Correlated wave functions and the absence of long-range order in numerical studies of the Hubbard model

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We present a formulation of the constrained path Monte Carlo method for fermions that uses trial wave functions that include many-body effects. This formulation allows us to implement a whole family of generalized mean-field states as constraints. As an example, we calculated superconducting pairing correlation functions for the two-dimensional repulsive Hubbard model using a BCS trial state as the constraint. We compared the results with the case where a free-electron trial wave function is used. We found that the correlation functions are *independent* of which state is used as the constraint, which reaffirms the results previously found by Zhang *et al.* [Phys. Rev. Lett. **78**, 4486 (1997)] regarding the suppression of long-range pairing correlations as the system size increases. [S0163-1829(99)03303-2]

I. INTRODUCTION

Since the discovery of high-temperature superconductivity, an enormous effort has been devoted to the theoretical study of two-dimensional electronic models. This effort is driven by the belief that the mechanism for superconductivity lies within the CuO_2 planes common to these materials and is dominantly electronic in origin. The two-dimensional repulsive Hubbard model has attracted the most attention as the simplest effective model possibly embodying the key electronic phenomena at low energies. Numerous works on this model have reproduced qualitatively the observed magnetic properties of the cuprates in the normal state. However, the search for superconductivity in the Hubbard model, although intensive and extensive, has yielded few positive indicators.[1,2]

Most of the present knowledge on the phase diagram of the two-dimensional repulsive Hubbard model has been obtained by combination of theorems and numerical studies of finite-size clusters. The numerical studies used Lanczos, variational Monte Carlo, and zero or finite-temperature quantum Monte Carlo techniques. In a superconducting phase, one expects the superconducting pairing correlation functions to exhibit off-diagonal long-range order (ODLRO), which is an indication of the Meissner effect.[3] With this in mind, a number of investigators have calculated pairing correlation functions in various symmetry channels. However, most calculations were limited to high temperatures and small system sizes. In the case of Monte Carlo studies these limitations were imposed by the fermion sign problem, which causes the variances of computed quantities and hence the computing time to grow exponentially with the increase in system sizes.

Recently, a new zero temperature quantum Monte Carlo method, the constrained path Monte Carlo (CPMC), was developed that overcomes the major limitations of the sign problem.[4] This method allows the calculation of pairing correlation functions at zero temperature without the exponential increase in computer time with system size. Using this method, Zhang *et al.*[1] calculated $d_{x^2-y^2}$-wave and extended s-wave pairing correlation functions versus distance in the ground state for lattices up to 16×16. They found that the $d_{x^2-y^2}$-wave correlations are stronger than extended s-wave correlations. However, as the system size or the interaction strength was increased, the magnitude of the long-range part of both correlation functions vanished.

Although the findings of Zhang *et al.*[1] provide evidence for the absence of ODLRO in the two-dimensional Hubbard model, the CPMC method is approximate and has a systematic error that is difficult to gauge. The systematic error is associated with the wave function used to constrain the Markov chains produced by the Monte Carlo procedure. More specifically, in the CPMC method the ground-state wave function is represented by an ensemble of Slater determinants. As these determinants evolve in imaginary time, the ones with a negative overlap with a constraining wave function are discarded. This procedure eliminates the sign problem but introduces an approximation that depends on the quality of the constraining wave function. Zhang *et al.*[1] used free-electron and unrestricted Hartree-Fock wave functions. More sophisticated choices of wave functions, particularly ones exhibiting strongly correlated electron effects, are typically difficult to implement, because of the increasing number of Slater determinants needed and the consequent increase in computing time.

In this work, we extended the formulation of the CPMC method in a way that allows the use of a wide variety of trial wave functions with only a small increase in computing time. As an illustration, we calculated the superconducting pairing correlation functions of the two-dimensional repulsive Hubbard model in the $d_{x^2-y^2}$-wave channel using as a constraint a BCS wave function that has superconducting ODLRO. We found that the resulting correlation functions are the same as those obtained using the free-electron and Hartree-Fock constraining wave functions. This reaffirms the results by Zhang *et al.*[1] regarding the vanishing of long-range pairing correlations as the system size increases.

