Exact Current DFT Study of Hooke's Atom in Magnetic Fields[1]

WUMING ZHU, SAMUEL TRICKEY, Physics and QTP, Univ. Florida — From exact analytical [1] and numerical solutions for Hooke's atom in a uniform external magnetic field, we construct the exact Kohn-Sham (KS)orbitals for current density functional theory (CDFT). We discuss the effects of the external B field relative to the harmonic confining potential on the exchange-correlation energy and various energy components, as well as exact exchange-correlation scalar and vector potentials. Exact density functional results are compared with results with several widely used approximate DFT functionals. Our exact CDFT results can be used as a check for any proposed CDFT functionals and as guidance for improvement of existing functionals. [1] "Analytical Solutions for States of the 3D Hooke's Atom in an External B Field", W. Zhu and S.B. Trickey to be published.

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