

Abstract Submitted  
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**Generalized density functional theory for effective potentials in many-body electronic structure** F. A. REBOREDO, P. R. C. KENT, Oak Ridge National Laboratory — We demonstrate the existence of different density functionals that retain selected properties of the many-body ground state in the non-interacting density functional solution. We focus on diffusion Monte Carlo applications that require trial wave functions with Fermion optimal nodes. The theory can be extended and used to understand current practices in several electronic structure methods [GW-BSE,CI,EPM] within a generalized density functional framework. The theory justifies and stimulates the search of optimal empirical density functionals and effective potentials but also cautions on the limits of their applicability. The theoretical concepts are tested against a near-analytic model that can be solved to numerical precision. Research performed at the Materials Science and Technology Division and the Center of Nanophase Material Sciences at Oak Ridge National Laboratory sponsored the Division of Materials Sciences and the Division of Scientific User Facilities U.S. Department of Energy.

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