d-wave state with multiplicative correlation factors for the Hubbard model

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A d-wave state wave function with multiplicative correlation factors for the Hubbard model is investigated using a variational Monte Carlo method. Employing a simple Gutzwiller-BCS wave function as a starting wave function, we consider improved wave functions with off-diagonal correlation factors. The Monte Carlo simulations are carried out on a square lattice with size 10×10 for $U = 8$ and next nearest neighbor transfer $t' = -0.09$. The ground-state energy is evaluated from an extrapolation. Our wave functions show that pair correlation functions are enhanced for a negative value of t'.

Keywords: Hubbard model, variational Monte Carlo method, BCS-Gutzwiller wave function, Off-diagonal correlation factors

I. Introduction

Strongly correlated electron systems have been investigated for many years in order to understand the mechanism of superconductivity of the high-T_c cuprate superconductors. Strong correlations between the itinerant electrons are believed to be crucial in cuprate high-T_c materials. Among the fundamental models for correlated electrons, the two-dimensional Hubbard model has been extensively studied since the proposal by Anderson.[1] The two-dimensional Hubbard model can be regarded as a simplified one-band model of three-band Cu-O network in the oxide superconductors.

An important question is whether the superconducting state is possible or not for the two-dimensional Hubbard model. This possibility has been controversial since the discovery of high-T_c oxide superconductors.[2–4] This possibility is supported by numerical calculations using the variational Monte Carlo method (VMC)[5–7] and recent quantum Monte Carlo method (QMC).[8] A Monte Carlo method employing constrained path approximation indicates, however, that the superconducting correlations are not enhanced in the ground state.[9] This disagreement should be clarified. Since the typical energy scale for superconductivity is very small compared to the bandwidth or U, a discrete structure of energy levels is sensitive for the ground state properties in finite systems. In fact it has been shown for the two-chain Hubbard model that the superconducting correlation functions are enhanced greatly if the level structures near the Fermi level become dense by modifying the value of the interchain transfer.[10–13] Since the standard Quantum Monte Carlo method suffers from a sign problem, the level spacings should be kept large in order to avoid a negative sign in QMC.[14,15] Thus it may be reasonable that the superconducting correlations are not enhanced in Quantum Monte Carlo simulations which have been done so far. It is required to consider the case where a sign problem occurs in order to investigate a possibility of superconductivity because in the variational Monte Carlo method the superconducting phase was suggested to exist in the region where the sign problem becomes serious.[6,7]

Our model is the 2D Hubbard model defined by

$$H = -t \sum_{\langle ij \rangle \sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + h.c.) - t' \sum_{\langle\langle j\ell \rangle\rangle \sigma} (c^{\dagger}_{j\sigma} c_{\ell\sigma} + h.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow}, \tag{1}$$

where $c^{\dagger}_{i\sigma}$ ($c_{i\sigma}$) is the creation (annihilation) operator of an electron with spin σ at the ith site. t is the transfer energy between the nearest-neighbor (n.n.) sites. $\langle ij \rangle$ denotes summation over all the n.n. bonds. We also examine the effect of t' between next-nearest neighbor (n.n.n.) sites. $\langle\langle j\ell \rangle\rangle$ denotes summation over the n.n.n. pairs. In this paper we investigate the region with small energy spacings near the Fermi level, where the sign problem is necessarily serious for the standard QMC. In QMC the following wave function is considered

$$\psi^{(m)}_{QMC} = \mathrm{e}^{-\Delta\tau K} \mathrm{e}^{-\Delta\tau UV} \cdots \mathrm{e}^{-\Delta\tau K} \mathrm{e}^{-\Delta\tau UV} \psi_0, \tag{2}$$

where ψ_0 is the non-interacting wave function. K and V indicate the kinetic and interaction parts of the Hamiltonian, respectively:

$$K = -t \sum_{\langle ij \rangle \sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + h.c.) - t' \sum_{\langle\langle j\ell \rangle\rangle \sigma} (c^{\dagger}_{j\sigma} c_{\ell\sigma} + h.c.), \tag{3}$$

$$V = \sum_i n_{i\uparrow} n_{i\downarrow}. \tag{4}$$

$\Delta\tau = \beta/m$ is assumed to be small. In the present paper we investigate a generalized wave function given as

$$\psi^{(m)} = \mathrm{e}^{-\lambda_m K} \mathrm{e}^{-\alpha_m V} \cdots \mathrm{e}^{-\lambda_1 K} \mathrm{e}^{-\alpha_1 V} \psi_0, \tag{5}$$

where λ_i and α_i are regarded as variational parameters to optimize the energy. Obviously $\psi^{(m)}$ has lower energy than that of $\psi^{(m)}_{QMC}$ if m is fixed. Since $\psi^{(m)}_{QMC}$ approaches the correct ground state wave function, $\psi^{(m)}$ is also expected to approach the correct ground state as $m \to \infty$. The purpose of this paper is to show the results for the superconducting ground state by a variational method using the off-diagonal wave function correlation factors.[16,17] It will be shown that the sign problem becomes less violent for $\psi^{(m)}$ if m is small. The ground state energy and correlation functions are calculated by our method. The paper is organized as follows. In the second section the wave functions are presented. The method of calculations is also briefly discussed. In the subsequent section we show our results for the BCS-Gutzwiller and off-diagonal BCS-Gutzwiller functions. The last section is assigned to a summary.

