Abstract Submitted
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Steps beyond the fixed-phase approximation in diffusion Monte Carlo[1] FERNANDO REBOREDO, Oak Ridge National Laboratory — The self-healing diffusion Monte Carlo algorithm (SHDMC) [Reboredo, Hood and Kent, Phys. Rev. B **79**, 195117 (2009); Reboredo, *ibid.* **80**, 125110 (2009)] is extended to study the ground and excited states of magnetic and periodic systems. The method converges to exact eigenstates as the statistical data collected increases if the wave function is sufficiently flexible. A recursive optimization algorithm is derived from the time evolution of the mixed probability density, which is given by an ensemble of electronic configurations (walkers) with complex weight. This complex weight allows the amplitude of the fixed-node wave function to move away from the trial wave function phase. This novel approach is both a generalization of SHDMC and the fixed-phase approximation [Ortiz, Ceperley and Martin, Phys Rev. Lett. **71**, 2777 (1993)]. The algorithm is demonstrated to converge to nearly exact solutions of model systems with periodic boundary conditions or applied magnetic fields for the ground state and low energy excitations. The computational cost is proportional to the number of independent degrees of freedom of the phase.

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