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Degenerate Open Shell Density Perturbation Theory MARK PALENIK, BRETT DUNLAP, Naval Research Lab — The density perturbation theory (DPT) methodology we have developed applies the Hohenberg-Kohn theorem to perturbations in density functional theory. At each order, the energy is directly minimized with respect to the density at all lower orders. The difference between the perturbed and unperturbed densities is expanded in terms of a finite number of basis functions, and a single matrix inversion in this space reduces the complexity of the problem to that of non-interacting perturbation theory. For open-shell systems with symmetry, however, the situation becomes more complex. Typically, the perturbation will break the symmetry leading to a zeroth-order shift in the Kohn-Sham potential. Because the symmetry breaking is independent of the strength of the perturbation, the mapping from the initial to the perturbed KS potential is discontinuous and techniques from perturbation theory for noninteracting particles fail. We describe a rigorous formulation of DPT for use in systems that display an initial degeneracy, such as atoms and $Fe_{55}Cp^*_{12}$ clusters and present initial calculations on these systems.

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