Correlated Motion in Three-Body Coulomb Systems

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As high-precision experiments become more sophisticated, and systems probed become more complex, it's important to ensure theory remains an essential tool for interpreting and predicting chemical systems and phenomena. Three-body Coulomb systems are the simplest that capture the effects of electron correlation and nuclear motion and are therefore of interest for atomic and molecular theory but also for systems containing various elementary particles such as muons and positrons.

High-accuracy, non-relativistic, quantum chemical calculations of the energy levels and wavefunctions of three-particle systems are calculated using a fast and efficient series solution method in a triple orthogonal Laguerre basis.[1] The method is adapted to calculate, in a single variational calculation, the critical mass or charge for bound state stability, and a Hartree-Fock implementation. The correlated motion of particles is quantified using radial and angular densities.

The effects of nuclear motion,[2] and high-accuracy benchmark electron correlation data,[3] will be presented. Exploring the correlated motion of electrons at low nuclear charge just prior to electron-detachment and attempting to capture this behaviour in future theoretical method developments, such as correlation functionals,[4] is an important step forward.

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4. A.L. Baskerville, M. Targema, H. Cox, *R. Soc. Open Sci*., 2022, **9**, 211333.