II. Formulation of superconductivity for off-diagonal correlation factors

A. Wave functions

The Gutzwiller-projected BCS-type wave function is defined as

$$\psi_S = P_G \psi_{BCS}, \tag{6}$$

$$\psi_{BCS} = \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow})|0\rangle. \tag{7}$$

The gap function is assumed to be d-type pairing: $\Delta_{\mathbf{k}} = \Delta_s(\cos k_x - \cos k_y)$. Coefficients $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$, which are variational parameters, should be determined to minimize the energy. We use the BCS form for $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ defined by

$$v_{\mathbf{k}}/u_{\mathbf{k}} = \Delta_{\mathbf{k}}/(\xi_{\mathbf{k}} + (\xi^2_{\mathbf{k}} + \Delta^2_{\mathbf{k}})^{1/2}), \tag{8}$$

where $\xi_{\mathbf{k}} = -2(\cos k_x + \cos k_y) - \mu$. The chemical potential μ is adjusted so that the expectation value of the electron number is equal to N_e. P_G is the well-known Gutzwiller operator given by

$$P_G = \prod_i (1 - (1-g) n_{i\uparrow} n_{i\downarrow}), \tag{9}$$

for a variational parameter g in the range of $0 \le g \le 1$. An approach with fixed electron number is employed in our previous papers.[6,7] In order to formulate an approach to consider the off-diagonal correlation operators, it is more convenient to use the BCS function directly without fixing the electron number. The two approaches are equivalent in the thermodynamic limit with optimized variational parameters. For this end the following simple transformation is introduced for the down spin:[18]

$$d_{\mathbf{k}} = c^\dagger_{-\mathbf{k}\downarrow}, \quad d^\dagger_{\mathbf{k}} = c_{-\mathbf{k}\downarrow}. \tag{10}$$

The up-spin electrons are unaltered, for which we use the notations $c_{\mathbf{k}} = c_{\mathbf{k}\uparrow}$ and $c^\dagger_{\mathbf{k}} = c^\dagger_{\mathbf{k}\uparrow}$. The vacuum $|0\rangle$ should read $|0\rangle = \prod_{\mathbf{k}} d^\dagger_{\mathbf{k}} |\tilde{0}\rangle$ if we write the vacuum for c and d particles as $|\tilde{0}\rangle$: $c_{\mathbf{k}}|\tilde{0}\rangle = d_{\mathbf{k}}|\tilde{0}\rangle = 0$. Then

$$\begin{aligned} \psi_{BCS} &= \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} c^\dagger_{\mathbf{k}} d_{\mathbf{k}})|0\rangle, \\ &= \prod_{\mathbf{k}} (u_{\mathbf{k}} d^\dagger_{\mathbf{k}} + v_{\mathbf{k}} c^\dagger_{\mathbf{k}})|\tilde{0}\rangle. \end{aligned} \tag{11}$$

The Gutzwiller projection operator is transformed to

$$P_G = \prod_i (1 - (1-g) c^\dagger_i c_i (1 - d^\dagger_i d_i)), \tag{12}$$

and the Hamiltonian has the form

$$H = -t \sum_{\langle ij \rangle} (c^\dagger_i c_j - d^\dagger_i d_j + h.c.) - t' \sum_{\langle\langle j\ell \rangle\rangle} (c^\dagger_j c_\ell - d^\dagger_j d_\ell + h.c.) + U \sum_i c^\dagger_i c_i (1 - d^\dagger_i d_i). \tag{13}$$

In terms of new operators the average electron number is written as

$$N_e = N + \sum_k \langle c^\dagger_k c_k - d^\dagger_k d_k \rangle. \tag{14}$$

The following wave functions are considered in this paper:[19]

$$\psi^{(1)}_S = e^{-\lambda K} e^{-\alpha V} \psi_{BCS}, \tag{15}$$

$$\psi^{(2)}_S = e^{-\lambda' K} e^{-\alpha' V} e^{-\lambda K} e^{-\alpha V} \psi_{BCS}, \tag{16}$$

$$\psi^{(3)}_S = e^{-\lambda'' K} e^{-\alpha'' V} e^{-\lambda' K} e^{-\alpha' V} e^{-\lambda K} e^{-\alpha V} \psi_{BCS}. \tag{17}$$

Our motivation to introduce the superconducting order parameter is to find more optimized wave functions in VMC.

B. Method of Monte Carlo calculations

The Monte Carlo method using the auxiliary fields, which has been developed in the projector Monte Carlo computations, is employed in this paper.[20,21] Following the discrete Hubbard-Stratonovich transformation,[22] the Gutzwiller operator is written as follows

$$\begin{aligned} P_G &= \prod_i (1 - (1-g) c^\dagger_i c_i (1 - d^\dagger_i d_i)) \\ &= \prod_i \exp(-\alpha c^\dagger_i c_i + \alpha c^\dagger_i c_i d^\dagger_i d_i) \\ &= (1/2)^N \sum_{\{s_i = \pm 1\}} \exp[\sum_i (2a s_i - \alpha/2)(c^\dagger_i c_i - d^\dagger_i d_i)], \end{aligned} \tag{18}$$

where $g = \mathrm{e}^{-\alpha}$ and $\cosh(2a) = \mathrm{e}^{-\alpha/2}$ for complex representation where a is a complex number. The real representation is also possible. s_i is the auxiliary field which

takes the value of ± 1 and N is the number of sites. The norm $\langle\psi_S|\psi_S\rangle$ is calculated as

$$\langle\psi_S|\psi_S\rangle = \text{const.} \sum_{\{u_i\}\{s_i\}} \times \langle\psi_0|\exp(h(u))\exp(h(s))|\psi_0\rangle, \quad (19)$$

where ψ_0 is the non-interacting wave function and the potential $h(s)$ is given by

$$h(s) = \sum_i (2as_i - \alpha/2)(n_i - \nu_i), \quad (20)$$

where $n_i = c_i^\dagger c_i$ and $\nu_i = d_i^\dagger d_i$. Then the norm is written as a sum of determinants,

$$\langle\psi_S|\psi_S\rangle = \text{const.} \sum_{\{u_i\}\{s_i\}} \times \det(\phi^\dagger \exp(V(u,\alpha))\exp(V(s,\alpha))\phi), \quad (21)$$

