

Self-healing Diffusion Quantum Monte Carlo Algorithms: Direct Reduction of the Fermion Sign Error in Electronic Structure Calculations

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Accurately solving the many electron Schrödinger equation for real materials is a holy grail of condensed matter physics and materials science. Currently Diffusion Monte Carlo (DMC) represents state of the art, both in terms of the accuracy that can be achieved and the number of electrons that can be treated (i.e. system complexity). To date a major limitation on the accuracy of DMC solution has been the so called fixed node approximation for the trial wave function that is used to guide the quantum Monte Carlo calculation – an approximation that allows one to circumvent the notorious “sign” problem associated with quantum Monte Carlo methods for Fermion systems.

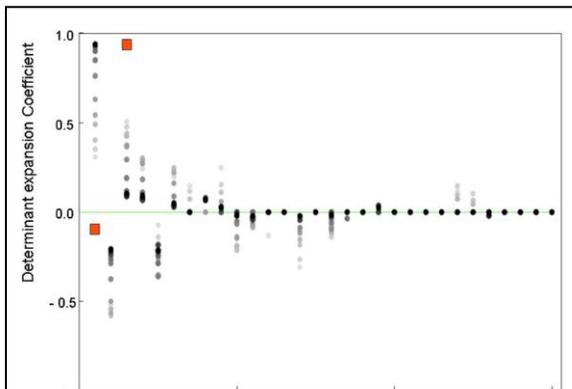
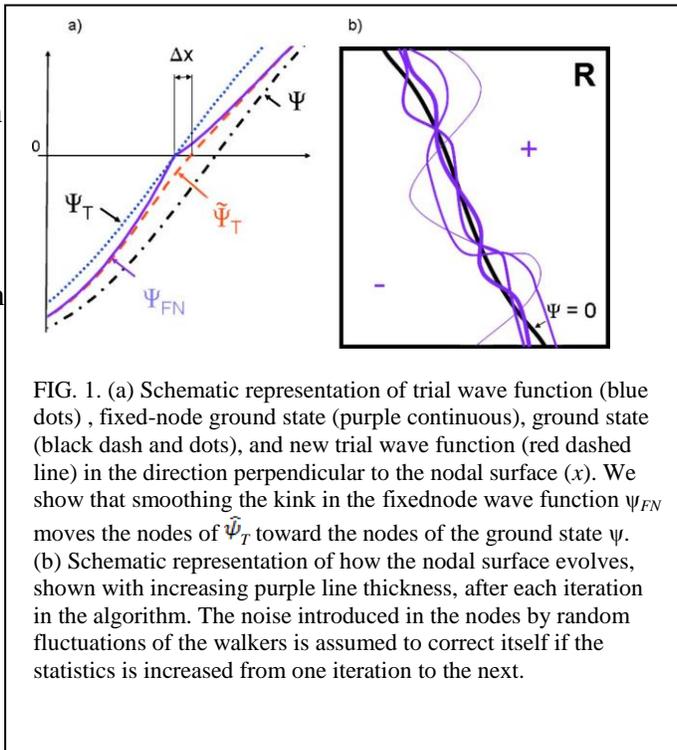


FIG. 2. Change in the values of the multideterminant expansion as the DMC self-healing algorithm progresses. Light gray colors denote older coefficients while darker ones denote more converged results. The initial nonzero coefficients are highlighted in red squares.

We have developed a self-healing Diffusion Monte Carlo (SH-DMC) method for calculating the ground-state properties of many electron systems. The method allows for systematic improvement of the nodal structure of the trial wave-function. The basic algorithm was recently published in Physical Review B. Ongoing tests on small systems (e.g. C20 and LiSr) support the possibility of treating correlated electron systems with unprecedented size and complexity.

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