

Abstract Submitted
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General degeneracy in density functional perturbation theory

MARK PALENIK, BRETT DUNLAP, Naval Research Lab — Degenerate perturbation theory from quantum mechanics is inadequate in density functional theory (DFT) because of nonlinearity in the Kohn-Sham (KS) potential. We develop the fully general degenerate DFT perturbation theory. The requirement that a differentiable map connects the unperturbed state to the perturbed state defines the unitary transformations and changes in Fermi-level occupation numbers at each order. The resulting methodology is applied to the iron atom ground state, which displays $3d-4s$ degeneracy, calculated with the VWN functional. By applying a perturbing quadrupole field, we demonstrate how the equations for the first-order density and first through third-order energies can be solved in a system where degeneracy appears both due to symmetry requirements and accidentally, between different representations of the symmetry group.

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