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Density-Matrix Based Fixed-Node and Fixed-Phase Approximation for Quantum Monte Carlo[1] JOHN SHUMWAY, Dept. of Physics and Astronomy, Arizona State University — We have generalized the fixed-node and fixed-phase approximations to use density matrices. For a given trial density matrix, we generate a quantum Monte Carlo algrithm that minimizes the free energy, subject to the nodal or phase restriction. This method has enabled us to perform efficient fermion path-integral simulations at all temperatures. In the T=0 limit the algorithm simulates two copies of the system that do not interact, but which are entangled through the nodal constraint. We illustrate the advantages of this density matrix formalism in applications to semiconductor nanostructures and small molecules. We are currently investigating the use of the Kubo formula and other linear response theories within the fixed-node approximation. (For simulation codes, preprints, and other information, see http://phy.asu.edu/shumway.)

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