ϕ is a $2N \times N$ matrix with first and second N components corresponding to c and d electron parts, respectively:

$$(\phi_0)_{ij} = \exp(i\mathbf{r}_i\cdot\mathbf{k}_j)v_{\mathbf{k}_j} \ (i = 1,\cdots,N; j = 1,\cdots,N), \quad (22)$$

$$(\phi_0)_{i+N,j} = \exp(i\mathbf{r}_i\cdot\mathbf{k}_j)u_{\mathbf{k}_j} \ (i = 1,\cdots,N; j = 1,\cdots,N). \quad (23)$$

In actual calculations the real representations are more convenient to evaluate the determinant where the elements of ϕ_0 are given by $\cos(\mathbf{r}_i\cdot\mathbf{k}_j)v_{\mathbf{k}_j}$ and $\sin(\mathbf{r}_i\cdot\mathbf{k}_j)v_{\mathbf{k}_j}$ for $i = 1,\cdots,N$, and $\cos(\mathbf{r}_i\cdot\mathbf{k}_j)u_{\mathbf{k}_j}$ and $\sin(\mathbf{r}_i\cdot\mathbf{k}_j)u_{\mathbf{k}_j}$ for $i = N+1,\cdots,2N$. $V(s,\alpha)$ is a diagonal $2N \times 2N$ matrix corresponding to $h(s)$:

$$V(s,\alpha) = \text{diag}(2as_1 - \alpha/2,\cdots,2as_N - \alpha/2, -2as_{N+1} + \alpha/2,\cdots,-2as_{2N} + \alpha/2). \quad (24)$$

diag$(a_1,\cdots)$ indicates a diagonal matrix with elements $a_1,\cdots$. Following the standard Monte Carlo method employed in Quantum Monte Carlo simulations, we can evaluate the expectation value for ψ_S. In order to consider the off-diagonal correlation factors, we evaluate the determinants given as

$$\langle\psi^{(m)}|\psi^{(m)}\rangle = \text{const.} \sum_{\{u_i^1\}\cdots\{u_i^m\}\{s_i^1\}\cdots\{s_i^m\}} \times \det(\phi^\dagger \exp(V(u^1,\alpha_1))\exp(-\lambda_1 K)\cdots\exp(-\lambda_1 K)\exp(V(s^1,\alpha_1))\phi_0), \quad (25)$$

where α_i and λ_i are variational parameters. K is a $2N \times 2N$ matrix corresponding to the kinetic part of the Hamiltonian, which is given by

$$K_{ij} = -t \quad (\text{if } (i,j) \text{ are nearest neighbor pairs } (i = 1,\cdots,N; j = 1,\cdots,N)), \quad (26)$$

$$K_{ij} = 0 \quad (\text{otherwise } (i = 1,\cdots,N; j = 1,\cdots,N)), \quad (27)$$

$$K_{i+N,j+N} = t \quad (\text{if } (i,j) \text{ are nearest neighbor pairs } (i = 1,\cdots,N; j = 1,\cdots,N)), \quad (28)$$

$$K_{i+N,j+N} = 0 \quad (\text{otherwise } (i = 1,\cdots,N; j = 1,\cdots,N)). \quad (29)$$

We optimize the ground state energy E_g with respect to g, Δ, μ, α_i and λ_i. It is of great help to employ the correlated measurements method in the process of searching optimum parameter values minimizing E_g.[23,24]

In one Monte Carlo step all the Hubbard-Stratonovich variables are updated once following the Metropolis algorithm. We perform several $5 \times 10^4 \sim 10^5$ Monte Carlo steps to evaluate the expectation values for optimum parameters.

III. Results of Monte Carlo calculations

A. Results for the Gutzwiller-BCS wave functions

The Gutzwiller-BCS wave function is investigated in this section. The 2D Hubbard model has been examined by many authors using the Gutzwiller-BCS function where the electron number is fixed.[5–7,25] Instead we show the Monte Carlo results using an algorithm without fixing the electron number since this algorithm can be applied to off-diagonal wave functions more easily. Two approaches should give the same results in the thermodynamic limit. On a finite lattice it is possibly expected that two algorithms give different results on a possibility of phase transition due to finite size effects. Thus an approach using an alternative algorithm works as a check of validity of the Gutzwiller-BCS wave function for the two-dimensional Hubbard model. Our purpose of this section is to show that both algorithms produce mostly the same results for the Gutzwiller-BCS wave function.

