Multi-determinant generalized Hartree-Fock wave functions in Monte Carlo calculations

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The quantum Monte Carlo algorithm is arguably one of the most powerful computational many-body methods, enabling accurate calculation of many properties in interacting quantum systems. In the presence of the so-called sign problem, the algorithm typically relies on trial wave functions to eliminate the exponential decay of signal-to-noise ratio, usually at the expense of a bias in the result. The quality of the trial state therefore is critical for accurate simulations. In this work, benchmark results of the ground state auxiliary-field quantum Monte Carlo method are reported for the Hubbard model on several geometries. We demonstrate that when multi-determinant generalized Hartree-Fock states are used as trial wave functions, the systematic errors can be systematically reduced to a low level and the results compare favorably with the exact diagonalization data.

I. INTRODUCTION

Strongly correlated materials, for example cuprate superconductors\textsuperscript{1} and heavy fermions,\textsuperscript{2,3} host a variety of remarkable phenomena such as high-$T_c$ superconductivity,\textsuperscript{4,5} metal-to-insulator transition,\textsuperscript{6} magnetism,\textsuperscript{7} quantum criticality,\textsuperscript{8} to name a few. The rich phases of these correlated materials offer great potential for energy and technology applications. Understanding and predicting their electronic and structural properties is one of the central missions of modern condensed matter physics and quantum chemistry. Nonetheless, the strongly correlated nature and complexity of the materials often pose great challenges to traditional theoretical methods. With the advances in hardware and algorithms, computational many-body techniques have become increasingly important in unlocking the underlying mechanisms of the physics emerging from strong correlations.

Over the past few decades, various numerical tools have been devised to solve the many-body Schrödinger equation for models as well as materials. Exact methods such as direct diagonalization and configuration interaction\textsuperscript{9} provide the most unbiased standard. However, the computational cost scales exponentially with system size since the methods deal directly with the Hilbert space of the Hamiltonian. Density functional theory (DFT),\textsuperscript{10} on the other hand, drastically reduces the computational cost by mapping the many-body problem onto an effective single-electron one through the use functionals that depend on the electron density. For its ability to handle large complex structures at a rather low computational cost, DFT has been widely used in the field of condensed matter physics, quantum chemistry, and material sciences. In spite of its success, limitations of DFT exist and treating strongly correlated systems with DFT remains challenging.\textsuperscript{11} It should be pointed out that progress has been made by combining DFT with other many-body techniques such as density-matrix renormalization group\textsuperscript{12} or dynamical mean-field theory.\textsuperscript{13,14}

In this regard, quantum Monte Carlo (QMC) methods offer an alternative route for tackling the problem of strong correlations. On the one hand, QMC methods treat electronic correlations directly without the need for empirical or approximate interactions. On the other hand, it offers a favorable algebraic scaling ($O(N^3) \sim O(N^4)$ where $N$ is the system size) compared to exact methods that typically scale exponentially with system size. For this reason, QMC methods can handle fairly large system sizes and provide near exact answers with controllable statistical errors. For example, in the study of helium-4 atoms under extreme pressure or temperature conditions, path integral Monte Carlo has been the choice of method.\textsuperscript{15}

For fermionic systems, however, the probability distribution used to sample the Hilbert space is no longer positive-definite due to the Pauli exclusion principle. Under this circumstance, statistical error grows exponentially and QMC loses its algebraic scaling, leading to the so-called sign problem.\textsuperscript{16,17} In most cases, there are approximate solutions to the sign problem which control the exponential decay of the signal-to-noise ratio. In the well-known fixed-node diffusion Monte Carlo (FNDMC) method,\textsuperscript{18} for example, a trial wave function is used to eliminate any moves that try to cross the nodal hyper-surface of the reference. In the same spirit, the ground state auxiliary-field quantum Monte Carlo (AFQMC) method implements the constrained-path approximation\textsuperscript{19,20} to retain positive random walkers. Under these approximations both QMC techniques regain the algebraic scaling, at the cost of a bias in the simulation results that depend sensitively on the quality of the trial wave function used to implement the constraint. Consequently, accurate trial wave functions are vital for the efficiency and correctness of simulations. In this work, we propose a class of multi-determinant mean-field trial wave functions for the AFQMC method. By comparing simulation results with exact diagonalization data, it is shown that the variational freedom of the proposed multi-determinant trial wave functions allow one to deliver accurate simulations.

