Excited-State Spherical DFT of Coulomb Systems

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Recently, Theophilou[1] proposed a novel version of the density functional theory by showing that the set of the spherical averages of the density around the nuclei determines uniquely the external potential in atoms, molecules and solids. Then, an extended version of this theorem[2,3] was put forward and a theory for subspaces was presented to treat degenerate states[4]. The spherical potential functional theory[5] was also developed.

Here, this novel theory is extended to individual excited states. The generalization is based on the methods developed in the series of papers[6–8] by Ayers, Levy and Nagy. Generalized Hohenberg-Kohn theorems are proved to the set of spherically symmetric densities using constrained search. A universal variational functional for the sum of the kinetic and electron-electron repulsion energies is constructed. The functional is appropriate for the ground state and all bound excited states. Euler equations and Kohn-Sham equations for the set are derived.

References

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