Phase Diagram and Pairing Symmetry of the Two-Dimensional t-J Model by a Variation Theory

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Two-dimensional $t$-J model is studied by a variational Monte Carlo method, using Gutzwiller-Jastrow-type wave functions. Various kinds of superconducting pairing symmetries are compared in order to determine the phase diagram of the ground state in the full $J/t$-$n$ plane. Near the half filling where the high temperature superconductivity is expected, the $d_{x^2-y^2}$ wave pairing state is always the most stable among various symmetries. The three-site term hardly changes the phase diagram in this regime. In the low electron density, the extended s-type wave becomes a quantitatively good state for large $J/t$ although the energy gain is small. The Gutzwiller wave function is shown to be the exact ground state in the low-electron-density limit for the supersymmetric case ($J/t = 2$).

KEYWORDS: high temperature superconductivity, t-J model, variation theory, pairing symmetry, three-site term, Monte Carlo method, phase diagram, Gutzwiller wave function, Gutzwiller approximation

§1. Introduction

Symmetry of Cooper pairs is considered as a key point to elucidate the mechanism of high-$T_c$ superconductivity. Many extensive experiments suggest that the unconventional $d_{x^2-y^2}$ anisotropic pairing is realized in high-$T_c$ oxides. Interesting phenomena due to this anisotropic pairing have been studied phenomenologically. Actually the two-dimensional (2D) $t$-$J$ model, which is considered as an effective Hamiltonian for the high-$T_c$ oxides, will probably have a ground-state with the $d_{x^2-y^2}$-wave pairing state for the reasonable parameters.

The 2D $t$-$J$ model is derived by regarding a singlet between the Cu spin and the hole’s spin on the neighboring O sites (Zhang-Rice singlet) as a mobile vacancy in the Heisenberg spin system. Different approaches, such as mean-field theories, $\omega$-variational studies, and exact diagonalization methods, support the $d_{x^2-y^2}$-wave pairing near half filling and for $J/t \sim 0.4$.

In this paper we study more extensively various pairing states in the whole parameter space ($J/t$ and electron density $n$) using a variational Monte Carlo method, and determine the phase diagram of the ground state.

It seems natural that the strong on-site repulsion between up-spin and down-spin electrons favors the anisotropic $d_{x^2-y^2}$-wave pairing. However, it is not at all apparent why, for example, the extended $s$-wave pairing state, which does not have the on-site pairing amplitude either, is not realized.

Furthermore, many discussions on the $d_{x^2-y^2}$-wave pairing have been limited to the low doping regime (near the half filling) and to small values of $J/t$. If we consider the wider range of parameter space, it is necessary to clarify the region where the $d_{x^2-y^2}$-wave is stable. For example, in the low-electron-density side a metallic state is expected, while in the large-$J/t$ region a phase separation is predicted. The relation between the phase separation and the $d_{x^2-y^2}$-wave state is not so clear. Actually from the phase diagram of the one-dimensional (1D) $t$-$J$ model, we expect that the superconducting state is next to the phase separation. But even if this is the case in 2D, we have to clarify the pairing symmetry of the neighboring superconducting state.

Meanwhile, in the low-electron densities, there may be a region where the $s$-wave pairing becomes stable. The two-electron problem is analytically solved to show a stable $s$-wave bound state for $J/t \geq 2$. This suggests that the extended $s$-wave pairing state is favorable for $J/t \geq 2$ in the low-density region. Actually in the 1D $t$-$J$ model, such a state was expected. For finite electron densities in the 2D case, we have to check this possibility. It is far from clear how this $s$-wave state relates to the $d_{x^2-y^2}$-wave state as well as to the phase separation.

For the supersymmetric case ($J/t = 2$), or on the edge of this extended $s$-wave region, we expect that the Gutzwiller wave function (GWF) becomes the exact ground state for $n \to 0$. This fact was predicted before in connection with the 1D $t$-$J$ model. It is very interesting to clarify the role of the GWF in the phase diagram.

With these aspects in mind, we focus on the following points in this paper. (1) How and why is the $d_{x^2-y^2}$-wave pairing stabilized, but not the other pairing states for the high-$T_c$ parameters? (2) The ranges of the stable $d_{x^2-y^2}$-wave state as well as other ones. Namely is there any possibility for the other pairing state to be realized in the phase diagram? (3) How large is the region

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where the phase separation takes place? (4) Is there any region where the extended s-wave state is stable in the low-electron density? (5) How are the variational states connected to the states in the low electron density limit and what happens at the supersymmetric case ($J/t = 2$)? (6) How does the three-site term affect the above results?

In order to study these questions on the phase diagram, we use the variational Monte Carlo (VMC) method. So far, the exact treatments like the quantum Monte Carlo methods have been often useless for the 2D $t$-$J$ model because of the minus sign problem. On the other hand, the present VMC method is free from such an obstacle and treats exactly the constraint of no doubly occupied sites. Accurate estimates of the expectation values are possible, which are indispensable to take advantage of merits of the variation theory.

As variational wave functions for superconductivity, we use Gutzwiller-projected BCS functions which were originally proposed by Anderson as a resonating valence bond state. It has been shown that the $d_{x^2-y^2}$-wave pairing state is the best variational state among Gutzwiller-projected BCS states near half filling. In this paper, we extend previous works to include a variety of pairing symmetries in the full parameter space of the 2D $t$-$J$ model with the three-site term. We construct a phase diagram of the ground state within the Gutzwiller-Jastrow-type wave functions. As will be seen later, the resultant 2D phase diagram shares some features with the 1D phase diagram.

The mean-field theories are sometimes useful to predict the behaviors of the system qualitatively. However, they treat the constraint of no double occupancy approximately. We are going to compare the obtained phase diagram with that predicted in the mean-field theories with the Gutzwiller approximation. It is found that a qualitatively correct phase diagram is obtained, but quantitatively we need some modifications for the Gutzwiller approximation.

The outline of this paper is as follows: In §2 we explain the model Hamiltonian and the variational wave functions. In §3 the relation between our variational states and the slave-boson mean-field theory is mentioned. Section 4 is devoted to the discussion on the metallic, magnetic and superconducting states for the high-electron-density or low-doping regime. We study the properties of the stable $d_{x^2-y^2}$-wave state and search for the origin of its stability in terms of the resonating valence bond theory. In §5 a phase diagram is constructed in the full $J/t$-$n$ plane, and properties of wave functions are described in the low electron density. We summarize in §6. In Appendix A the energy of the Hubbard model is shown for a comparison in §4.1. The brief summary of the Gutzwiller approximation is given in Appendix A.

A part of the present results was published before.

§2. Model and Trial Wave Functions

We consider the $t$-$J$ model defined in the Hilbert space without double occupancy of electrons. In this paper we include the so-called “three-site term” or “pair-hopping term”, $\mathcal{H}_3$, which is usually neglected but is present in the effective Hamiltonian derived from the Hubbard model. Thus our model is written as

$$\mathcal{H} = \mathcal{H}_t + \mathcal{H}_J + \mathcal{H}_3,$$

$$\mathcal{H}_t = -t \sum_{\langle i,j \rangle} (c_{i\sigma}^+ c_{j\sigma} + c_{j\sigma}^+ c_{i\sigma}),$$

$$\mathcal{H}_J = J \sum_{\langle i,j \rangle} \left( S_i \cdot S_j - \frac{1}{4} n_i n_j \right),$$

$$\mathcal{H}_3 = -\frac{J^{(3)}}{4} \sum_{j,\tau \neq \tau'} c_{j,-\sigma}^+ c_{j,-\sigma} c_{j+\tau,\sigma}^+ c_{j+\tau',\sigma},$$

where $(i, j)$ represents the sum over the nearest-neighbor pairs. $\tau$ and $\tau'$ run as vectors pointing to the nearest-neighbor sites. We take $t$ as the energy unit in the following. This model has four parameters: $J/t$, $J^{(3)}/J$, electron density $n = N/N_a$ and magnetization $m = (N_u - N_d)/N_a$, where $N (= N_d + N_u)$ is the total electron number, $N_a$ the number of sites and $N_o$ the number of electrons with spin $\sigma$. We study mostly the nonmagnetic case ($m = 0$).