The paper is organized as follows: in Sec. II we briefly describe the CPMC technique emphasizing aspects of the new formulation. In Sec. III, we define the Hamiltonian and

pairing correlation functions and present our results. In Sec. IV, we discuss our conclusions.

II. METHOD

In this section we summarize the main features of the CPMC method. For a more detailed description of the method see Ref. 4. In the CPMC method, the ground-state wave function $|\Psi_0\rangle$ is projected in imaginary time τ from a known initial wave function $|\Psi(\tau=0)\rangle=|\Psi_T\rangle$ by a branching random walk in an over-complete space of Slater determinants $|\phi\rangle$,

$$|\phi\rangle=\prod_{i,\sigma}^{N_\sigma} \phi_{i\sigma}^\dagger|0\rangle, \quad \phi_{i\sigma}^\dagger=\sum_{j=1}^{N} c_{j\sigma}^\dagger \Phi_{ji}^\sigma, \qquad (1)$$

where $c_{j\sigma}^\dagger$ creates and electron in orbital j with spin σ ($n_{j\sigma}=c_{j\sigma}^\dagger c_{j\sigma}$), and

$$\langle\phi|\phi'\rangle\neq\delta_{\phi\phi'} \qquad (2)$$

with N the number of available single-particle states (for the Hubbard model corresponds to the total number of lattice sites) and N_σ the number of particles with spin σ. The total number of electrons is given by $N_e=N_\uparrow+N_\downarrow$.

The projection corresponds to finding the ground state from the long-time solution of the imaginary-time representation of Schrödinger's equation specified by a Hamiltonian $\hat{H}$,

$$\frac{\partial|\Psi\rangle}{\partial\tau}=-(\hat{H}-E_0\hat{1})|\Psi\rangle \qquad (3)$$

with E_0 the ground-state energy ($\hbar$ is set to 1).

Provided $N_0=\langle\Psi_0|\Psi(0)\rangle\neq0$ and $\hat{H}$ being time independent, the formal solution

$$|\Psi(\tau)\rangle=e^{-\tau(\hat{H}-E_0\hat{1})}|\Psi(0)\rangle \qquad (4)$$

has the property

$$\lim_{\tau\to\infty}|\Psi(\tau)\rangle=N_0|\Psi_0\rangle. \qquad (5)$$

On the computer this large τ limit is accomplished by breaking up τ in small time steps $\Delta\tau$ and iterating the equation

$$|\Psi^{n+1}\rangle=e^{-\Delta\tau(\hat{H}-E_T\hat{1})}|\Psi^n\rangle, \qquad (6)$$

where E_T is a guess at the ground-state energy E_0 and $\Delta\tau N_s=\tau$ with N_s the number of imaginary time steps. As $\tau\to\infty$, the iteration becomes stationary, i.e., $\partial|\Psi\rangle/\partial\tau=0$, and if E_T is adjusted to equal E_0, then $|\Psi(\tau\to\infty)\rangle=N_0|\Psi_0\rangle$.

The propagation in imaginary time is done in the following way: in the space of Slater determinants, we write $|\Psi_0\rangle=\Sigma_\phi\chi(\phi)|\phi\rangle$ and choose $\chi(\phi)>0$. By being positive, the function $\chi(\phi)$ describes the distribution of Slater determinants representing the ground state. The Monte Carlo process samples from this distribution. This process is implemented by the application of a Trotter decomposition and a Hubbard-Stratonovich transformation to the iteration in Eq. (6) and converting it into

$$|\Psi^{n+1}\rangle=\int d\mathbf{x}\, P(\mathbf{x})B(\mathbf{x})|\Psi^n\rangle, \qquad (7)$$

where $\mathbf{x}$ is to be interpreted as a multidimensional random variable distributed according to $P(\mathbf{x})$ and $B(\mathbf{x})$ is an operator approximating $e^{-\Delta\tau\hat{H}}$ for a given value of the random variable, whose general structure is a product of exponentials of operators linear in $c^\dagger c$. For each time step $\Delta\tau$, $B(\mathbf{x})$ has the property of transforming one Slater determinant into another. The Monte Carlo method evaluates the multidimensional integral (7) by using an ensemble of random walkers represented by Slater determinants $|\phi\rangle$. For each walker, it samples $\mathbf{x}$ from $P(\mathbf{x})$ and then obtains the new Slater determinant by multiplying

