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Magnetic Field Effects upon Exchange-Correlation in the Hooke's Atom[1] WUMING ZHU, SAMUEL TRICKEY, Quantum Theory Project and Department of Physics, University of Florida, Gainesville, FL 32611 — Extending Density Functional Theory (DFT) to coulombic systems in a non-vanishing magnetic field in a computationally feasible way is highly desirable. Even though the current DFT (CDFT) formalism is long-established, there still are no generally applicable, reliable $E_{xc}, \mathbf{A}_{xc}$ functionals analogous with the LDA. Progress can be made by comparison study on a solvable correlated system. Hooke's atom is well-known in ordinary DFT because its Schrödinger equation can be solved exactly for some coupling strengths and numerically with high accuracy for the rest. Hence exact Kohn-Sham quantities are readily available. Using our extensions (exact and numerical) to non-zero B-field, we examined the effects on exchange- correlation holes and energies and considered possible ways to include the essential ones in $E_{xc}, \mathbf{A}_{xc}$. In our tests, the CDFT vorticity variable, ν, turns out to be a computationally difficult quantity which may not be appropriate in practice to describe external B field effects on $E_{xc}, \mathbf{A}_{xc}$.

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