The three-site term, $\mathcal{H}_3$, shows up in the effective Hamiltonian of the Hubbard model in the strong coupling regime ($U \gg t$) in this case $J^{(3)}$ is equal to $4t^2/U (= J)$. For the electron-doped high-$T_c$ cuprate (Nd system), the doped electrons directly enter the Cu orbitals, so that the Hubbard model becomes an adequate model, and thus we should assume $J^{(3)} = J$.

On the other hand, if the effective Hamiltonian is derived from a hole-doped CuO$_2$ model including Cu $d_{x^2-y^2}$ and O 2$p$ orbitals, $J^{(3)}$ could be negative. Therefore in this paper we use $J^{(3)}$ as a parameter and discuss its effect on the phase diagram.

For this Hamiltonian, we study Gutzwiller-Jastrow-type variational wave functions defined as:

$$\Psi = \prod_{j,\ell} \prod_{\sigma \sigma'} \left[ 1 - \eta(r_{j\ell}) \right] n_{j\sigma} n_{\ell\sigma'},$$

with $r_{j\ell} = |r_j - r_{\ell}|$. The function $\Phi$ is a one-body mean-field-type wave function; we consider (1) a simple Fermi sea $\Phi_F$ as a metallic state, (2) a Hartree-Fock antiferromagnetic (AF) function for the AF ordered state, and (3) a BCS wave function with various pairing symmetries. So far these types of wave functions have been widely used for the small-doping region. In this paper, we study these states in the whole parameter regime.

The AF state is defined as:

$$\Phi_{AF} = \prod_{k,\sigma} \left[ \hat{u}_k c_{k\sigma}^+ + \text{sgn}(\sigma) \hat{v}_k c_{k+K\sigma}^+ \right] |0\rangle,$$

with

$$\hat{u}_k = \frac{1}{2} \left[ 1 - \frac{\varepsilon_k}{\sqrt{\varepsilon_k^2 + \Delta_{AF}^2}} \right]^{1/2},$$

where $\varepsilon_k$ and $\Delta_{AF}$ are the single-particle energy and the AF gap parameter, respectively.
\[ \tilde{v}_k = \left[ \frac{1}{2} \left( 1 + \frac{\varepsilon_k}{\sqrt{\varepsilon_k^2 + \Delta_{AF}^2}} \right) \right]^{1/2}. \]

Here, sgn(\(\sigma\)) takes either +1 or −1 according as \(\sigma = \uparrow\) or \(\downarrow\); \(\varepsilon_k = -2t(\cos k_x + \cos k_y)\) and the wave vector \(K = (\pi, \pi)\) represents the AF reciprocal lattice vector. \(\Delta_{AF}\) is an AF variational parameter; \(\Phi_{AF}\) is reduced to the simple Fermi sea \(\Phi_F\) as \(\Delta_{AF} \to 0\).

The BCS wave function is given as:

\[ \Phi_{SC} = \prod_k \left[ u_k + v_k c_{k\uparrow}^\dagger c_{-k\downarrow} \right] |0\rangle, \tag{2.7} \]

with

\[ a_k = \frac{\Delta k}{\varepsilon_k - \mu + \sqrt{(\varepsilon_k - \mu)^2 + \Delta_k^2}}. \tag{2.8} \]

For most cases we take \(\mu\) as the chemical potential for the noninteracting system, \(\mu_0\). However the optimal value of \(\mu\) ought to change due to the correlation. We will check the \(\mu\) dependence of the variational energy in §4.3.

The pairing symmetry of \(\Delta_k\) is chosen as follows:

\[ \Delta_k = \begin{cases} \Delta_k \sin k_x \sin k_y & \text{(i) s wave} \\ \Delta_k (\cos k_x + C \cos k_y) & \text{(ii) } d_{xy} \text{ wave} \\ \Delta_k (\cos k_x + e^{i\theta} \cos k_y) & \text{(iii) s+d wave} \\ \Delta_k (\cos k_x + e^{i\theta} \cos k_y) & \text{(iv) s+id wave}, \end{cases} \tag{2.9} \]

In each case \(\Delta \geq 0\) is a variational parameter and when \(\Delta = 0\), \(\Phi_{SC}\) is reduced to the simple Fermi sea, \(\Phi_F\). Note here that the expectation value of the order parameter \(\langle c_{k\uparrow}^\dagger c_{-k\downarrow} \rangle = \Delta_{SC}\) is not necessarily equal to \(\Delta\). \(\Delta_{SC}\) is to be calculated as an expectation value in the variational state. Actually \(\Delta_{SC}\) is largely reduced from \(\Delta\) near the half filling due to the strong electron correlation.

By changing the value of \(C\) (\(-1 \leq C \leq 1\)) and \(\theta\) (\(0 \leq \theta \leq \pi\)) in the cases (iii) and (iv), various symmetries are continuously realized. For example, \(\Delta_k\) of the case (iii) is rewritten as:

\[ \Delta_k = \Delta_s (\cos k_x + \cos k_y) + \Delta_d (\cos k_x - \cos k_y), \tag{2.10} \]

with \(\Delta_s = \Delta(1 + C)/2\) and \(\Delta_d = \Delta(1 - C)/2\). Thus the state with \(C = -1\) represents the pure \(d_{xy}\) symmetry, the state with \(C = 0\) s+d state, and the state with \(C = 1\) the pure extended s state, respectively. For the case \(-1 < C < 1\), the wave function has different gap amplitudes in the directions of \(x\) and \(y\) axes, which conflicts with the symmetry of the lattice. On the other hand, \(\Delta_k\) of the state (iv) represents a complex mixture of the \(d_{xy}\) and extended s states. Especially at \(\theta = \pi/2\), \(\Delta_k\) is the so-called s+id state.

Many-body effects are introduced into eq. (2.5) by a two-body Jastrow correlation factor

\[ \mathcal{P} = \prod_{j,k} \prod_{\sigma \sigma'} \left[ 1 - \left( \eta(\tau_{jk}) \right) n_{j\sigma} n_{k\sigma'} \right]. \tag{2.11} \]

This factor reduces the amplitude of the wave function according to the charge configuration. By requiring \(\eta(0) = 0\), the local constraint of the prohibition of double occupancy (Gutzwiller projection) is strictly satisfied. For \(r \neq 0\), we consider two cases: (a) \(\eta(r) = 1\), which is nothing but the Gutzwiller projection \(\mathcal{P}_d = \prod_{k=0}^{N_b} \left[ 1 - \left\{ \eta(r_{jk}) \right\} n_{j\sigma} n_{k\sigma'} \right] |0\rangle\) and (b) an intersite correlation factor,

\[ \eta(r) = \left[ \frac{L}{\pi} \sqrt{\sin^2 \left( \frac{\pi x}{L} \right) + \sin^2 \left( \frac{\pi y}{L} \right)} \right]^{\nu}. \tag{2.12} \]

Here \(L\) is the linear dimension of the lattice: \(N_a = L \times L\). We abbreviate this correlation factor as \(\mathcal{P}_{\text{TLL}}\). It works as repulsive Jastrow correlation for \(\nu > 0\) and attractive one for \(\nu < 0\), and is reduced to \(\mathcal{P}_d\) for \(\nu = 0\). This factor is a Tomonaga-Luttinger-liquid (TLL) type and has been investigated in detail for the 1D systems and the 2D systems. Here we choose this form only for its simplicity as an intersite factor. Alternatively one can use a short-range correlation factor but the difference of the optimized variational energy between the two choices is negligibly small.

§3. Relation between Variation Theory and Slave-Boson Mean-Field Approximation

The phase diagram and physical properties of the 2D \(t-J\) model were extensively studied in the slave-boson mean-field approximation. Thus it is important to clarify the relation to the present variation theory. In the slave-boson mean-field approximation, the electron operator at site \(i\) and spin \(\sigma\) is decoupled as

\[ c_{i,\sigma} = b_{i,\sigma} f_{i,\sigma}, \tag{3.1} \]

where \(b_{i,\sigma}\) is a slave-boson operator which represents the vacant site (holon), and \(f_{i,\sigma}\) is a fermion (spinon) operator.