$$|\phi^{n+1}\rangle=B(\mathbf{x})|\phi^n\rangle. \qquad (8)$$

Once the Monte Carlo procedure converges, the ensemble of $|\phi\rangle$ represents $|\Psi_0\rangle$ in the sense that their distribution is a Monte Carlo sampling of $\chi(\phi)$. In this sense, the CPMC approach is a sort of stochastic configuration interaction method.

To specify the ground-state wave function completely, only determinants satisfying $\langle\Psi_0|\phi\rangle>0$ are needed because $|\Psi_0\rangle$ resides in either of two degenerate halves of the Slater determinantal space [in general, a manifold of dimension $N_e(N-N_e)$], separated by a nodal hypersurface $\mathcal{N}$ defined by $\langle\Psi_0|\phi\rangle=0$. The sign problem occurs because walkers can cross $\mathcal{N}$ as their orbitals evolve continuously in the random walk. Asymptotically in τ they populate the two halves equally, leading to an ensemble that tends to have zero overlap with $|\Psi_0\rangle$. If $\mathcal{N}$ were known, one would simply constrain the random walk to one half of the space and obtain an exact solution of Schrödinger's equation. In the CPMC method, without *a priori* knowledge of $\mathcal{N}$, we use a constraining wave function, which we usually take to be the trial wave function $|\Psi_T\rangle$, and require the Slater determinants to satisfy $\langle\Psi_T|\phi\rangle>0$. Thus, the quality of the calculation clearly depends on $|\Psi_T\rangle$. In the past only free-electron or Hartree-Fock wave functions were implemented, mainly due to their simplicity and the novelty of the method. However, it is desirable to use more sophisticated wave functions that include many-body effects. For example, to study superconductivity it is interesting to implement trial wave functions that exhibit ODLRO, like a BCS wave function.

Our goal is to use trial wave functions of the type (i.e., a Bogoliugov transformation of the vacuum $|0\rangle$, $\langle0|0\rangle=1$)

$$|\Psi_T\rangle=\prod_k (u_k+v_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger)|0\rangle, \qquad (9)$$

where the product includes all values of momentum $k=(k_x,k_y)$ in the first Brillouin zone and $|u_k|^2+|v_k|^2=1$ to ensure normalization ($\langle\Psi_T|\Psi_T\rangle=1$). Other than satisfying the normalization condition, the parameters u_k and v_k can be chosen arbitrarily.

Equation (9) represents a wave function that does not have a fixed particle number N_e. To represent a fixed electron number, $|\Psi_T\rangle$ needs to be projected onto that particular subspace. The resulting wave function is a linear combination of a large number of Slater determinants[5] (large in the sense that the number grows very rapidly with system size

and particle number to the point where it becomes impractical to use). Alternatively, one can work in an extended space with different electron numbers. To do that, we follow Yokoyama and Shiba[6] and perform a particle-hole transformation on one of the spin species:

$$d_k = c^\dagger_{-k\downarrow},$$
$$c^\dagger_k = c^\dagger_{k\uparrow}. \tag{10}$$

Using this transformation and noting that the new vacuum $|\tilde{0}\rangle$ is related to the old one by

$$|0\rangle = \prod_k d^\dagger_k |\tilde{0}\rangle \tag{11}$$

we can rewrite $|\Psi_T\rangle$ in terms of the new c and d operators:

$$|\Psi_T\rangle = \prod_k (u_k d^\dagger_k + v_k c^\dagger_k)|\tilde{0}\rangle \tag{12}$$

so that $|\Psi_T\rangle$ is represented by a single Slater determinant. Since we are interested in projecting out the ground state with a fixed electron number, we have to use the propagator $e^{-\tau(\hat{H} - E_0\hat{1} - \mu\hat{N}_e)} = \hat{\mathcal{U}}(\tau)$ and choose μ, the chemical potential, to select the desired number of electrons $N_e = \langle\Psi_0|\hat{N}_e|\Psi_0\rangle/\langle\Psi_0|\Psi_0\rangle$ ($\hat{N}_e = \Sigma_{j\sigma} n_{j\sigma}$). At the end of the projection the ground-state wave function will have a fixed number of electrons given by the choice of μ.

