Optimization of nodes of many-body wave functions

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A great deal of effort has been invested by various researchers in trying to find ways to go beyond the fixed-node approximation in projector Monte Carlo methods applied to continuum fermionic systems. Particularly notable is the work of Kalos, but also of Anderson, attempting to devise exact fermionic algorithms, and, the work of Ceperley on the release-node algorithm. However, at present none of these methods are comparable in efficiency to the commonly used fixed-node approximation. An alternative approach is to devise sufficiently accurate trial wave functions that the fixed-node error is small enough to be ignored. There are two obstacles to success in this approach. First, one is always limited by the chosen form of the trial wave function. Second, there is at present no efficient method for optimizing many-body nodes. Here we discuss the second issue.

The variance minimization method has become the standard method for optimizing many-body wave functions. It is highly effective for Jastrow parameters, but not as effective for parameters in the determinants because for the determinantal parameters reductions in the variance and the energy are not strongly correlated. In recent years many methods have been proposed for energy optimizing quantum Monte Carlo wave functions. Of these, the three highly efficient methods are: 1) The generalized eigenvalue method of Nightingale and Melik-Alaverdian, which was proposed by them for linear parameters only but extended by us to nonlinear parameters. 2) The effective fluctuation potential (EFP) method of Fahy, Filippi and coworkers, and the recent perturbative EFP of Schautz, Scemama and Filippi. We show that the latter can be more simply derived as first-order perturbation theory in a nonorthogonal basis. 3) The modified Newton method of Umrigar and Filippi[1] and of Sorella[2]. We show that the three methods are related to each other and point out that a control parameter can be employed in each of them to make them totally stable. We use these methods to optimize all the parameters in the Jastrow and the determinantal parts of the wave function and point out that different issues arise in optimizing the Jastrow and the determinantal parameters. By systematically increasing the number of determinants we find that seemingly similar systems, such as C_2 and Si_2 have vastly different fixed-node errors for single-determinant wave functions and that fixed-node errors for some simple systems can be as large as 1 eV. In contrast, the optimized multideterminantal wave functions yield energies in excellent agreement with experiment.

The methods described above can be straightforwardly extended to minimizing directly the fixed-node diffusion Monte Carlo energy and therefore the nodes of the trial wave functions.

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[2] S. Sorella, Phys. Rev. B 71, 241103 (2005).