The mean-field approximation using this slave-boson representation gives a d-wave pairing state as the ground state near half filling. In this state, the fermion (spinon) degrees of freedom have a BCS order parameter

\[ \langle f_{i,\uparrow}^\dagger f_{i+\pi,\downarrow} \rangle = -\langle f_{i,\uparrow}^\dagger f_{i+\pi,\downarrow} \rangle, \tag{3.2} \]

and its wave function is the same with eq. (2.7).

On the other hand, the slave bosons are assumed to form a boson condensate. Since the slave bosons have hard-core nature or two bosons cannot occupy the same site, it is not clear whether the bosons really form a boson condensate in the two (or quasi-two) dimensional systems. In the slave-boson mean-field approximation, however, the hard-core nature is neglected and thus the ground-state for the bosons is written as

\[ \langle b_{k=0}^\dagger \rangle^{N_b} |0\rangle, \tag{3.3} \]

where \(N_b\) is the number of holes.

We can take account of the hard-core nature by using a Gutzwiller projection operator for bosons

\[ \mathcal{P}_d(b_{k=0}^\dagger)^{N_b} |0\rangle, \tag{3.4} \]

instead of (3.3). Even in this case, the wave-function amplitude for the slave boson is equal to 1 for any boson configurations.

The electronic wave-function in the slave-boson scheme is the product of the fermion and boson wave functions. Therefore the ground-state obtained in the slave-boson mean-field theory is equal to eq. (2.7); our variational calculations take full account of the effect of
the Gutzwiller projection. The VMC method enables us to estimate accurate expectation values even in the presence of the Gutzwiller projection. We use square lattices with $L = 10-26$ for the metallic states and $L = 10-20$ for the ordered states; mainly the system with $L = 10$ is used for $\Psi_{SC}$, because the size dependence is negligible for $L \geq 10$ as far as energy is concerned. The periodic($x$)-antiperiodic($y$) boundary conditions are used and $N_{\sigma}$ is chosen so as to satisfy the closed-shell condition. To suppress statistical errors, we take sufficient sample numbers ($3 \times 10^{5} - 2 \times 10^{6}$) and Metropolis trials (50 at maximum for each electron) between the samplings.

To treat the coherent states for the superconductivity, two VMC schemes have been applied: one by using the grand canonical scheme and one by fixing the electron number. The results of the two methods ought to coincide in the thermodynamic limit. The former scheme has a merit in calculating the order parameter directly, but it needs much longer CPU time. In this work we adopt the latter scheme.

§4. Pairing Symmetry in Low-Doping Regime

In this section we study the region of high electron density or low doping, laying emphasis on the stable pairing symmetry of superconductivity. In §4.1 we study metallic states as a starting point, since the other states with AF order or superconducting order parameter reduces to the GWF when the order parameter vanishes. The energy gain due to the occurrence of the order is discussed in comparison with the variational energy of the GWF. The instability of metallic states against the phase separation and the effect of the Jastrow correlation factor are described. Next we investigate various pairing states for the half-filled case in §4.2 and for less-than-half-filled cases in §4.3. We show that the ordered states are free from the instability against the phase separation for a small value of $J/t$. Finally in §4.4 we look at the properties of the stable $d_{x^2-y^2}$-wave state.

4.1 Metallic states

First, we consider the GWF, $\Psi_{G} = \mathcal{P}_{G}\Phi_{F}$, as a metallic state. In Fig. 1 three energy components: transfer energy $E_{t} = \langle H_{t} \rangle$, exchange energy $E_{J} = \langle H_{J} \rangle$ and the three-site contribution $E_{3} = \langle H_{3} \rangle$ are plotted as a function of $n$; size dependence is almost negligible in this scale.

Near the half filling, $E_{J}$ is upward convex. This means that when $J/t \to \infty$ the system must have a phase separation. In order to study this kind of phase separation in the small-$J/t$ region, it is necessary to study the $n$ dependence of variational energies more carefully. Figure 2 shows the close-up of this dependence near the half filling. On one hand, $E_{t}/t$ and $E_{3}/J$ are linear with respect to $\delta \equiv 1 - n$; on the other hand, $E_{J}/J$ does not behave linearly but

$$E_{J}/J = E_{J}(\delta = 0)/J + \text{const.} \times \delta^{0.7}, \quad (4.1)$$

for wide range of $n$. This $\delta$-dependence means that the total energy $E = E_{t} + E_{J} + E_{3}$ is always upward convex for any non-zero value of $J/t$. Thus the GWF is unstable in itself against the phase separation.

As shown in Appendix A, this is in sharp contrast with the GWF in the Hubbard model, for which both $E_{t}/t$ and $E_{J}/U$ are proportional to $\delta$ as $\delta \to 0$. The total energy is always downward convex, leading to no phase separation. This indicates that as long as the 2D GWF is concerned, the $t$-$J$ model for $J/t > 0$ is not connected to the Hubbard model near the half filling.

We study this instability also for the TLL-type function $\Psi_{TLL} = \mathcal{P}_{TLL}\Phi_{F}$, which Valenti and Gros studied. The results are summarized in Table I, indicated as TLL. As $n \to 1$ (i.e. $\delta \to 0$), intersite correlation factors generally become less effective, so that the occurrence of the phase separation near the half filling is not affected even by this intersite correlation factor. Namely, as far as a form of $\mathcal{P}\Phi_{F}$ is assumed, the instability against the phase separation is inevitable. Later when we study the projected BCS state, this phase separation is removed.

4.2 Half-Filled Case

First, let us look at the results for the half filling. Figure 3 shows the variational energy for the the case (iii) in eq. (2.9) for various values of $C$. For the $d_{x^2-y^2}$-wave case ($C = -1.0$), $E_{J}/J$ is symmetric with respect to $\Delta/t = 2$ and thus has two minima at $\Delta/t \sim 0.57$ and 7. (This fact was not discussed in the previous VMC calculations.) As the parameter $C$ increases, the minimal value monotonically increases, as seen in the inset, where the scale is expanded. Thus the $d_{x^2-y^2}$ wave has the lowest energy in the class of variational states (iii). For the extended s wave ($C = 1.0$) where there is no dependence on $\Delta$ of the variational energy. This is because $\mu = 0$ at half filling and thus $\delta k_{F}$ becomes a constant, which means that $\Psi_{SC}$ is equivalent to $\Psi_{G}$.

In Fig. 4 we show the variational energy for the $s+id$-wave function (iv) in eq. (2.9). As in the inset the energy minima for $\pi/2 \leq \theta \leq \pi$ are degenerate within the error bars. This degeneracy is due to the SU(2) symmetry of the Heisenberg model; it was proved that under the Gutzwiller projection the state with $\pi/2 \leq \theta \leq \pi$ are all the same state.

These VMC calculations for the projected BCS-type wave functions $\Psi_{SC}$ are consistent with the slave-boson mean-field theory. However, the actual ground state at half filling should be an AF magnetically ordered state. In fact, $\Psi_{AF} = \mathcal{P}_{AF}\Phi_{AF}$ is slightly stabler than $\Psi_{SC}$ and the best variational state among the present states. This feature is in contrast with 1D systems, where ordered states—AF and $s$-type superconducting—have higher energies than the GWF. The expectation values of $(\mathbf{S}_{i} \cdot \mathbf{S}_{j})$ for the nearest-neighbor $i$ and $j$ are $-0.3206$ for $\Psi_{AF}$ and $-0.3199$ for the $d_{x^2-y^2}$ or the $s+id$ state, which are close to the best estimation $-0.3346$.