The changes in the CPMC method necessary to use the BCS form of a correlated wave function are minor. Instead of matrices Φ^σ for up and down spin of sizes $N \times N_\sigma$ to represent the random walkers, they, as well as the trial wave function $|\Psi_T\rangle$, are now represented by a single matrix of size $2N \times N$. The increase in computation time caused by the increase in the size of the matrices depends on the system size and the number of particles. A rough estimate gives the increase as the factor $3N/N_e$. For example, for a 6×6 system with $N_e = 26$ this is $2.89N/N_e$. The closer we get to half-filling ($N_e = N$) the smaller the increase. In general, for the filling fractions studied here, the increase in computer time is approximately four.

III. CALCULATION AND RESULTS

The Hamiltonian is the usual Hubbard Hamiltonian on a square lattice with periodic boundary conditions:

$$\hat{H} = -t \sum_{\langle ij\rangle,\sigma} (c^\dagger_{i,\sigma} c_{j,\sigma} + c^\dagger_{j,\sigma} c_{i,\sigma}) + U\sum_i n_{i\uparrow} n_{i\downarrow}, \tag{13}$$

where t is the nearest-neighbor hopping matrix element and U is the on-site Coulomb repulsion. We set $t = 1$ so that all energies are measured in units of t. In terms of the operators c and d defined by the transformation (10) the Hamiltonian has the form

$$\hat{H} = -t\sum_{\langle ij\rangle} (c^\dagger_i c_j + c^\dagger_j c_i - d^\dagger_i d_j - d^\dagger_j d_i) + U\sum_i n^c_i(1 - n^d_i), \tag{14}$$

where $n^c_i (n^d_i)$ denotes the occupation in the c (d) orbital. This transformed Hamiltonian corresponds to a two-band spinless fermion model.

We computed the ground-state energy and the superconducting pairing correlation functions in the $d_{x^2-y^2}$-wave channel using the following definitions:

$$P_d(\vec{R}) = \langle \Delta^\dagger_d(\vec{R}) \Delta_d(0)\rangle, \tag{15}$$

where the pair-field operator is

$$\Delta_d(\vec{R}) = \sum_\delta f_d(\vec{\delta})[c_{\vec{R}\uparrow} c_{\vec{R}+\vec{\delta}\downarrow} - c_{\vec{R}\downarrow} c_{\vec{R}+\vec{\delta}\uparrow}] \tag{16}$$

with $\vec{\delta} = \pm\hat{x}, \pm\hat{y}$, $f_d(\pm\hat{x}) = 1$, and $f_d(\pm\hat{y}) = -1$. $\vec{R}$ denotes the position in the lattice in units of the lattice constant, which is taken to be unity.

We used trial wave functions of the form (9) with u_k and v_k given by the BCS relation

$$\frac{v_k}{u_k} = \frac{\Delta_k}{\epsilon_k - \mu + \sqrt{(\epsilon_k - \mu)^2 + |\Delta_k|^2}}, \tag{17}$$

where ϵ_k is a single-particle energy and Δ_k is the gap, $\Delta_k = \Delta f(k)$. Δ is a variational c number and $f(k)$ represents the symmetry of the pairing, which we choose to be $d_{x^2-y^2}$, $f(k) = \cos(k_x) - \cos(k_y)$.

We concentrated on the $d_{x^2-y^2}$-wave channel in part because the existence of ODLRO in the extended s-wave channel is conditioned upon the existence of ODLRO in the isotropic s-wave channel.[7] Since the possibility of pairing in the isotropic s-wave channel is highly unlikely for the repulsive Hubbard model, so is the chance of pairing in the extended s-wave channel. Moreover, these statements have been verified numerically by us and by Zhang et al.[1] Also, it has been increasingly established experimentally that the order parameter in the superconducting cuprates has $d_{x^2-y^2}$-wave symmetry.

