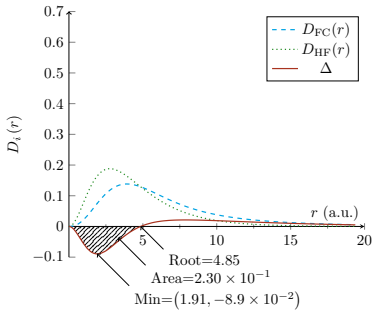

Figure 1: Coulomb Hole Δ at $Z = Z_C^{FC}$

References

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2. H. Cox and A. L. Baskerville, *Adv. Quantum Chem.* **77** (2018), 201.
3. A. L. Baskerville, A. W. King and H. Cox, *R. Soc. Open Sci.* **6** (2019), 181357.