4.3 Symmetry of Cooper pairs in less-than-half-filling

Now, we consider less-than-half-filled cases. We concentrate on the $s+id$-type wave function, (iv) of eq. (2.9), which contains the $d_{x^2-y^2}$ and extended $s$-wave states.
All the other states give higher energy than the $s+i\!d$-type state. For example, the $s+i\!d$-type-wave states (iii) in eq. (2.9) with $-1 < C < 1$ always give higher variational energy as in the half-filled case. As for the $d_{xy}$ wave state (ii), we find that each energy component is a monotonically increasing function of $\Delta/t$ for every electron density. Thus there is no chance for the $d_{xy}$ wave to be stabilized. The behavior of the conventional s-wave state (i) is very similar to the extended s wave in the high density regime; the energy is always higher than the $d_{x^2-y^2}$ wave for small $\delta$.

Let us return to the $s+i\!d$-type state. Figures 5(a)-(c) show the energy components of the $s+i\!d$-type wave function. As a typical electron density, we use $\delta = 0.12$ ($n = 0.88$). The $d_{x^2-y^2}$ wave ($\theta = \pi$) is the most favorable except the three-site term. Thus, when there is no three-site term ($J^{(3)} = 0$), the $d_{x^2-y^2}$-wave state has always the lowest variational energy $\Psi_0$. As an example, we show in Fig. 6 the total energy $E/t$ for $J/t = 0.25$ and several values of $\theta$. The situation does not change for $J/t \leq 2.0$.

Here we mention the effect of the three-site term $H_3$. The variational energy for the extended s wave is lowered in the presence of $H_3$. We have found, however, that the most stable state is still the $d_{x^2-y^2}$ wave, even when the value of $J^{(3)}/J$ is as large as 1.0. On the contrary, the $d_{x^2-y^2}$ wave is further stabilized in the ferromagnetic case ($J^{(3)} < 0$). The situation does not change for any value of $J/t$ and for electron densities $n = 0.52-0.96$.

Figure 7 shows the optimal variational energy for the $d_{x^2-y^2}$-wave state for $n \sim 1$ and $J/t = 0.5$. In comparison with the metallic GWF, there is a definite energy gain due to the superconducting order parameter. In Fig. 7 we also plot the data of the AF state, $\Psi_{AF} = P_d \Phi_{AF}$ and the $\pi$-flux state. Just at half filling $\Psi_{AF}$ is slightly lower than the $d_{x^2-y^2}$-wave state. However even at $\delta = 0.02$ the $d_{x^2-y^2}$-wave state has a lower energy, so that the AF state disappears immediately when holes are doped in the 2D Heisenberg system.

The $\pi$-flux state, which is equivalent to the $s+i\!d$ state at half filling, has exactly the same energy with the $d_{x^2-y^2}$-wave state for $n = 1$. For the doped case, however, the $\pi$-flux state has much higher variational energy than the $d_{x^2-y^2}$ wave. It is even higher than the AF state. Therefore it is not likely that the $d_{x^2-y^2}$-wave state is mixed with the $\pi$-flux state.

Finally, we refer to the $\mu$ dependence of the energy. We calculate the total energy for some $J/t$ by varying the value of $\mu$ in eq. (2.8). The smaller $J/t$ is, the more weakly $E/t$ depends on $\mu$. As an example, the result for $J/t = 0.5$ is plotted in Fig. 8, where $\Delta_{opt}/t \sim 0.55$. The energy improvement by optimal $\mu$ upon the value for $\mu_0$ is slight. Thus the use of the noninteracting value $\mu_0$ is justified for small $J/t$ to some extent. Therefore, we include each energy component for some variational states; the optimal functions are used for the TLL, AF and $d_{x^2-y^2}$-wave states. The differences from the GWF value are shown.

First of all, we notice that the metallic state with Jastrow correlation (indicated as TLL) has slightly lower kinetic energy ($< 1\%$) than the GWF. This is because the Jastrow (repulsive) correlation factor tends to separate the electrons so as to gain the kinetic energy. However, its gain is so small that TLL state cannot overcome the $d_{x^2-y^2}$-wave state.

In contrast to this, the other ordered states (AF, d, s+i\!d state) unanimously gain the exchange energy, namely $\langle S_i \cdot S_j \rangle$ and $-\Delta n_i n_j/4$, but all of them lose the kinetic energy. As the doping increases the energy gain for the exchange term becomes smaller and smaller. Finally, at some doping, the energy gain due to the AF order or superconducting order vanishes. This tendency gives the $n$-dependences of the variational energy shown in Fig. 7.

Comparing the $d_{x^2-y^2}$-wave with the AF states, we can see that the loss of the kinetic energy is always smaller than that for the AF state, while the gain of the exchange energy is larger for the $d_{x^2-y^2}$ wave for every electron density. This makes the $d_{x^2-y^2}$ state the best variational state.

In Table I, we also include the energy components for the $s+i\!d$ and extended s states. For comparison we borrow the same value of $\Delta/t$ with the optimal $d_{x^2-y^2}$ case, namely $\Delta/t = 0.7, 0.55, 0.40,$ and $0.25$ for $n = 0.96, 0.88, 0.80,$ and $0.72,$ respectively. As for the exchange term $\langle S_i \cdot S_j \rangle$, the $d_{x^2-y^2}$-wave state has a large exchange energy. For example at $n = 0.88$ ($\delta = 0.12$) it gains 29% of the exchange term of the GWF. The s+i\!d-wave also gains the exchange term similar to the $d_{x^2-y^2}$ wave, but its magnitude is slightly smaller. For the extended s wave the energy gain is very small. This is the reason why the $d_{x^2-y^2}$-wave state is favored by the exchange term $J$. We discuss this phenomena in terms of the resonating valence bond (RVB) representation of the wave functions.

Equation (2.7) can be rewritten as

$$\Psi_{SC} = P_d \prod_k a_k \exp \left[ \sum_{i,j} a_{i,j} c_{i,j}^\dagger c_{i,j}^\dagger \right] |0\rangle, \quad (4.2)$$

where $a_{i,j}$ is Fourier transform of $a_k$. If we fix the electron number by projecting out the $N$ electron states, we obtain

$$P_N \Psi_{SC} = P_d \prod_k a_k \frac{1}{(2\pi)^N} \left[ \sum_{i,j} a_{i,j} c_{i,j}^\dagger c_{i,j} \right]^N |0\rangle. \quad (4.3)$$

This form of the wave function is the superposition of various RVB configurations. Each valence bond (VB) is represented by $c_{i,j} c_{i,j}^\dagger$, whose amplitude is $a_{i,j}$.

By investigating the actual form of $a_{i,j}$ from the definition in eq. (2.8) for various symmetries, we can see the difference between the $d_{x^2-y^2}$ wave and s+i\!d, or extended s wave. The main difference is that, among the dominant $a_{i,j}$’s, the next-nearest neighbor bond exactly
vanishes for the $d_{x^2−y^2}$ state, i.e.
\[ a_{i,i+x+y} = \sum_k \cos(k_x + k_y) \frac{\Delta_k}{\varepsilon_k - \mu + \sqrt{(\varepsilon_k - \mu)^2 + \Delta_k^2}} = 0, \]  
(4.4)

because of the antisymmetric nature for exchanging $k_x$ and $k_y$. On the other hand, for the $s$-id and extended $s$ cases, $a_{i,i+x+y}$ has a comparable amplitude with the nearest-neighbor $a_{i,i+x}$ or $a_{i,i+y}$.

Due to this main difference, the RVB amplitude for the nearest-neighbor bond for the $d_{x^2−y^2}$ state is more enhanced than the $s$-id or extended $s$ state. As a result, the $d_{x^2−y^2}$-wave state is the most favorable for the exchange energy. (Reversely we can say that the next-nearest-neighbor exchange energy favors the extended $s$-wave state.) To see this more closely, the spin structure factor,
\[ S(q) = \frac{1}{N_a} \sum_{j,k} 4 \langle S_j^z S_k^z \rangle e^{i(q_j - q_k)}, \]  
(4.5)
is compared in Fig. 9 for the optimized $d_{x^2−y^2}$ wave and extended $s$ wave. The antiferromagnetic correlation is enhanced for the $d_{x^2−y^2}$ wave, which leads to the gain in the exchange energy.

