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Wavefunction correction scheme for non fixed-node diffusion Monte Carlo

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Abstract. Wavefunction correction scheme, which was developed as a variance reduction tool for the pure and fixed-node diffusion Monte Carlo (DMC) computations by Anderson and Freihaut, is applied to the DMC computations of fermions without using the fixed-node constraint. This technique is found to be suitable for the non fixed-node calculations because of the significant decreases observed in the computation efforts in the benchmark computations for calculating results with certain statistical error values.

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Key words: quantum Monte Carlo, diffusion Monte Carlo, fermions

1 Introduction

Antisymmetry condition of the wavefunction on identical particle exchanges complicates the electronic structure calculations of the fermionic many-body systems. The projector quantum Monte Carlo (QMC) methods [1, 2], facilitating imaginary time evolution of an initial quantum state, are accurate tools for such fermionic calculations. However, the evolution in imaginary time tends to the symmetric bosonic ground state instead of the antisymmetric fermionic ground state, resulting in the famous *fermion sign problem* [3]. Most of the attempts for an exact imposition of the antisymmetry condition in the projector methods facilitate plus and minus signed *walkers* diffusing and canceling each other whenever encounters occur [4]. Usual population control mechanism in these methods can only stabilize the difference between the plus and minus signed populations and therefore cancellations of opposite signed walkers are essential for controlling the total population. Population control problem arises for larger systems since the plus and minus signed walker encounter rate is very low in the higher dimensional configuration spaces. The antisymmetric guiding functions used in the

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recently developed fermion Monte Carlo method [5] increase the stability of the non fixed-node DMC to some extent. However, it was shown that these developments were not enough for the resolution of the sign problem [6]. Therefore, applications of the exact methods are currently limited to a small number of fermions.

Wavefunction correction scheme was developed for the projector QMC computations as a variance reduction tool [7]. The difference between the true ground state wavefunction and a trial wavefunction is sampled in this technique instead of the ground state wavefunction itself. This technique is used as an efficiency improvement in the projector QMC computations of bosons [7–9] as well as fixed-node projector QMC computations of fermions [9].

In the current study, wavefunction correction scheme is applied to plus-minus cancellation facilitating computations of the fermionic systems without using the fixed-node approximation. Reduction of the computation times to acheve certain precision values with the usage of the wavefunction correction scheme in such QMC calculations are investigated on some simple benchmark systems. Calculations are carried out using the diffusion Monte Carlo (DMC) [1, 2, 10] method but the correction scheme is applicable to other projector QMC methods as well.

2 Method of computation

DMC, an highly accurate QMC method, relies on the fact that the form of the imaginary time Schrödinger equation is a diffusion equation with a source term:

$$\partial_\tau \Psi(\mathbf{x},\tau) = \frac{1}{2}\nabla^2 \Psi(\mathbf{x},\tau) - [V(\mathbf{x}) - E_R]\Psi(\mathbf{x},\tau), \tag{1}$$

where $\mathbf{x}$ is the position vector in the configuration space of the physical system. The potential energy $V(\mathbf{x})$ defines the interactions between the particles and with external sources. DMC treats the wavefunction $\Psi(\mathbf{x},\tau)$ as a density distribution of some number of hypothetical particles, also called as walkers, diffusing in the $D \times N$ dimensional configuration space, D being the number of space dimensions and N being the number of identical particles. These walkers are subjected to a branching process according to the source term of the diffusion equation which is the term including the potential energy $V(\mathbf{x})$ in the Schrödinger equation. Population control is established by controlling the rate of the branching process via adjustments of the reference energy E_R which is an overall energy shift. The evolution in imaginary time τ projects out the ground state component of an arbitrary initial wavefunction $\Psi(\mathbf{x},0)$ in the long τ limit [10]. The DMC method uses short time propagator and thus the calculated expectation value result has a time step error which can be made insignificant by a time step extrapolation.

When the fixed-node constraint is not enforced the sign problem manifests itself as the problem of imposing the antisymmetry condition. Minus signed walkers arise in such non fixed-node calculations, breaking down the population control mechanism for large systems even with the cancellations of opposite signed walkers.