The Monte Carlo simulations are carried out on the square lattice with size 10×10. The parameters of the Hamiltonian are chosen as $t' = -0.09$ and $U = 8$ in units of t. The average number of electrons is given by $N_e = 80$. The energy gain due to pair condensations is maximum around the value of $t' = -0.1$.[7] We adjust the chemical potential in the wave function so that the expectation

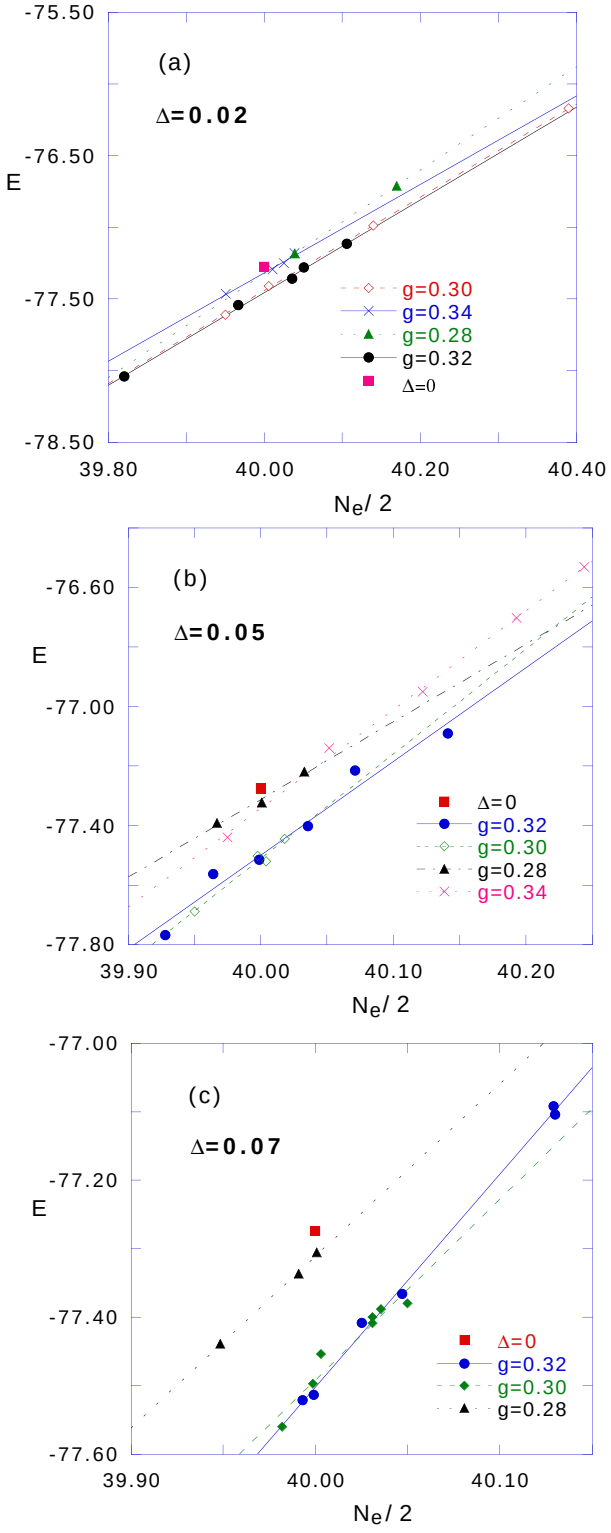

FIG. 1. Energy vs N_e for the BCS-Gutzwiller function for $\Delta = 0.02$ (a), 0.05 (b), and 0.07 (c).

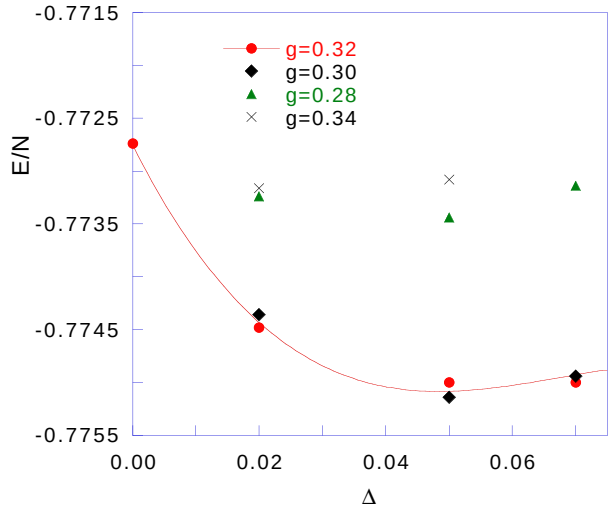

FIG. 2. Energy vs Δ for the BCS-Gutzwiller function.

