

Application of Density-Matrix Correlation Functional to Transition Metal Impurities*

R. G. Hennig and A. E. Carlsson

Washington University in St. Louis

Abstract

Correlation effects are difficult to treat for transition metals in many types of hosts, such as enzymes, zeolitic catalysts, and high- T_c superconductors. We prove that for Anderson-type Hamiltonians the exchange-correlation energy is a functional of the local moments of the density matrix. An exact inequality based on the second moment of the density matrix for the exchange-correlation functional in terms of the one-particle density matrix¹ is extended to arbitrary band fillings by a rigorous decomposition of the wave function in tight-binding theory. The inequality, used as an approximation to the exchange-correlation functional, yields exact results for simple dimer molecules with either on-site or inter-site Coulomb interactions. Exact results for the energy of small Hubbard and Anderson clusters show that the method is very accurate for isolated interaction centers, but larger errors are present for coupled interaction centers. We implemented this method in a variational density-matrix algorithm, with cubic system size scaling and applied it to Anderson-type impurities in arbitrary hosts using the recursion method. Several physical properties including the occupancy of the impurity states and the bond strength of the impurity to the bulk as well as charge and spin fluctuations are calculated.

*Supported by NSF grant DMR-9971476.

¹A. E. Carlsson. Phys. Rev. B 56, 12058 (1997)