Next we consider the difference in the kinetic energy in Table I. The ordered states always lose the kinetic energy compared with the GWF. Without taking account of the Gutzwiller projection, we can estimate
\[ \langle c_{i,\uparrow}^\dagger c_{j,\uparrow} \rangle = \frac{1}{N_a} \sum_k e^{-i k(r_i - r_j)} |v_k|^2 = \frac{1}{4N_a} \sum_k \frac{\epsilon_k - \mu}{E_k} (\cos k_x + \cos k_y). \]  
(4.6)

In the case of $\Delta = 0$, $(\epsilon_k - \mu)/E_k = \text{sign}(\epsilon_k - \mu)$, but in the presence of $\Delta$, the amplitude of $\langle c_{i,\uparrow}^\dagger c_{j,\uparrow} \rangle$ generally reduces. This causes the loss of the kinetic energy for the ordered state. Since there is a zero point at $k_x = \pm k_y$ on the Fermi surface for the $d_{x^2−y^2}$-wave state, the loss is the least among the superconducting states. This fact also favors the $d_{x^2−y^2}$ symmetry.

Finally we discuss the $\langle \bar{n}_i n_j / 4 \rangle$ term. For example, the GWF gives $\langle \bar{n}_i n_j / 4 \rangle = -0.1925$ for $n = 0.88$ case. This is understood from the fact that $\langle \bar{n}_i \rangle = 0.88$, then $\langle \bar{n}_i \rangle^2/4 = 0.1936$. As shown in Table I, the value of this term for the other states does not change so much from that of the GWF. For example, $\langle \bar{n}_i n_j / 4 \rangle$ changes only 0.5% for the $d_{x^2−y^2}$ wave. Actually the charge-density correlation function in the real space shows that, in the $d_{x^2−y^2}$ case, the amplitude of the nearest and next-nearest neighbors is slightly enhanced. This is in contrast to the GWF which shows dips at those sites due to the exchange hole. Meanwhile, the extended $s$ wave scarcely modifies the GWF value. Thus, we expect that an attractive correlation factor gives more energy gain. We check the effect of the intersite correlation factor by introducing eq. (2.11) to the $d_{x^2−y^2}$-wave state: $P_{\text{TLL}} \Phi_{\text{SC}}$. However, we have found that the energy is hardly affected by the intersite correlation. Therefore the stability of the $d_{x^2−y^2}$ state is mainly caused by the energy gain of the exchange term which is understood from the RVB picture as discussed above.

§5. Phase Diagram

In this section, we construct a phase diagram in the whole $J/t$-$n$ plane. First of all we show the summary of the phase diagram in Fig. 10. In the following subsections we describe the details of determining the phase boundaries.

In §5.1 we discuss the phase boundary between the $d_{x^2−y^2}$-wave state and the metallic state. The stabilization of the extended $s$ wave in the low electron density is studied in §5.2. The properties of the GWF around the supersymmetric case ($J/t = 2$) is discussed in §5.3. In §5.4 the phase separation in the large $J/t$ region is studied. We consider in §5.5 the effect of the three-site term on each phase.

5.1 Range of $d_{x^2−y^2}$ wave

To begin with, we determine the phase boundary between the $d_{x^2−y^2}$-wave state and the metallic state. Here we use the GWF as the metallic state, because the energy gain due to the intersite Jastrow correlation factors is very small. Figures 11 and 12 show the energy components of the $d_{x^2−y^2}$-wave function for various electron densities ranging from $n = 1$ down to 0.04.

The kinetic energy $E_t/t$ shown in Fig. 11 goes to 0 as the electron density approaches either 0 or 1. The latter is due to the Gutzwiller projection, $P_4$. Furthermore $E_t/t$ is a monotonically increasing function of $\Delta/t$ in every density. This means that the kinetic energy does not favor the superconductivity for every electron density. On the other hand, $E_s/J$ shown in Fig. 12 decreases at finite values of $\Delta/t$. The exchange term gives the attractive force in the $d_{x^2−y^2}$ channel as expected. Thus the $d_{x^2−y^2}$ state is not realized without the exchange interaction ($J/t = 0$). For finite $J/t$, the variational energy
\[ E = t \times (E_t/t) + J \times (E_s/J) \]  
(5.1)
has a minimum at a finite value of $\Delta/t$. The obtained optimal values of $\Delta/t$ are plotted in Fig. 13. From this figure the phase boundary is estimated for every electron density. For example, $\delta = 0.2$ ($n = 0.8$) case the phase boundary is at $J/t = 0.1$. This boundary is shown by a solid line with solid triangles in Fig. 10. For the higher doping case $n \lesssim 0.64$ [Fig. 13(b)], it is difficult to determine the boundary definitely, because small $\Delta$ seems to be realized for small value of $J/t$. However, this residual small $\Delta$ is not so meaningful practically, because the energy gain is as small as that of the TLL (metallic) state. Therefore, we estimate the phase boundary by extrapolating the straight fitting lines as indicated in Fig. 13(b). The boundary thus determined is represented by a dashed line with reversed triangles in Fig. 10.

5.2 Range of extended $s$ wave

Next we discuss the stability of the extended $s$ wave in the low density region. As shown by the analytic treatments in the $n \to 0$ limit, the free elec-
electron state is unstable against the s-wave bound state for 
\( 2 < J/t < 3.4367 \). We will discuss this possibility of the 
extended s wave in the finite electron densities.

In Figs. 14 and 15 we show the expectation values of energy components for the extended s wave. [The result of s-wave symmetry (1) of eq. (2.9) is quantitatively similar to that of the extended s wave.] The kinetic energy, \( E_{k} / t \), rapidly approaches zero as \( \Delta t \) increases. As regards \( E_{k} / J \), energy gain is hardly seen for small doping as shown in Fig. 15(b). This is consistent with the result in the half filling where \( E_{k} / t \) does not depend on \( \Delta \) as discussed before. On the other hand for small electron densities [Fig. 15(a)], \( E_{k} / J \) appreciably decreases. This is the cause of the stability of the extended s wave in the low density.

In Fig. 16 we plot the total energy for \( n = 0.04 \) as an example. No energy gain from the GWF can be seen for \( J/t \leq 2 \), while the energy gradually decreases for \( J/t > 2 \). This is consistent with the analysis of two electron systems, where the electrons form a s-wave bound state for \( J/t \geq 2 \).

For finite electron densities, the stable region of the extended s wave is shown in Fig. 10. Since the energy gain is very small and the same order with that obtained by a metallic state with an intersite correlation factor, it is not easy to determine accurately the boundary of the extended s wave.

In Fig. 16 we also plot the energy gain due to the intersite correlation factor, \( \Psi_{TLL} \). For \( J/t < 2.0 \), the optimal value of \( \nu \) in eq. (2.12) is positive, which corresponds to the repulsive Jastrow factor. For example, we get \( \nu_{\text{opt}} \sim 0.25 \) (0.20, 0.14, 0.06) for \( J/t = 0 \) (0.5, 1.0, 1.5). Just at \( J/t = 2.0 \) we find that the Jastrow factor does not reduce the variational energy, which indicates that the GWF is a good variational function for this “supersymmetric” case as in 1D. We will come back to this point shortly. For \( J/t > 2.0 \), \( \nu_{\text{opt}} \) is negative, namely, \( \nu_{\text{opt}} \sim -0.09 \) (−0.19, −0.27) for \( J/t = 2.5 \) (3.0, 3.5). This means that effective attractive interaction exists between electrons.

