NEW INSIGHTS INTO DFT FROM ELECTRONS ON A SPHERE

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In recent years, there has been growing interest in the quantum mechanics of pairs of confined electrons. The helium atom, of course, has been studied from the early days and the Hooke's Law atom ("hookium") was introduced in the 1960s. But, more recently, accurate solutions have also been found for pairs of electrons trapped inside a ball ("ballium" [1]) and on its surface ("spherium" [2]) and these are now being used for the development of new functionals in density functional theory (DFT).

Spherium is a particularly attractive model because it is defined by a single parameter (the radius R of the sphere) and varying this parameter takes us smoothly from a weakly correlated system (small R) dominated by dynamical correlation, to a strongly correlated system (large R) dominated by static correlation.

I will review the quantum mechanics of spherium and show how this system can be used as the starting point for a new way of understanding and improving DFT.

[1] PF Loos and PMW Gill, *J Chem Phys* 132 (2010) 234111.
[2] PF Loos and PMW Gill, *Phys Rev Lett* 103 (2009) 123008.

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