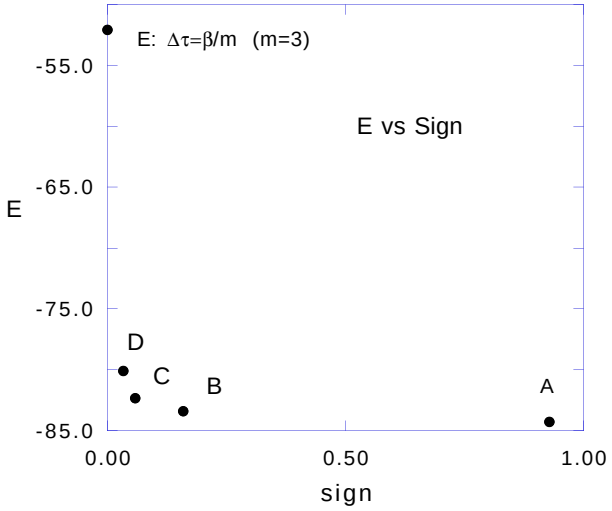

FIG. 3. The expectation value of sign $\langle s \rangle$ for several values of parameters λ and α. The parameters are the following. A: $g = 0.221$, $\lambda = 0.194$, $g' = 0.263$, $\lambda' = 0.138$, $g'' = 0.280$, $\lambda'' = 0.064$; B: $g = 0.1$, $\lambda = 0.2$, $g' = 0.15$, $\lambda' = 0.2$, $g'' = 0.2$, $\lambda'' = 0.1$; C: $g = 0.08$, $\lambda = 0.2$, $g' = 0.08$, $\lambda' = 0.2$, $g'' = 0.08$, $\lambda'' = 0.1$; D: $g = 0.08$, $\lambda = 0.25$, $g' = 0.08$, $\lambda' = 0.25$, $g'' = 0.08$, $\lambda'' = 0.25$; E: $g = 0.0695$, $\lambda = 0.333$, $g' = 0.0695$, $\lambda' = 0.333$, $g'' = 0.0695$, $\lambda'' = 0.333$ ($\Delta\tau = \beta/m$ ($\beta = 1$, $m = 3$)). The value for E is evaluated from an extrapolation.

value of the electron number equals N_e. We have applied the periodic and antiperiodic boundary conditions along the y and x directions, respectively, to avoid a situation where the gap function $\Delta_{\mathbf{k}}$ vanishes on the node. Since we have a constraint to fix the average electron number, there is one variational parameter in practice for the projected BCS wave function. It has been shown that the d-wave state is the most favorable one compared with s-wave and extended s-wave states.[7] Thus we show the results for the d-wave state: $\Delta_{\mathbf{k}} = \Delta(\cos k_x - \cos k_y)$.

We show the energy as a function of the average electron number for fixed g and Δ in Figs.1(a), (b) and (c). The average electron number decreases with an introduc-

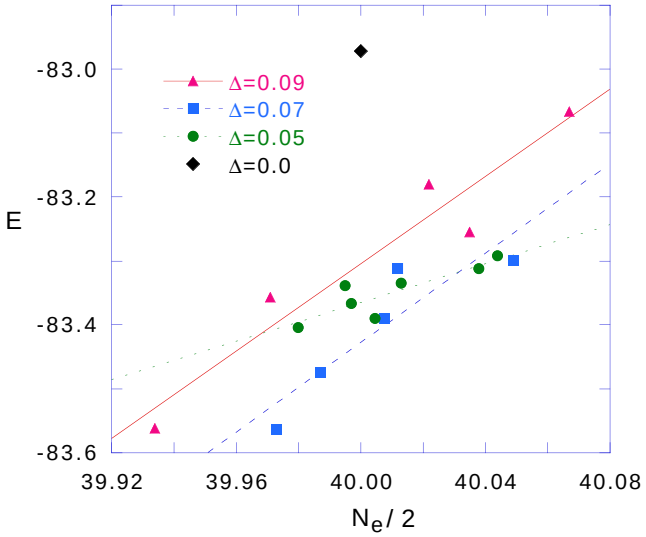

FIG. 4. The energy versus N_e for $\psi_S^{(1)}$. The values of Δ are shown in the figure.

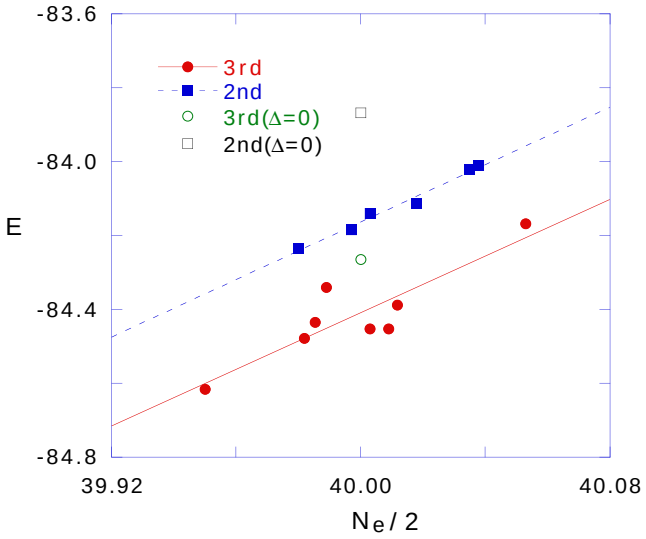

FIG. 5. Energy versus N_e for $\psi_S^{(2)}$ and $\psi_S^{(3)}$. $\Delta = 0.05$ for $\psi_S^{(2)}$ and $\Delta = 0.07$ for $\psi_S^{(3)}$.

tion of Δ if the chemical potential is fixed. In Fig.2 the energy is shown as a function of Δ for which the expectation value of the electron number is equal to $N_e = 80$. The figure clearly indicates that the energy has a minimum at a finite value of Δ. The behavior as a function of Δ is very similar to that obtained by the algorithm with fixed electron number. It is thus supported that the ground state is superconducting if calculations are based on the BCS-Gutzwiller function. The d-wave BCS state is stable for a negative value of t' around the value of -0.1 for the 10×10 square lattice. This value is highly dependent on the system size. Recent calculations for large N up to 22×22 for the BCS-Gutzwiller function[26] indicate that the superconducting condensation energy remains finite in the thermodynamic limit for restrict values of t' and electron density.

