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Self-healing diffusion quantum Monte Carlo algorithms: Theory and Applications[1] F.A. REBOREDO, P.R.C. KENT, M.L. TIAGO, Oak Ridge National Laboratory, R.Q. HOOD, Lawrence Livermore National Laboratory — We present a method to obtain the fixed node ground state wave function from an importance sampling Diffusion Monte Carlo (DMC) run. The fixed node ground state wave-function is altered to obtain an improved trial wave-function for the next DMC run. The theory behind this approach will be discussed. Two iterative algorithms are presented and validated in a model system by direct comparison with full configuration interaction (CI) wave functions and energies. We find that the trial wave-function is systematically improved. The scalar product of the trial wave-function with the CI result converges to 1 even starting from wave-functions orthogonal to the CI ground state. Similarly, the DMC total energy and density converges to the CI result. In the optimization process we find an optimal non-interacting nodal potential of density-functional-like form. An extension to a model system with full Coulomb interactions demonstrates that we can obtain the exact Kohn-Sham effective potential from the DMC data. Subsequently we apply our method to real molecules such as benzene and find that we can improve the ground state energy as compared with the single determinant result even starting from random wave-functions. Results for other molecular systems and comparison with alternative methods will be presented.

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