Abstract Submitted
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Systematic reduction of sign errors for excited states in many-body problems[1] FERNANDO REBOREDO, Oak Ridge National Laboratory — A recently developed self-healing diffusion Monte Carlo algorithm (SHDMC) is extended to the calculation of excited states. SHDMC is a recursive approach that improves systematically the nodes of the trial wave function by locally smoothing the kinks of the fixed-node wave function [Reboredo, Hood and Kent PRB **79**, 195117 (2009)]. The smoothed-fixed-node wave-functions of inequivalent nodal pockets of excited states are estimated simultaneously from the mixed probability density. The decay of the wave-function into lower energy states is avoided by i) removing the projection of the improved trial-wave function into previously calculated eigenstates; and ii) adjusting the reference energy in each nodal pocket. It is demonstrated, in a model system, that the algorithm converges to many-body excited states in bosonic and fermionic cases [Reboredo PRB **80**, 125110 (2009)]. The computational cost of SHDMC scales linearly with the number of independent degrees of freedom of the nodal surface, while its accuracy improves systematically with the nodal degrees of freedom and as the statistical data collected increases.

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