We used two different trial wave functions: one with $\Delta = 0.5$, which corresponds to a BCS superconducting state, and the other one with $\Delta = 0$, which corresponds to the free-electron case. In both cases we choose the parameter μ in the BCS wave function so that $\langle\Psi_T|\hat{N}_e|\Psi_T\rangle = N_e$ where N_e is the number of electrons we are interested in. While the free-electron wave function has a fixed number of electrons ($\sigma_{N_e} = \sqrt{\langle\hat{N}_e^2\rangle - \langle\hat{N}_e\rangle^2} = 0$), the BCS wave function with $\Delta \neq 0$ has components with different electron numbers so that $\sigma_{N_e} \neq 0$. It is important to notice that in general the parameter μ in the BCS wave function is different than the one used in the propagator $\hat{\mathcal{U}}(\tau)$. The latter one is set so that at the end of the propagation the ground state has the desired number of electrons N_e.

To illustrate the difference between these two wave functions, in Fig. 1 we plot the variational value of the $d_{x^2-y^2}$-wave correlation functions versus distance, that is $\langle\Psi_T|\Delta^\dagger_d(\vec{R})\Delta_d(0)|\Psi_T\rangle$, for the two trial wave functions in a 10×10 system with $U = 4$ and $N_e = 82$, so that the filling fraction is $n_e = N_e/N = 0.82$. This filling corresponds to a closed-shell case, that is, the free-electron ground state is nondegenerate. In the free-electron case the correlations die
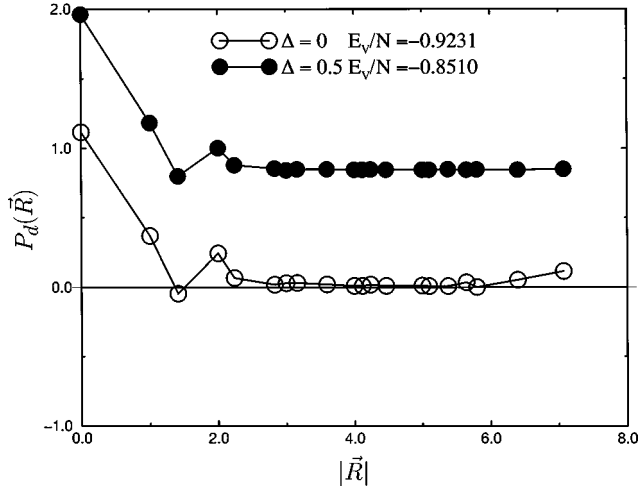
FIG. 1. Variational value of the pairing correlations versus distance $|\vec{R}|$ for two different trial wave functions in a 10×10 system. Parameters are $U=4$ and filling fraction $n_e = 0.82$. The BCS wave function exhibits ODLRO.

out rapidly with distance, while in the BCS case the existence of ODLRO is evident in the sense that for long distances, the correlation functions approach a finite value given by the square of the superconducting order parameter Δ^{SC}:

$$\Delta^{SC} = \frac{4}{N}\sum_k f(k) u_k v_k = \frac{4}{N}\sum_k f(k) \frac{\Delta_k}{\sqrt{(\epsilon_k - \mu)^2 + \Delta_k^2}}. \tag{18}$$

The overlap between the two normalized trial wave functions is $\langle \Psi_T(\Delta=0)|\Psi_T(\Delta=0.5)\rangle = 0.0076$, so the two wave functions are close to being orthogonal.