5.3 Supersymmetric Case

Now we investigate the supersymmetric case (\( J/t = 2 \)) more in detail. For this special parameter, the GWF is shown to be exact in the low density limit. Actually, the two-electron problem can be solved analytically. We consider the GWF with two electrons,

\[
\Psi_{G} = \prod_{j}[1 - n_{j} n_{j}] c_{k=0}^{\uparrow} c_{k=0}^{\downarrow} |0\rangle
\]

\[
= \sum_{i,j}(1 - \delta_{i,j} c_{i}^{\dagger} c_{j}^{\dagger} c_{i}^{\dagger} c_{j}^{\dagger} |0\rangle. \tag{5.2}
\]

If \( H \) (including \( H_{TLL} \)) is applied to this state, the resultant equation is written as,

\[
\mathcal{H}\Psi_{G} = -2z t \Psi_{G} + \{2t - J - (z - 1)J(3)\} \Xi, \tag{5.3}
\]

where \( z \) is the number of nearest neighbor sites (here \( z = 4 \)) and

\[
\Xi = \sum_{i,\tau} c_{i+\tau}^{\dagger} c_{i}^{\dagger} |0\rangle. \tag{5.4}
\]

This means that if the condition

\[
2t - J - (z - 1)J(3) = 0 \tag{5.5}
\]

i.e.

\[
\frac{J}{t} = \frac{2}{1 + (z - 1)J(3)/J} \tag{5.6}
\]

is satisfied, the GWF is an exact eigenstate with energy \(-2zt\), irrespective of \( N_{a} \) [in fact \( \langle \Psi_{G}|\Xi|\Psi_{G}\rangle/\langle \Psi_{G}|\Psi_{G}\rangle = O(1/N_{a}) \)]. The energy is identical with the noninteracting case. As will be mentioned in §5.5, the free electron state has no instability against the bound-pair states of both s and d waves when eq. (5.6) holds. Thus the GWF is shown to be the exact ground state. This property does not depend on the lattice form and dimension.

One can interpret this as the same aspect with the 1D \( t-J \) model. Namely the electron hopping term, which favors the electrons mutually apart, and the exchange term, which works attractively, are well balanced and a kind of “noninteracting” state is realized.

5.4 Region of phase separation

As was shown, a phase separation appears in the 2D \( t-J \) model for the large \( J/t \) region. Here we discuss it from our variational calculations. The phase separation occurs between the Heisenberg system (without hole) and a hole-rich phase. For the small-\( n \) region, the state with phase separation is approximated as a state with the Heisenberg island and the remaining vacuum. The energy of this state is

\[
E_{\text{PS}} = n E_{\text{Heis}} = -1.1693nJ, \tag{5.7}
\]

where \( E_{\text{Heis}} \) is the ground state energy of the 2D Heisenberg model. Comparing this energy with the optimized variational energies of the GWF, the d\( _{x^2-y^2} \) wave and extended s-wave states, we determine the phase boundary, which is also shown in Fig. 10.

In Fig. 16, the energy \( E_{\text{PS}} \) is also plotted; since the \( J/t \)-dependence is strong, we can determine the phase boundary accurately in the small electron density region. Table II summarizes the phase boundary (\( J_{c}/t \)) obtained in this way. The extrapolation of these values to \( n = 0 \) leads us to \( J_{c}/t = 3.437 \), which is quite close to the exact value 3.4367.

As shown in Fig. 16 the GWF is a good trial function in the low-electron density and the variational energy has weak \( J/t \) dependence. Therefore we can broadly estimate \( J_{c}/t \) as \( n \to 0 \) from the GWF. In the limit of \( n \to 0 \) the energy components of the GWF are analytically expressed as \( E_{1}/t = -4n \), \( E_{2}/J = -n^{2} \), \( E_{3}/J(3) = -3n^{2} \). These values are the same with the free electron system, because double occupation can be substantially neglected. Using \( E_{\text{GWF}} = -4n \) and \( E_{\text{PS}} \) in eq. (5.7) we obtain the phase boundary

\[
J_{c}/t = 4/E_{\text{Heis}}/J = 3.42. \tag{5.8}
\]
As \( n \) increases, our estimation of the phase boundary becomes inaccurate. For one thing, we have assumed that the phase separation takes place between the Heisenberg island and the vacuum. Another thing is that we have compared variational energies with the accurate energy of the phase separation with \( E_{\text{fin}} \). Nevertheless our estimation of the phase boundary agrees well with other results up to fairly high density \( (n \lesssim 0.9) \).

5.5 Effect of the three-site term on the phase diagram

Next, we consider the effect of the three-site term on the variational energies and the phase diagram. In Figs. 17 and 18, \( E_\delta/J^{(3)} \) is shown for the \( d_{x^2-y^2} \) wave and extended s-wave states, respectively. For the \( d_{x^2-y^2} \) case, \( E_\delta/J^{(3)} \) behaves similarly to \( E_\delta/t \), while for the extended s wave it decreases with increasing \( \Delta/t \) and its shape resembles that of \( E_\delta/J \) rather than \( E_\delta/t \).

First consider the boundary between the \( d_{x^2-y^2} \) wave and the metallic phase. In Fig. 19 we plot the \( \Delta_{\text{opt}}/t \) for the \( d_{x^2-y^2} \) wave for some values of \( J^{(3)}/J \) and \( n = 0.8 \). The phase boundary of the \( d_{x^2-y^2} \) wave, \( J_{\text{c}}/t \), where \( \Delta_{\text{opt}} \) vanishes, scarcely changes from that for \( J^{(3)} = 0 \). This aspect is common for other densities \((n = 0.52-0.96)\). Thus, the region of the \( d_{x^2-y^2} \) wave hardly changes at least for \( n > 0.64 \) by the three-site term.

The phase boundary of the extended s wave, on the contrary, depends on the three-site term considerably. For the extended s wave, \( E_\delta/J^{(3)} \) decreases with increasing \( \Delta/t \) as shown in Fig. 18. Thus the extended s wave becomes stabler for \( J^{(3)}/J > 0 \) and its region expands. The shift of the boundary is also shown in Fig. 10 by an arrow for \( E_\delta/J^{(3)} = 0.5 \). Inversely, for \( J^{(3)}/J < 0 \) the energy of the extended s wave increases so that its region disappears for the case of \( J^{(3)}/J = -0.5 \), namely the GWF is stable for every value of \( J/t \).

This behavior is consistent with the analysis of two-electron problem. If we solve the two electron problem including \( H_3 \), we obtain the eigenvalue equation

\[
\frac{1}{\pi a} K\left(\frac{1}{a}\right) = \frac{J}{4t} (1 + 3J^{(3)}/J) \left[ \frac{2}{\pi} K\left(\frac{1}{a}\right) - 1 \right]
\]  

(5.9)

for the two-electron bound state with the extended s symmetry, where \( a = -E/4t \geq 1 \) and \( K(k) \) is the complete elliptic integral of the first kind. Equation (5.9) has a solution when

\[
\frac{J}{4t} (1 + 3J^{(3)}/J) \geq \frac{1}{2}.
\]

(5.10)

As a result, for fixed \( J^{(3)}/J \), the critical value above which the two electrons form a bound state is

\[
J_c/t = \frac{2}{1 + 3J^{(3)}/J}.
\]

(5.11)

This value is exactly the same with the condition eq. (5.6) where the GWF becomes an exact eigenstate. For \( J^{(3)}/J = 0.5 \), this critical value is \( J/t = 4/5 \). This value coincides with the boundary shown in Fig. 10 which we determine from the VMC calculations. When \( J^{(3)}/J \leq -1/3 \), there is no solution for the two-electron bound state.

The phase boundary to the phase separation is also estimated. The shifted boundaries for \( J^{(3)}/J = \pm 0.5 \) are shown with open circle and dotted line in Fig. 10. For \( J^{(3)}/J = 0.5 \) the extended s-wave state becomes so stable that the phase separation does not take place for small \( n \). On the other hand, for \( J^{(3)}/J = -0.5 \) the extended s-wave state is not stabilized and thus the phase separation expands to smaller \( J/t \) region.

§6. Summary and Discussions

By using the variational Monte Carlo method, we have studied the \( t-J \) model with the three-site term for the square lattice, and obtained a phase diagram in the full \( J/t-n \) plane. We have used Gutzwiller-Jastrow-type wave functions describing metallic, antiferromagnetic, and various singlet-pairing superconducting states: the BCS-like \( s \), \( d_{xy} \), \( s+d \)-type, and \( s+i \)-type waves, which include the \( d_{x^2-y^2} \) and extended s waves.

