The variational two-electron reduced-density-matrix method for extended systems

Nicholas C. Rubin and David A. Mazziotti

Department of Chemistry and The James Franck Institute,

The University of Chicago, Chicago, IL 60637 USA

Abstract

The variational two-electron reduced-density-matrix method is formulated for single and multiband extended systems. Two single band lattice models of strongly correlated materials are used to test approximate N-representability beyond what is found in a molecular setting. The first of these systems is the repulsive U Hubbard model with linear and ladder lattice topologies. The second model contains only two-body interactions and is unique among typical spin models in that it does not have a mean-field reference wave function. The ground state wave functions from all Hamiltonians in the model with only two-body interactions have the same 1-electron reduced density matrix; consequently, one-electron theories are largely inapplicable. The superconducting η-pairing ground states make the model a unique tool for demonstrating the necessary N-representability in highly correlated environments. A one-dimensional polymer represented by Crystalline-orbital Hartree-Fock theory provides formalism for studying the electronic structure in a general multiband system. We demonstrate that time-reversal symmetry, which is implicitly included in position space electronic structure calculations, must be explicitly included as an N-representability constraint on the 2-RDM when using a momentum space basis. The necessity of these equality constraints is demonstrated by the accurate recovery of the binding energy of two polymers and the symmetry of their natural orbital occupations.