The rest of the paper is organized as follows. Sec-
II. METHOD

A. Multi-determinant generalized Hartree-Fock wave function

In this work we employ trial wave-functions consisting of non-orthogonal Slater determinant expansions of the form:

\[ |\Phi\rangle = \sum_{i=1}^{n_d} c_i |\varphi_i\rangle, \tag{1} \]

where \( |\varphi_i\rangle \) are Slater determinants and \( c_i \) are linear variational parameters. As opposed to Slater determinant expansions built from particle-hole excitations from a given reference determinant, typically employed in quantum Monte Carlo calculations, we do not enforce orthonormalization between different Slater determinants in the expansion, hence \( \langle \varphi_i | \varphi_j \rangle \neq 0 \). In fact, each Slater determinant is represented as an orbital rotation from a given reference

\[ |\varphi_i\rangle = e^{-\sum_{p,q} Z_{pq} \hat{c}_p^\dagger \hat{c}_q} |\varphi_{\text{ref}}\rangle, \tag{2} \]

where \( Z \) is an unitary matrix.

The trial wave function is generated using a version of the projected Hartree-Fock (PHF) algorithm developed in the Scuseria group at Rice University. The algorithm directly minimizes the energy \( E = \langle \Phi | \hat{H} | \Phi \rangle / \langle \Phi | \Phi \rangle \) using a BFGS-like technique and analytical energy gradients. We refer the readers to Ref. 21 for the relevant equations. There are two different approaches within the algorithm, the few-determinant (FED) algorithm and the resonating Hartree-Fock (ResHF) approach. In the FED algorithm, the Slater determinant expansion is generated iteratively, adding and optimizing one determinant in each iteration to an already existing expansion. During each iteration, determinants \( |\varphi_i\rangle \) \((i = 1, 2, \ldots, n_d - 1)\) obtained from previous iterations are kept fixed and the energy is minimized with respect to the orbital rotation matrix of the new determinant and all linear coefficients. This process continues until a given number of determinants is generated. At this point, the linear coefficients are re-optimized by solving the associated eigenvalue problem. In the FED theory, symmetry projectors can be incorporated straightforwardly. The resulting single- or multi-reference symmetry-projected FED wave functions have been shown to be quite accurate. However, we will not focus on symmetry restoration in our calculations.

In the ResHF approach the energy, \( E \), is minimized with respect to all variational parameters in the trial wave-function, including the rotation matrices of all determinants and all linear coefficients. In this work, ResHF trial wave-functions are produced using FED generated trial wave-functions as input. We use the same BFGS-like direct optimization algorithm used for FED, but include all parameters simultaneously in the optimization.

The mean-field orbital used in the FED and ResHF theories could be restricted-HF (RHF), unrestricted-HF (UHF), or generalized HF (GHF) wave functions. The three types of state represent different levels of symmetry-breaking. In the present study, we will mainly focus on using GHF determinants in which all symmetries of the Hamiltonian are broken except for the total particle number. However, it is argued that the GHF wave function contains the most variational freedom (at the mean-field level) comparing to the RHF or UHF states. In the following, we will demonstrate the flexibility of the symmetry-broken multi-determinant GHF wave function in QMC calculations through the combined strength of the FED and ResHF theories.

B. AFQMC and the Constrained-Path approximation

The AFQMC technique implemented in this study works in the second-quantized framework. It is based on the projection equation

\[ |\Psi_0\rangle = \lim_{\tau \to \infty} e^{-\tau \hat{H}} |\Psi_T\rangle, \tag{3} \]

where \( \tau \) is the imaginary time and \( |\Psi_T\rangle \) is a trial wave function that has a finite overlap with the many-body ground state \( |\Psi_0\rangle \) of the Hamiltonian \( \hat{H} \). In actual numerical calculations, the projection is realized iteratively

\[ |\Psi^{(\ell+1)}\rangle = e^{-\Delta \tau \hat{H}} |\Psi^{(\ell)}\rangle, \tag{4} \]

where the discrete imaginary time step \( \Delta \tau \) is chosen to be a small positive number.

In a numerical calculation, the small-time projector is first approximated by implementing the second-order Trotter-Suzuki break-up of the Hubbard-Stratonovich (HS) transformation:

\[ e^{-\Delta \tau \hat{H}} \approx e^{-\Delta \tau \hat{K}/2} e^{-\Delta \tau \hat{V}} e^{-\Delta \tau \hat{K}/2}, \tag{5} \]

where \( \hat{K} \) and \( \hat{V} \) denote the part of \( \hat{H} \) that is quadratic and quartic in fermion operators respectively. The error of the approximation is of the order \( O(\Delta \tau^2) \) and can be reduced systematically using higher order break-up formulas. The quartic term is further decomposed using the Hubbard-Stratonovich (HS) transformation

\[ e^{-\Delta \tau \hat{V}} = \int ds \, P(s) e^{\hat{v}(s)}. \tag{6} \]

In this identity, \( P(s) \) is a probability distribution function of the HS fields \( s \) and its functional form is determined by the quartic term \( \hat{V} \) of the Hamiltonian. \( \hat{v}(s) \)
is an one-body operator that depends on \( s, \Delta \tau, \) and the matrix elements of \( V \) (only the \( s \)-dependence is shown explicitly).