The variational energy $E_v = \langle \Psi_T | \hat{H} | \Psi_T \rangle$ is much larger for the BCS trial wave function than for the free-electron trial wave function. In general we find that the variational energy increases monotonically with the parameter Δ of the

BCS wave function, as it is shown in Fig. 2 for a 10×10 system with $U=4$ and $\langle \hat{N}_e \rangle = 82$. This variation contrasts previous results obtained with the variational Monte Carlo method, which found that a nonzero value of Δ minimizes the variational energy.[6,8,9] However, in these cases, a Gutzwiller factor was included in the wave function that projected out totally or partially the states with double occupancy. It seems that the inclusion of this factor is crucial to obtain a minimum of the variational energy at a finite value of Δ. Within our method it is both inconvenient and unnecessary to use trial wave functions that are non-Fock states such as the Guztwiller wave function:

$$|\Psi_G\rangle = \prod_i (\hat{1} - g n_{i\uparrow} n_{i\downarrow})|\Psi_{FOCK}\rangle \tag{19}$$

with g a variational parameter that determines the average number of doubly occupied sites. (When $g=1$, double occupation is completely suppressed.) Such states are inconvenient because they do not propagate as single Slater determinants. However, since we are doing a projection in imaginary time onto the ground state of the system, it is not necessary to improve the variational energy of our trial state.

In the large U limit, the Hubbard model can be mapped onto the t-J model. This strong coupling limit was used in Refs. 8 and 6 to calculate the energy, making a comparison with our work difficult. However, we can do a comparison with Ref. 9 since they used the Hubbard Hamiltonian to calculate the energy. In their Fig. 1, they report the variational energy per site as a function of Δ for a 6×6 system with $U=8$, 32 electrons, periodic boundary conditions in the x direction and antiperiodic in the y direction. From their figure, the minimum value for the energy per site is $-0.655\,23$ and corresponds to a value of $\Delta=0.1$. The variational energy per site that we obtain for the same system but with periodic boundary conditions in both directions is $0.027\,26$. The difference can likely be accounted for by the fact that we did not project our wave function onto a fixed particle number and second, we did not use a Gutzwiller factor. However, the
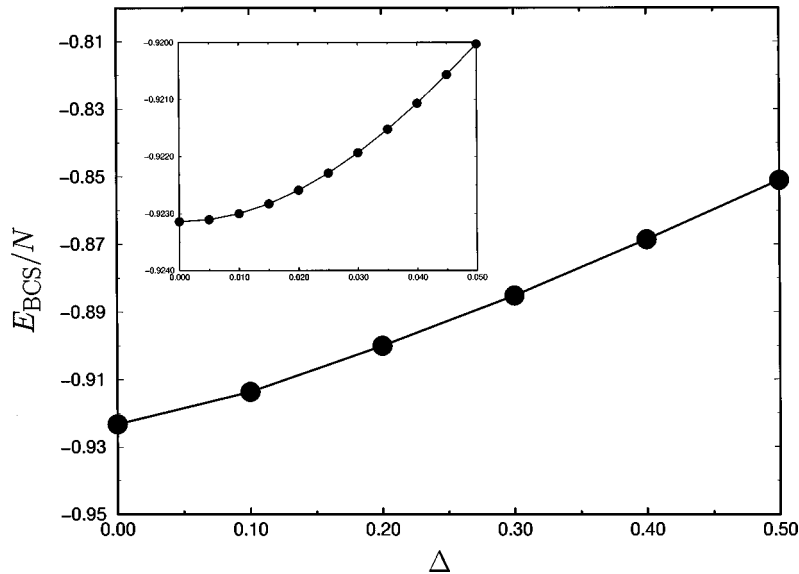