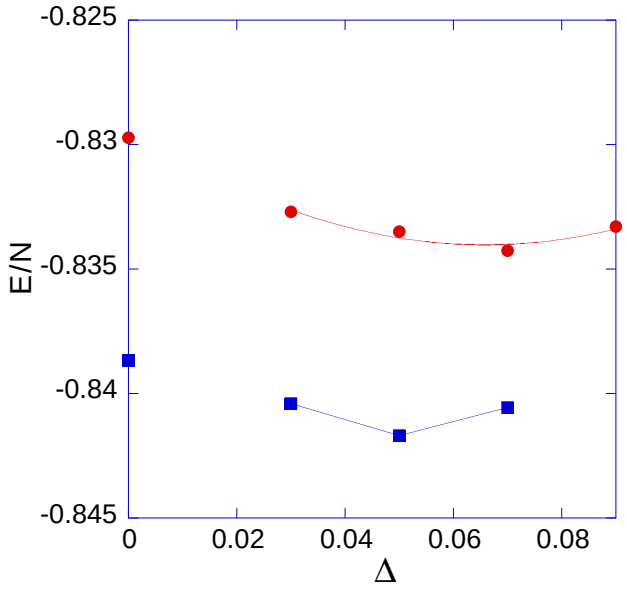

FIG. 6. Energy as a function of Δ for $\psi_S^{(1)}$ and $\psi_S^{(2)}$ from the top.

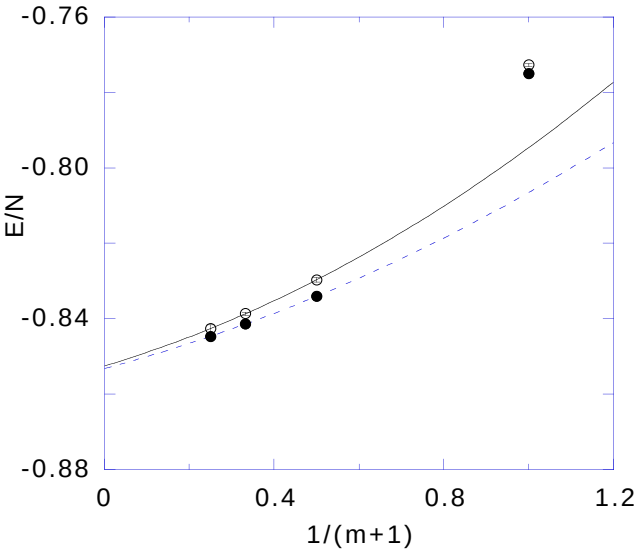

FIG. 7. Energy versus $1/(m+1)$. The upper and lower curves correspond to the normal and d-wave state, respectively.

B. Off-diagonal Gutzwiller wave functions

Now we turn to show Monte Carlo results for the BCS-Gutzwiller function with off-diagonal correlation factors. The wave functions which we consider here are given by eqs.(12)−(14). In the limit $\Delta \to 0$ they are reduced to off-diagonal Gutzwiller functions given as

$$\psi_G^{(1)} = \mathrm{e}^{-\lambda K} P_G \psi_F, \tag{30}$$

$$\psi_G^{(2)} = \mathrm{e}^{-\lambda' K} P_G \mathrm{e}^{-\lambda K} P_G \psi_F, \tag{31}$$

$$\psi_G^{(3)} = \mathrm{e}^{-\lambda'' K} P_G \mathrm{e}^{-\lambda' K} P_G \mathrm{e}^{-\lambda K} P_G \psi_F, \tag{32}$$