Using Eqs. (5) and (6), the iterative projection equation can be cast as

\[
|\Psi^{(\ell+1)}\rangle = \int ds P(s) \tilde{B}(s) |\Psi^{(\ell)}\rangle, \tag{7}
\]

where we have used \( \tilde{B}(s) \) to denote collectively the product of one-body projectors \( e^{-\Delta \tau \hat{K}/2} e^{\hat{\psi}(s)} e^{-\Delta \tau \hat{K}/2} \). The integral equation is then realized by importance-sampled branching random walks in the space of Slater determinants. At every step, \( \tilde{B}(s) \) is applied to each walker \( |\phi^{(\ell)}\rangle \) in a population by drawing a component of the HS field \( s \) from the distribution \( P(s) \). This process generates a new collection of walkers for the next iteration. The walker population varies along the way of projection due to fluctuating weights. Once converged, the resulting walkers, together with their weights, give a stochastic representation of the ground state wave function \( |\Psi_0\rangle \) at any step. Observables such as energy and correlation functions can be measured periodically.

Within the AFQMC approach just described, the sign problem occurs because of the symmetry between the walkers with opposite overall signs \( \{|\phi\rangle\} \) and \( \{-|\phi\rangle\} \).\(^{20}\) The two sets are degenerate and cannot be distinguished by the random walks. If uncontrolled along the projection, the Monte Carlo representation of the ground state wave function will eventually become an equal mixture of + and – walkers. The overall Monte Carlo signal therefore decays (exponentially fast) with imaginary time, leading to the sign problem.\(^{33}\) The sign problem can be eliminated by removing walkers that have zero overlap with the ground state, \( \langle \Psi_0 | \phi \rangle = 0 \), because these walkers will no longer contribute to the representation of the ground state in the future.\(^{20}\) Since the exact ground state \( |\Psi_0\rangle \) is typically unknown, the constrained-path approximation\(^{19,26}\) uses the trial wave function to enforce the constraint, \( \langle \Psi_T | \phi \rangle = 0 \), at each step of the projection. As a consequence, the AFQMC algorithm under the constrained-path approximation (the combined technique will be called CPMC in the following discussions) is not exact and the results will have a systematic error that depend on the quality of the trial wave function. Previous benchmarks for the single-band repulsive Hubbard model have shown that the constrained-path error is typically very small with single-determinant mean-field type trial wave functions.\(^{20,27,28,34,35}\) While there are proposals for more elaborate trial states which give accurate results,\(^{27,28,35}\) we will show below that the symmetry-broken MR GHF state provides a robust and computationally economic route for accurate CPMC calculations.

### III. RESULTS AND DISCUSSION

#### A. Benchmark platform

We choose to demonstrate the symmetry-broken multi-determinant GHF state by solving the ground state of the repulsive Hubbard model using the CPMC algorithm. The model is defined by the Hamiltonian

\[
\hat{H} = -t \sum_{\langle ij \rangle \sigma} \left( \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \hat{c}_{j\sigma}^\dagger \hat{c}_{i\sigma} \right) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}, \tag{8}
\]

where \( \hat{c}_{i\sigma}^\dagger \) (\( \hat{c}_{i\sigma} \)) are the spin-\( \sigma \) (\( \sigma = \uparrow, \downarrow \)) electron creation (annihilation) operator at site \( i \). \( U > 0 \) is the on-site Coulomb repulsion. \( t \) is the hopping integral between two near-neighbor sites \( i \) and \( j \). Throughout this work, we use \( t \) as the unit of energy and set \( t = 1 \). Due to the local nature of the Hubbard interaction, we choose to work with the spin-decomposition HS transformation\(^{36}\) in the calculations.

Fig. 1 depicts the geometries of several \( L_1 \times L_2 \) lattices considered in our calculations. Here \( L_1 \) and \( L_2 \) are the linear dimension along the Bravais lattice vector \( a_1 \) and \( a_2 \) respectively. Both bipartite and geometrically frustrated lattices are considered, and periodic boundary conditions are assumed in all simulations.