FIG. 2. BCS variational energy per site as a function of Δ for the same system as in Fig. 1. The energy increases monotonically with Δ. The inset shows smaller values of Δ where Ref. 9 finds a minimum.
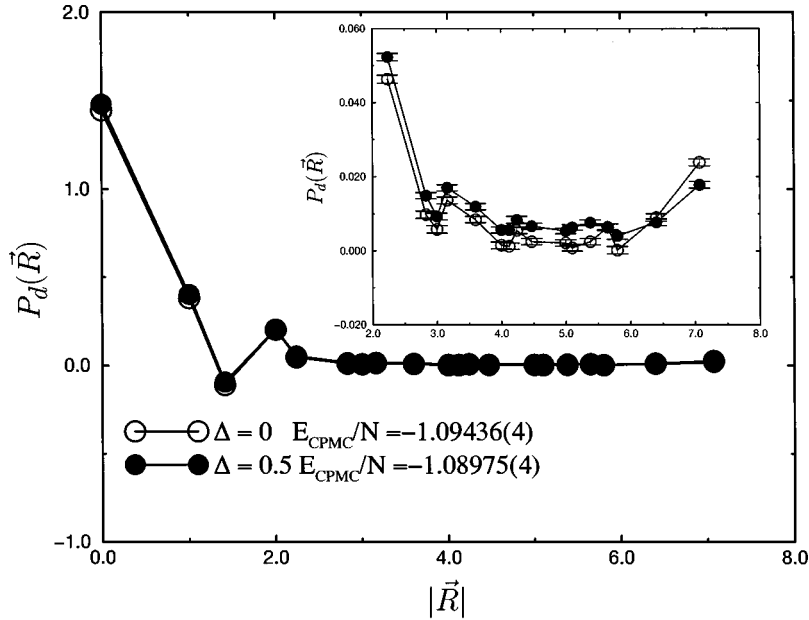
FIG. 3. Pairing correlation functions in the $d_{x^2-y^2}$-wave channel given by the CPMC method for same system as in Fig. 1. The inset shows the long range part in detail. The results are the same for the two different trial wave functions: the correlations decay quickly with distance. Errors bars are smaller than the size of the symbols.

ground-state energy per site calculated with the CPMC method is -0.7272 ± 0.0005, which is considerably lower than their value.

As a check of our algorithm we compared the correlation functions and ground-state energy given by the CPMC method using the free-electron trial wave function with results by Zhang et al.,[10] who used the original formulation of the CPMC, for a 6×6 system with $U=4$ and $N_e=26$ and an 8×8 system with $U=8$ and $N_e=50$. We found excellent agreement with their results.

In Fig. 3 we plot the resulting correlations functions given by the CPMC calculation with the two trial wave-functions used in Fig. 1, for 10×10 with $U=4$. It is clear that the results are essentially the *same* no matter what trial wave function is used. The long-distance magnitude of the correlation functions is very small, smaller than the free-electron case.

Similar calculations to the ones presented in Fig. 3 were done for 12×12, 8×8 and 6×6 systems with different values of U and dopings corresponding to closed shells cases. The results are consistently the same: the correlation functions are the same no matter what trial wave function is used. The ground-state energy, however, is always larger when the BCS wave function is used. The difference between the two ground-state energies is larger for larger U. When the BCS wave function is used, we find that there are more nodal crossings; that is, more walkers are discarded because their overlap with the trial wave function is negative. We believe this is why the energy is higher in the case of the BCS wave function.

We did not use systems larger than 12×12 in part because as system size increases, it becomes more difficult to select μ in the propagator to get the desired number of electrons. This is because the energy levels are getting closer in larger systems. Also, we found that the correlation functions are the same no matter which trial wave function is used for

6×6, 8×8, 10×10 and 12×12 systems. This evidence is enough to conclude that the correlation functions are independent of which trial wave function is used.

IV. CONCLUSIONS

We presented a formulation of the CPMC method that uses trial wave functions that include correlation effects and have components of different electron numbers. Instead of projecting it onto a subspace with fixed number of electrons, we used a particle-hole transformation in one of the spin species to write such trial wave functions as only one Slater determinant.

Because of the increase in the size of the matrices used, this formulation involves a small increase in computing time compared to the original formulation. The increase in CPU time is roughly $3N/N_e$. For the dopings considered in this work it comes to a factor of approximately 4.

This formulation is very general and allows the implementation of a whole family of mean-field wave functions. Following Bach, Lieb, and Solovej[11] we call this class of functions generalized Hartree-Fock states, i.e., states that are ground states of some quadratic mean-field Hamiltonian in Fock space that do not necessarily conserve particle number. Possible examples include spin-density wave, charge-density wave, and superconductivity.

As an illustration, and because of its importance in high-temperature superconductivity, we used a BCS trial wave function with $d_{x^2-y^2}$-wave symmetry to calculate the superconducting pairing correlation functions in the ground state for the two-dimensional repulsive Hubbard model. We compared this result with the one using the free-electron trial wave function. We studied 6×6, 8×8, 10×10, and 12×12 systems for different values of U and dopings and found that the results for the correlation functions are inde-

pendent of which trial wave function is used for the constraint.

