Hooke's atom: A toy model for DFT

JAVIER DOMINGUEZ-CALVO[1] , RUBEN FERRADÁS[1] and EDUARD MATITO[1,2]

[1]*Donostia International Physics Center (DIPC), Donostia, Euskadi, Spain,*
[2]IKERBASQUE, Basque Foundation for Science, Bilbao, Euskadi, Spain
javier.dominguez@dipc.org

ABSTRACT

Coulombic many-electron quantum systems are in almost every case impossible to solve analytically. However, we can find one notable exception to the rule in the Harmonium Atom (HA) [1][2], or Hooke's Atom, that can be exactly solved under some conditions. Such a system is defined as electrons tied to a chargeless center by harmonic interactions and repelled from each other by the Coulomb force. This is just a theoretical model as no real electron actually behaves this way. However, HA densities resemble molecular interactions, with peaks of probability of finding electrons at certain positions in space. Having exact solutions makes HA a perfect toy model for use to simulate other non-analytical counterparts.

The system is defined by the confinement parameter, or in other words, the strength of the harmonic interaction. Exact wave functions can be obtained for an infinite but countable number of different confinement parameters of the two-electron system. In all those cases, an analytical expression of the wave function can be obtained, giving rise to many DFT related properties in analytical form, such as electron densities or even exchange-correlation potentials for different values of electron-electron interaction.

This work dwells on the retrieval and characterization of exact electronic densities for several harmonic strengths, as well as the first-order reduced density matrix and exact correlation potentials. Exact expressions of such properties will allow us to test density functional approximations of these properties under different correlation regimes, opening the possibility to the design of more relative approximations.

References

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