#### B. Results

We begin by making two remarks. Firstly, we note that RHF or UHF orbitals can be considered as special cases

![FIG. 1. Geometries considered in this work: (a) 4 x 4 square lattice, (b) 3 x 2 honeycomb lattice, (c) 4 x 3 triangular lattice, and (d) 2 x 2 kagome lattice. In each panel, the colors represent different basis in a unit cell. a1 and a2 are Bravais lattice vectors. The square lattice has a1 = (a, 0) and a2 = (0, a), while the lattice vectors are a1 = (a, 0) and a2 = a(\( \frac{1}{2}, \frac{\sqrt{3}}{2} \)) for the rest of the geometries. We set the lattice constant a = 1.](4d5404489f9f47e682522e18df37a0f0)
of the GHF wave function with vanishing off-diagonal spin components \((\hat{c}_i^\dagger \hat{c}_j)\). To demonstrate the advantage of using the GHF state at the variational level, Fig. 2 gives a simple comparison for the half-filled Hubbard triangular lattice at \(U = 4\). The figure shows that the GHF wave function clearly has the lowest variational energy regardless of \(n_d\).

Secondly, while the total number of electrons in a GHF wave function is conserved, the particle number for each spin component \((\hat{n}_\uparrow)\) and \((\hat{n}_\downarrow)\) does not because spin-flip terms are now explicitly included in the GHF orbitals. Therefore, simulations using GHF-type walkers will typically break the symmetry between \((\hat{n}_\uparrow)\) and \((\hat{n}_\downarrow)\) as well as the CPMC energy as a function of imaginary projection time \(\tau\) for the half-filled \(4 \times 3\) Hubbard triangular lattice. In this example, a 10-determinant GHF trial wave function is adopted. Walkers are initialized by a single-determinant GHF wave function. It can be clearly seen that although the energy converges reasonably well to the exact energy (apart from the Trotter error), the density does not. Therefore throughout this work, we will initialize random walkers using free-electron wave functions\(^{37}\) in which \((\hat{n}_\uparrow)\) and \((\hat{n}_\downarrow)\) are fixed at the desired value.

In Fig. 4, we choose to demonstrate typical Trotter approximation behaviors in our calculations. The sample system is a 4-hole doped \(2 \times 2\) kagome lattice at \(U = 8\). Since this is a closed-shell filling, we compare the \(\Delta\tau\)-dependence of a free-electron (FE) trial wave function to that of a 200-determinant GHF state optimized using the ResHF theory (dubbed ResHF-optimized). The multi-determinant trial wave function clearly has a weaker time-step dependence. Similar comparisons are also observed in other simulations. The relatively weaker \(\Delta\tau\)-dependence seems to be typical in calculations using multi-determinant trial states.\(^{35}\) In this example, the extrapolated energy is lower than the exact data for the FE trial wave function. In other words the mixed estimator \(E = \langle \Psi_T | \hat{H} | \Phi \rangle / \langle \Psi_T | \Phi \rangle\) used to compute the energy is not always variational. Unlike the real-space fixed-node method,\(^{18}\) random walkers in CPMC are represented by over-complete non-orthogonal Slater determinants. As a result, walkers removed by the constraint are not necessarily orthogonal to the remaining walkers, breaking the equivalence between the variational and mixed estimators. For detailed discussions and proposals of constructing variational energy estimators, we refer the readers to Ref. 38. In the present study we will not address the issue.

As mentioned in Section II, we use a two-step approach to generate GHF trial wave functions. For a given \(n_d\), a FED GHF wave function is constructed. The ResHF theory is applied subsequently to optimize all determinants simultaneously. In principle, both FED and ResHF-optimized GHF states can serve the role of trial state. To examine their performance, we first compare the deviation of their variational energy from the exact ground state energy in Fig. 5. The system under consideration is the half-filled \(2 \times 2\) kagome lattice at \(U = 8\). Indeed, by adding more configurations to the multi-determinant expansion, the relative error in variational energy can be
reduced systematically for both type of wave functions. In this particular example, however, one is able to gain a substantial improvement over the FED state by applying the ResHF theory. For example, at \( n_d = 200 \), the deviation (defined as \( |E - E_{\text{ex}}|/|E_{\text{ex}}| \times 100\% \), where \( E_{\text{ex}} \) is the exact energy) of the ResHF variational energy is \( \sim 0.64\% \) while that of the FED variational energy is about 4.22\%. Similar comparisons are also observed in other lattice geometries.