Most of the calculations presented in this work correspond to closed shell cases, that is, electron fillings with a nondegenerate free-electron ground state. To check the consistency of our results we also studied some open shell cases like a 6×6 system with 32 electrons ($n_e = 0.89$), $U = 8$ and periodic boundary conditions. We used three different trial wave functions: one free-electron wave function with a fixed number of electrons, another free-electron wave function but with some paired electrons in the Fermi surface and a BCS wave function with $\Delta = 0.1$. The CPMC result is consistent with those of the closed shell cases: the superconducting pairing correlation functions, which vanish for large distances, are independent of the trial wave-function used. Technically, the open shell case is more difficult because in general the free-electron trial wave functions do not have translational invariance. For this reason, one finds different values of the correlation functions for the same distance $|\vec{R}|$ but different directions in the lattice. To overcome this problem we averaged the correlation functions for a given $|\vec{R}|$ over all possible directions in the lattice. This procedure is also used for the closed shell cases but is more relevant in the open shell case where the differences are caused by a broken symmetry introduced by the trial wave function as opposed to small statistical fluctuations due to the Monte Carlo process.

These results reaffirm the previous ones by Zhang *et al.*[1] implying the absence of ODLRO in the $d_{x^2-y^2}$-wave channel of the two-dimensional repulsive Hubbard model. We do not dismiss the possibility of ODLRO existing in some exotic channel or for some combination of quasiparticle operators instead of the bare ones.[12] This work has only investigated the channels commonly studied. Although it is not rigorously proven that the absence of ODLRO implies no Meissner effect and consequently no superconductivity, it is reasonable to think that a model without apparent ODLRO is inappropriate as a model of the superconducting phase for the high-temperature superconducting materials.

The lack of clear numerical evidence of $d_{x^2-y^2}$-wave superconductivity upon doping and the abundance of clear numerical evidence of antiferromagnetism at half filling makes it hard to see how a theory, like the SO(5) phenomenology, can apply to the Hubbard model as some have recently suggested.[13] This phenomenology requires the antiferromagnetic long-range order at half-filling to transform into $d_{x^2-y^2}$-wave superconducting long-range order in the doped states. If the low lying excited states have approximate SO(5) symmetry, why then does the strong antiferromagnetic state transform into something that is so hard to find? The two-dimensional repulsive Hubbard model seems to be an inappropriate candidate for the SO(5) phenomenology.

[1] Shiwei Zhang, J. Carlson, and J. E. Gubernatis, Phys. Rev. Lett. **78**, 4486 (1997).

[2] See, for example, Elbio Dagotto, Rev. Mod. Phys. **66**, 763 (1994).

[3] G. L. Sewell, J. Math. Phys. **38**, 2053 (1997).

[4] Shiwei Zhang, J. Carlson, and J. E. Guberntis, Phys. Rev. Lett. **74**, 3652 (1995); Phys. Rev. B **55**, 7464 (1997).

[5] J. P. Bouchaud, A. Georges, and C. Lhuillier, J. Phys. (France) **49**, 553 (1988).

[6] H. Yokoyama and H. Shiba, J. Phys. Soc. Jpn. **57**, 2482 (1988).

[7] Shoucheng Zhang, Phys. Rev. B **42**, 1012 (1990).

[8] Claudio Gross, Phys. Rev. B **38**, 931 (1988).

[9] T. Nakanishi, K. Yamaji, and T. Yanagisawa, J. Phys. Soc. Jpn. **66**, 294 (1997).

[10] Shiwei Zhang, J. Carlson, and J. E. Gubernatis (private communication).

[11] V. Bach, E. H. Lieb, and J. P. Solovej, J. Stat. Phys. **76**, 3 (1994).

[12] E. Dagotto and J. R. Schrieffer, Phys. Rev. B **43**, 8705 (1991).

[13] W. Hanke, R. Eder, E. Arrigoni, A. Dorneich, S. Meixner, and M. G. Zacher, cond-mat/9807015 (unpublished).