Main results are summarized in the phase diagram shown in Fig. 10. Remarkable points which we have confirmed and found are:

(1) At half filling, many pairing states including the \( d_{x^2-y^2} \) and the \( s+i \)-wave states are degenerate and the most stable, in accordance with the analysis of the local SU(2) symmetry. Nevertheless, the antiferromagnetic state is more stable here.

(2) For plausible parameters of high-\( T_c \) superconductors, the \( d_{x^2-y^2} \) wave is the most stable state among various pairing symmetries. The range of the \( d_{x^2-y^2} \) wave hardly changes even if the three-site term is added. Substantially, there is no chance to realize \( s+d \), \( s+i \)-d, and extended s waves in this region.

(3) The \( d_{xy} \) wave always has higher energy than the GWF except for extraordinarily large negative value of \( J^{(3)} \).

(4) In the region of low electron density and \( J/t > 2.0 \), the extended s wave becomes a good state, which almost reproduces the exact value of the phase boundary for \( n \to 0 \). However the energy gain from the GWF is small. This phase corresponds to the low-electron-density phase predicted in the 1D \( t-J \) model, which consists of two-electron singlet bound-pairs.

(5) Metallic states \( \Phi_F \) are unstable in itself against the phase separation for \( n \sim 1 \) and \( J/t > 0 \). This is in contrast with the cases of the 1D \( t-J \), and 1D and 2D Hubbard models.

(6) For the supersymmetric case \( (J/t = 2) \), the GWF is exact in the \( n \to 0 \) limit and behaves like the non-interacting state in the low-electron-density region just like the 1D \( t-J \) model. The GWF is also a very good trial wave function in the region up to \( n \lesssim 0.25 \).

Our result that the \( d_{x^2-y^2} \) wave is stable for the parameters of high-\( T_c \) oxides confirms the early VMC results. The obtained phase diagram is consistent with the one by the high-temperature expansion and is qualitatively similar to that of the VMC calculations by Dagotto et al. We suspect, however, that the qualitative and/or quantitative differences between the previous VMC works and the present one are attributed to some insufficient or erroneous numerical treatments of the former works.
We should not consider the results (1)-(5) are completely decisive because of the approximate trial functions used. However, the results of the relative stability among various pairing symmetries are persuasive, because we do not give partial treatment to a specific symmetry.

We also calculate the variational energies using the Gutzwiller approximation. In contrast to the VMC method, the Gutzwiller approximation assumes the effect of the projection as some statistical weights. The details are summarized in Appendix B. Figure 20 shows the obtained variational energy for various superconducting states including the d$_{x^2-y^2}$ and extended s waves for $n \sim 1$ and $J/t = 0.5$. The variational energies for the metallic GWF is also plotted. This figure is to be compared with Fig. 7 where the same calculation is carried out using the VMC method. The Gutzwiller approximation gives a similar result. In Fig. 20 there is a small region in the vicinity of $n = 1$ where s+id state is realized, which was found before. This is due to the violation of the SU(2) symmetry in the approximation.

Figure 21 shows the phase diagram determined from the Gutzwiller approximation. As expected from the good coincidence of the variational energy with the VMC results, the obtained phase diagram resembles Fig. 10 determined from the VMC method. Thus, the Gutzwiller approximation gives broadly reasonable results.

In the following we compare our results with other works.

As for the stability of the d$_{x^2-y^2}$-wave pairing, our result is common with one for the 2D d-p model. Using similar variational wave functions for this model, Asahata and Oguri recently showed that the d$_{x^2-y^2}$-wave pairing state appears in the borders of metallic and AF regions in the phase diagram. On the other hand, concerning the possibility of the extended s wave, it is pointed out that modification of the Fermi surface structure in $\Phi$ of eq. (2.5) is important.

As shown by previous VMC calculations the ferromagnetic region with full momentum corresponding to Nagaoka’s theorem exists in the region $0.6 \lesssim n < 1$ and $J/t \lesssim 0.1$. On the other hand, according to the high-temperature-expansion partial ferromagnetism appears in the similar region. In this paper, we have not discussed this ferromagnetism in detail, since it is confined in a small parameter range. The relation among the above two calculations and our present results is an interesting issue left for future studies.

Kagan and Rice showed that the p-wave pairing is the leading instability for small values of $J/t$ and low-electron densities by means of the t-matrix technique. In this paper we have not discussed this possibility, because its energy gain seems extremely small. It is rather difficult to detect a tiny energy gain by the ordinary VMC calculations; moreover such a small energy gain is easily overcome by introducing the Jastrow correlation factors in the metallic states.

Another interesting issue is the possibility of spin-charge separation in the 2D systems. From the density correlation function, Putikka et al discussed the spin-charge separation. However as claimed later, it is not yet conclusive. To study TLL states for the metallic phase, a VMC-method and a Green function Monte Carlo method have been used. In this paper we have taken account of this possibility by adopting a TLL-type correlation factor. Consequently, the energy gain thereof is very small and it is not likely that the ground-state becomes a Tomonaga-Luttinger liquid state in the present variational scheme.

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**Appendix A: The GWF for the Hubbard Model**

In this appendix, we show the behavior of $E/t$ as a function of $n$ ($n \sim 1$) for the 2D Hubbard model:

$$\mathcal{H}_{\text{hub}} = -t \sum_{\langle i,j \rangle \sigma} \left( c_{i,\sigma}^\dagger c_{j,\sigma} + c_{j,\sigma}^\dagger c_{i,\sigma} \right) + U \sum_j n_{j\uparrow} n_{j\downarrow},$$

with the GWF:

$$\Psi_G(g) = \prod_j \left[ 1 - (1 - g)n_{j\uparrow}n_{j\downarrow} \right] \Phi_F.$$

The optimized results near the half filling is shown in Fig. 22; $E/t$ behaves linearly as $\delta \to 0$, although size dependence becomes a little larger as $n$ approaches 1. This linear behavior is in sharp contrast with the result of the $t$-$J$ model as discussed in §4.1.

This discordance may be intuitively understood as follows. By neglecting higher-order terms, $\mathcal{H}$ of eq. (2.1) is a canonical transformation of the Hubbard Hamiltonian:

$$\mathcal{H} = e^{-iS} \mathcal{H}_{\text{hub}} e^{iS}.$$

Therefore, the expectation value with respect to the GWF is written as

$$\langle \Psi_G | \mathcal{H} | \Psi_G \rangle = \langle \Psi_G | e^{-iS} \mathcal{H}_{\text{hub}} e^{iS} | \Psi_G \rangle$$

$$= \langle \bar{\Psi} | \mathcal{H}_{\text{hub}} | \bar{\Psi} \rangle$$

where $\bar{\Psi} = e^{iS} \Psi_G$. Consequently, we should adopt modified functions $\bar{\Psi}$ for the Hubbard model to obtain a similar behavior.

Nevertheless, in 1D, where the modified wave functions are much better, there exists no conflict between the two models even within the GWF. And this GWF-result is consistent with the exact analysis, which shows that the Hubbard model is connected to the $t$-$J$ model for every $n$ in the strong coupling limit. Anyway, it is necessary to confirm by some reliable method that
the t-J model is connected to the Hubbard model also for 2D metallic states.

Appendix B: Gutzwiller Approximation

In this Appendix we summarize the Gutzwiller approximation for the 2D t-J model. This approximation is extensively studied in connection with the VMC calculations. In order to compare with the present results, we only have to include the estimation of the \( \langle n, n_j/4 \rangle \) term.