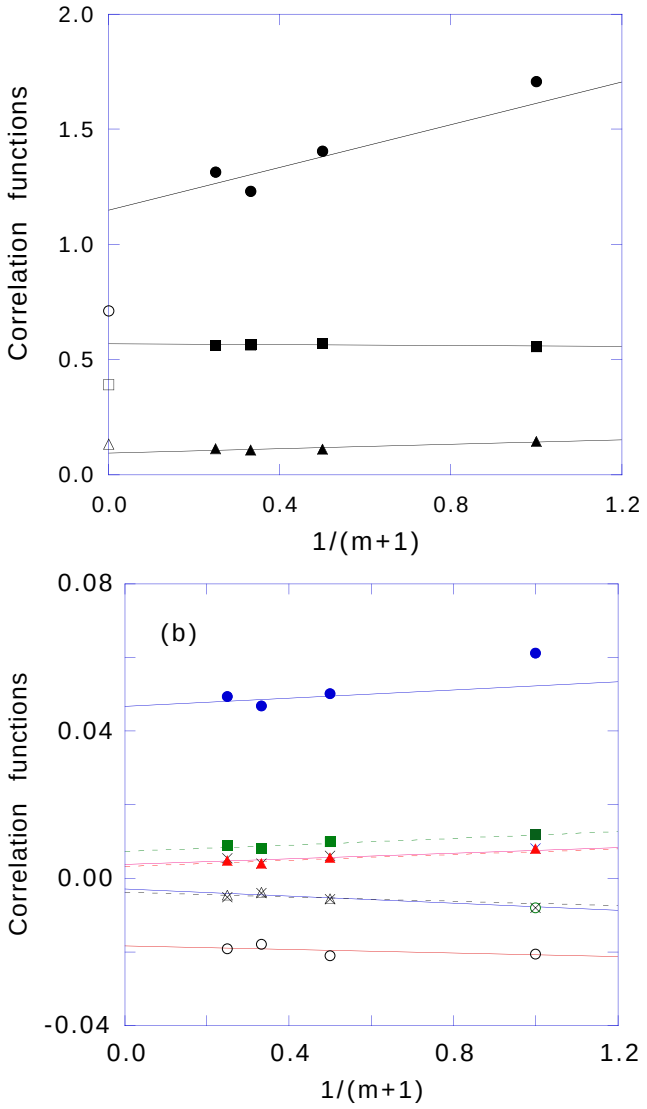

FIG. 8. Pair correlation functions versus $1/(m+1)$ for the ground state. In (a) from the top $\sum_\ell D_{yy}(\ell)$, $D_{yy}(\ell=0)$ and $D_{yy}(\ell=1)$ are shown. In (b) from the top $D_{yy}(\ell=2)$, $D_{yy}(\ell=3)$, $D_{yy}(\ell=4)$, $D_{yy}(\ell=5)$, $D_{yx}(\ell=5)$, $D_{yx}(\ell=3)$ and $D_{yx}(\ell=2)$. Symbols on the vertical axis indicate the values for $U=0$ where from the top $\sum_\ell D_{yy}(\ell)$, $D_{yy}(\ell=0)$ and $D_{yy}(\ell=1)$ are shown.

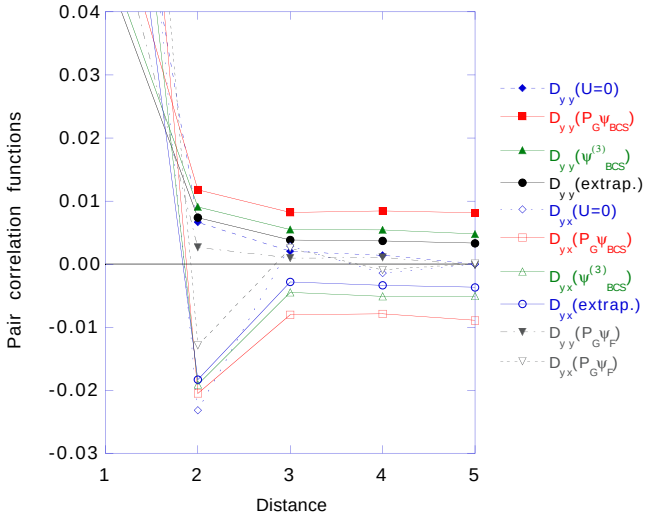

FIG. 9. Pair correlation functions D_{yy} and D_{yx} as a function of the distance. The extrapolated values are also shown by circles.

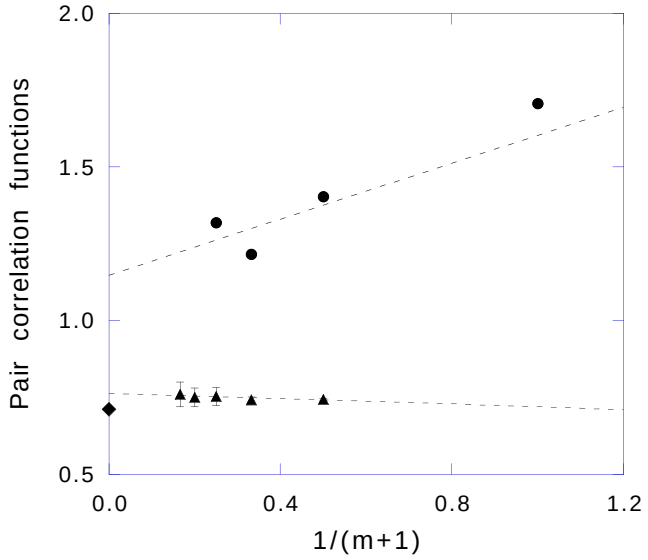

FIG. 10. Pair correlation functions $\sum_\ell D_{yy}(\ell)$ versus $1/(m+1)$. For circles an initial state is the d-wave BCS state, and for triangles an initial state is chosen as the normal state. The diamond indicates the value for $U=0$.

where ψ_F is the Fermi sea occupied by the conduction electrons up to the Fermi energy. If we can calculate the energies for $\psi_S^{(1)}$, $\psi_S^{(2)}$, $\cdots$, $\psi_S^{(m)}$,$\cdots$, we can estimate the correct ground state energy from an extrapolation with respect to $1/m$. This is also true for the wave functions $\psi_G^{(1)}$, $\psi_G^{(2)}$, $\cdots$. It will be shown that we obtain the same ground state energy for both the sequence of wave functions.

C. Negative signs for the off-diagonal correlation factors

Before going into the description of our results, we discuss a negative sign problem which is crucial for Quantum Monte Carlo simulations in many fermion systems. It is well known that a sign problem occurs in Quantum Monte Carlo simulations for the wave function

$$\psi_{QMC} = \mathrm{e}^{-\Delta\tau K}\mathrm{e}^{-\Delta\tau UV}\cdots\mathrm{e}^{-\Delta\tau K}\mathrm{e}^{-\Delta\tau UV}\psi_0, \quad (33)$$

where $\Delta\tau=\beta/m$. For our parameters ($t'=-0.09, U=8$ and $N_e=80$) a simulation with ψ_{QMC} suffers from a sign problem even for small m. In Fig.3 the sign $\langle s\rangle$ is shown for $m=3$: a comparison is made between ψ_{QMC} and $\psi_G^{(3)}$ where ψ_{QMC} is regarded as a special case with parameters $\lambda=\lambda'=\lambda''=\Delta\tau$ and $\alpha=\alpha'=\alpha''=\Delta\tau U$ for $\psi_G^{(3)}$. In this figure the sign versus energy is shown for several values of parameters. It is remarkable that the sign takes a finite definite value if the variational parameters are close to optimum parameters for $m=3$. The optimized

parameters produce no sign problem in our case. Thus if we consider $\psi^{(m)}$ (which is a generalization of ψ_{QMC}) the sign problem is reduced and the expectation values are evaluated definitely in simulations.