This comparison between FED and ResHF-optimized wave functions carries over to CPMC calculations. Also in Fig. 5, results of a series of CPMC simulations using FED and ResHF-optimized GHF trial wave functions are plotted for \( n_d \) up to 200 determinants. Both calculation results are approaching the exact energy monotonically as more determinants are included and optimized. At \( n_d = 200 \), the FED trial wave function gives \( E_{\text{CPMC}} = -5.60252(28) \), corresponding to a relative error \( \sim 0.388\% \). Using the ResHF-optimized GHF state as the trial wave function, the CPMC ground state energy is \( E = -5.62334(11) \), which is 0.018\% (in relative error) away from the exact energy.

We would like to mention that in our benchmark calculations (see Table I), there are several closed-shell hole-doped systems under periodic boundary conditions where both FED and ResHF-optimized states give almost comparable results. Furthermore, we found in our benchmark data that there are situations where the CPMC energy does not improve systematically. It turns out that these exceptions are caused by poor FED determinants. Therefore, as in any numerical mean-field calculations, it is necessary to use different initial configurations and make sure the FED result converge properly. When care is taken, the combined FED and ResHF theory can produce high quality trial states for Monte Carlo simulations.

We list detailed benchmark calculations results in Table I. In each test case, we have used both FED and ResHF-optimized trial wave functions consisting of as many as 200 determinants. In the table \( n_d \) represents the number of ResHF-optimized determinants that gives the best agreement with the exact diagonalization result. Energies reported in the table have been extrapolated to the \( \Delta \tau \to 0 \) limit following the example of Fig. 4.

The table shows the advantage of optimizing FED determinants for both mean-field and many-body calculations. Although in a few instances the FED and ResHF-optimized states appear to have the same variational energy, the latter still leads to a better agreement in Monte Carlo calculations. Generally speaking, at weak couplings \( U < W \), where \( W \) is the bandwidth of the tight-binding Hamiltonian, the data suggest that a handful number of determinants on the order \( n_d \sim \mathcal{O}(10) \) is sufficient to reduce the constrained-path systematic error in the calculation results regardless of the geometries. On half-filled bipartite lattices, in particular, a single-determinant GHF trial state is able to generate essentially exact results for the square and honeycomb lattices at \( U = 4 \), a situation that is consistent with previous reports. At \( U = 8 \) (\( U \sim W \)) the number of determinants that gives the best agreement goes up to the order \( \mathcal{O}(10^2) \). This behavior is to be expected since, at the ansatz wave function level, strong correlations (in the sense that \( U \gtrsim W \)) typically require multi-determinantal wave functions to capture correlation effects. For extremely correlated systems where \( U > W \), it is very likely that more than \( \mathcal{O}(10^3) \) are required for the result to converge. A possible alternative option would be using the Gutzwiller projector, an approach shown to be quite effective at large couplings. However, we will leave the construction of trial states by Gutzwiller-projecting GHF...
determinants for future investigations.

Finally, it is worth mentioning that on the slightly doped square lattice, competing phases such as incommensurate magnetic ordering, charge inhomogeneity, and possibly $d$-wave superconducting state may exist and compete with each other. Without restoring the symmetry of the exact ground state in the trial wave functions, the Monte Carlo results appear to have relatively larger deviations, as can be observed in Table I. Apart from this challenging scenario, the benchmark data generally suggest that the combined FED and ResHF theories is able to generate high quality symmetry-broken trial wave functions that can much reduce the systematic errors caused by the constrained-path approximation.

IV. SUMMARY

In this work, we have studied the performance of multi-determinant generalized Hartree-Fock trial wave function in CPMC calculations. By comparing the results with exact eigenenergies available on small clusters, it is shown that the optimized multi-determinant GHF state is able to produce satisfactory benchmark results without explicitly restoring the symmetries of the Hamiltonian at a manageable computational cost. The quality of the multi-determinant GHF state can be systematically improved by including more determinants in the FED and ResHF calculations. The combined (symmetry-broken) FED-ResHF GHF approach thus promises a flexible and straightforward technique for accurate Monte Carlo calculations.

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lattices is obtained from Ref. 41 and 42 respectively. The rest of the exact data are obtained from using the ALPS library.

The symbol $\Delta$ shows percentage relative error defined as $\Delta = \frac{E_{\text{Fed}} - E_{\text{Res}}}{E_{\text{Res}}} \times 100\%$, where $E$ is the variational or CPMC energy. The exact energy of the 4\times4, 2\times3, 3\times4, and 4\times4 lattices are obtained from Ref. 41 to 43 respectively. The rest of the exact data are obtained from using the ALPS library.

In the case of open-shell fillings, we have implemented a small twist boundary condition ($\sim O(10^{-3})$) to break the degeneracy.

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