D. Results for the off-diagonal wave functions

In Fig.4 we show the energy versus N_e for $\psi_S^{(1)}$, where the d-type symmetry is assumed. Obviously the d-wave state has lower energy than that of the normal state. Similarly the energy as a function of N_e is shown for $\psi_S^{(2)}$ and $\psi_S^{(3)}$ in Fig.5. Then the energy as a function of Δ is in Fig.6. In Table I the variational parameters used in the simulation are presented. We show the energy versus $1/(m+1)$ in Fig.7 where dashed and solid curves correspond to the energies for $\psi_S^{(m)}$ and $\psi_G^{(m)}$, respectively. Both curves predict the same values in an extrapolation to the limit $m \to \infty$. The correlation functions of BCS pair operators were calculated for $\psi_S^{(m)}$ ($m = 1, 2$ and 3) in order to check the superconducting nature of the ground state. Pair correlation functions are defined as

$$D_{\alpha\beta}(\ell) = \langle \Delta_\alpha^\dagger(i+\ell)\Delta_\beta(i)\rangle, \tag{34}$$

where $\Delta_\alpha(i)$, $\alpha = x, y$, denote the annihilation operators of singlet electron pairs on nearest neighbor sites as:

$$\Delta_\alpha(i) = c_{i\downarrow}c_{i+\hat{\alpha}\uparrow} - c_{i\uparrow}c_{i+\hat{\alpha}\downarrow}, \tag{35}$$

where $\hat{\alpha}$ denotes a unit vector in $\alpha(= x, y)$ direction. The results for optimum parameters are shown in Figs.8(a) and 8(b) as a function of $1/(m+1)$. It is possible to extrapolate pair correlation functions to the limit $1/(m+1) \to 0$ by straight lines. The extrapolated values versus the distance ℓ are shown in Fig.9 with available data for $U = 0$ and BCS wave functions. The pair correlation functions are enhanced largely compared with the non-interacting ones showing a clear contrast to the normal state Gutzwiller function. Let us compare the expectation values of $\sum_\ell D_{yy}(\ell)$ for $\psi_S^{(m)}$ and $\psi_G^{(m)}$ in Fig.10. If we choose the normal state as an initial trial wave function, the superconducting correlation functions are enhanced only slightly for small m ($m = 1, \cdots, 5$). The large-m calculations are required to confirm the possibility of superconductivity. The convergence of the wave function is not so fast as compared with the convergence of energy.

IV. Summary

We have investigated the ground state property of the two-dimensional Hubbard model using the Gutzwiller and off-diagonal wave functions. The strong correlation among electrons are properly treated by the Monte Carlo method. In particular, the possibility of superconductivity was examined in connection to the oxide superconductors. The Monte Carlo simulations have been carried out on the square lattice with size 10×10 for $U = 8$, $t' = -0.09$ and $N_e = 80$. Monte Carlo calculations are not an easy task for this set of parameters since the sign problem inevitably occurs because of the small level spacings around the Fermi energy.

We have examined the d-wave states with multiplicative correlation factors. First we have examined the ground state using the Gutzwiller ansatz. The energy has a minimum for finite value of Δ implying a possibility of superconductivity. Second, the first order off-diagonal wave function is examined for which we have determined the optimum values of parameters. The ground state is again superconducting for the improved wave functions. The second and third order improved wave functions are also investigated to estimate the ground state energy. The minimum of the ground state is located at a finite value of Δ, which strongly suggests that the ground state is superconducting. The superconducting correlation functions are also evaluated for the ground state. We have extrapolated the expectation values to the limit of $m \to \infty$. The extrapolated values obviously indicates that the superconducting correlation functions are enhanced compared to the non-interacting case.

We have investigated a generalized version of the wave function employed in the standard Quantum Monte Carlo method. As is shown in the text the sign problem is softened for small m if we shift the values of parameters in exponentials. A direction along which the parameters are shifted from the QMC values β/m coincides with the direction to find a minimum of the ground state energy. If we can continue the evaluations for larger m, the ground state is tractable more correctly.

Our results indicate a possibility of superconductivity due to an electronic origin for the Hubbard model. The Hubbard model has been investigated intensively using the Gutzwiller ansatz. We believe it important to examine the ground state property employing improved wave functions. A comparison with other methods such as fixed-node or constrained path Monte Carlo methods should be made for larger systems as well as for smaller ones[17] in the region where the sign problem arises.

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TABLE I. Variational parameters used in the simulation for 10×10, $U = 8$ and $t' = -0.09$.

wave function	g	Δ	λ	g'	λ'	g''	λ''
$P_G\psi_{\rm BCS}$	0.32	0.05	–	–	–	–	–
$\psi^{(1)}_{BCS}$	0.074	0.07	0.092	–	–	–	–
$\psi^{(2)}_{BCS}$	0.13	0.05	0.17	0.24	0.065	–	–
$\psi^{(3)}_{BCS}$	0.22	0.07	0.20	0.26	0.14	0.28	0.0635

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