In the Gutzwiller approximation, the expectation value

\[
\langle \psi_0 | P d \psi_0 \rangle,
\]

is approximated by

\[
\frac{2\delta}{1+\delta} \langle \psi_0 | \epsilon_i \sigma c_{ij,\sigma} | \psi_0 \rangle,
\]

where \( \delta \) is the doping rate \((\delta = 1-n). \) Similarly the exchange term is given by

\[
\langle \psi_0 | P d S_i \cdot S_j P d | \psi_0 \rangle = \frac{4}{(1+\delta)^2} \langle \psi_0 | S_i \cdot S_j | \psi_0 \rangle.
\]

For the \( \langle n, n_j/4 \rangle \) term, we introduce the following approximation,

\[
\langle \psi_0 | P d n_i n_j P d | \psi_0 \rangle = \frac{4}{(1+\delta)^2} \langle \psi_0 | n_i n_j | \psi_0 \rangle.
\]

Using these approximations, self-consistent equations are given by

\[
\Delta_k = \frac{1}{N_a} \sum_{k'} \gamma_k^{k'} \frac{\Delta_{k'}}{2E_{k'}}\),
\]

\[
\xi_k = \frac{1}{4g_s J + \frac{1}{4} \sum_{k'} \gamma_k^{k'} \frac{\xi_{k'}}{2E_{k'}}},
\]

\[
\delta = \frac{1}{N_a} \sum_k \frac{\xi_k}{E_k},
\]

where

\[
\gamma_k = 2(\cos k_x + \cos k_y), \quad E_k = \sqrt{\xi_k^2 + |\Delta_k|^2}, \quad g_t = \frac{2\delta}{1+\delta}, \quad g_s = \frac{4}{(1+\delta)^2}, \quad \bar{\mu} = \mu + \frac{1}{N_a} \frac{\partial \langle H \rangle}{\partial \delta}.
\]

These self-consistent equations are numerically solved for the \( d_{x^2+y^2} \), \( s+id \) and extended s-wave states.
To confirm the θ dependence, we calculate each energy component as a function of θ, by fixing Δ/t at 0.6, which is the optimal value of the d^2_0 - y^2 wave for J/t = 0.5. Both E_1/t and E_3/J are monotonically decreasing functions except for the very vicinity of θ = 0. On the contrary, E_3/J(3) is an monotonically increasing function of θ, although the increment is relatively small.

This feature is essentially the same for the high density region. In this sense, even in the d-wave superconducting state, effective repulsive force between electrons works for J/t < 2.0.

For the bound state with d-wave symmetry, we find

\[ J_c - J_c^{(3)} = \frac{4t}{8/\pi - 2} \approx 7.32t. \]

Fig. 1. Energy components of the Gutzwiller wave function as a function of electron density. Each Symbol represents a system size: solid circle (L = 26), upward triangle (20), downward triangle (16), circle (14), square (12) and diamond (10). Curves are a guide for the eyes.

Fig. 2. Data of Fig. 1 are re-plotted. E_1/t and E_3/J(3) are plotted versus 1−n in (a), and E_3/J versus (1−n)^0.7 in (b). Symbols have the same meanings with Fig. 1.

Fig. 3. Energy expectation values at half filling for the case (iii) (s+d-type wave) of eq. (2.9) for several values of C (−1.0, −0.6, −0.4, 0, 0.4, 0.6, 1.0). The inset is the magnification of the minimum area around ∆/t = 0.57. Symbols for the value of C are common in the inset. The system used is L = 10, and the sample number is 3 × 10^4. The value of Green function Monte Carlo method is E/J = −1.1693.2

Fig. 4. Energy expectation values at half filling for the case (iv) (s+id-type wave) for several values of θ (0, π/4, π/2, 3π/4, π). The inset is the magnification of the minimum area around 0.5 − 2. Symbols of θ are common with the inset. The system used is L = 10, and the sample number is 3 × 10^4.

Fig. 5. Expectation values of three energy components for s+id-type wave and for some value of θ (0, π/4, π/2, 3π/4, π) in the same energy scale. Electron density is chosen at n = 0.88. The system used is L = 10, and the sample number is 3 × 5 × 10^4. Since there are large statistical fluctuations in E_3/J and E_3/J(3) for small θ and large ∆/t, we show the data of two Monte Carlo runs for θ = 0.

Fig. 6. Total energy of s+id-type wave for some value of θ (0, π/4, π/2, 3π/4, π). J(3)/J = 0. The inset is the magnified figure of the minimum area. Symbols of θ are common with the inset. The system used is L = 10, and the sample number is 3 × 5 × 10^4.

Fig. 7. Comparison of total energies among four variational states as a function of n near the half filling (J(3) = 0). Symbols have the same meaning with Figs. 1 and 2. The arrow on the right axis represents the accurate value obtained by the Green function Monte Carlo method.
Fig. 8. Total energy of the $d_{x^2-y^2}$-wave state versus $\mu/t$ for some values of $\Delta/t$. Note that the scale is small. The arrow on the horizontal axis indicates the noninteracting value of $\mu$. $3 \times 10^3$ samples are used. $L = 10$.

Fig. 9. Comparison of spin structure factors between the GWF, the optimized $d_{x^2-y^2}$ wave ($\Delta/t = 0.55$), and the extended $s$ wave ($\Delta/t = 0.55$). The path of $q$ is $\Gamma(0,0) \rightarrow X(\pi,0) \rightarrow M(\pi,\pi) \rightarrow \Gamma$. The system with $L = 10$ and $5 \times 10^4$ samples are used.

Fig. 10. Phase diagram for the ground state of the 2D $t$-$J$ model. Basically it represents the case of $J^{(3)}/J = 0$. The shifts due to finite $J^{(3)}/J$ are shown by shadowed arrows with their values. The exact phase boundary between the $s$-wave bound state and the phase separation for $n \rightarrow 0$ is shown by a solid arrow on the abscissa. For detailed explanations, see the text.

Fig. 11. Expectation values of transfer energy of the $d_{x^2-y^2}$ wave for (a) low density ($n = 0.04, 0.12, 0.16, 0.24, 0.32, 0.36, and 0.44$) and (b) high density ($n = 0.52, 0.60, 0.64, 0.72, 0.80, 0.88$, and $0.96$). $L = 10$ and the sample number is $3 \times 5 \times 10^4$.

Fig. 12. Expectation values of exchange energy of the $d_{x^2-y^2}$ wave for (a) low density ($n = 0.04 - 0.52$) and (b) high density ($n = 0.60 - 1.0$). $L = 10$. The sample number is $3 \times 5 \times 10^4$.

Fig. 13. Optimized value of $\Delta/t$ for the $d_{x^2-y^2}$ wave as a function of $J/t$ (a) in the high density ($n = 0.64 - 0.96$) and (b) in the medium density ($n = 0.32 - 0.60$). In (a) we fit the data with curves, and in (b) with straight lines. The arrow on the vertical axis in (a) is the value for $n = 1.0$.

Fig. 14. Expectation values of transfer energy of the extended $s$ wave for (a) low density ($n = 0.04 - 0.44$) and (b) high density ($n = 0.52 - 0.96$). $L = 10$ and the sample number is $3 \times 5 \times 10^4$.

Fig. 15. Expectation values of exchange energy of the extended $s$ wave for (a) low density ($n = 0.04 - 0.52$) and (b) high density ($n = 0.60 - 1.0$). $L = 10$ and the sample number is $3 \times 5 \times 10^4$. Since for large $\Delta/t$ statistical fluctuations are large, the results of two trials are depicted for a few values of $n$.

Fig. 16. Comparison among some variational energies as a function of $J/t$ for $n = 0.04$ for the $t$-$J$ model ($J^{(3)} = 0$). For $J/t \leq 2$ the optimal extended $s$ wave is reduced to the GWF. Note that the scale is small. $L = 10$ and the sample number is $2 \times 10^3$.

Fig. 17. Expectation values of three-site term of the $d_{x^2-y^2}$ wave for (a) low density ($n = 0.04 - 0.52$) and (b) high density ($n = 0.60 - 0.96$). $L = 10$ and the sample number is $3 \times 5 \times 10^4$.

Fig. 18. Expectation values of the three-site term of the extended $s$ wave for (a) low density ($n = 0.04 - 0.52$) and (b) high density ($n = 0.60 - 0.96$). $L = 10$ and the sample number is $3 \times 5 \times 10^4$. For the large value of $\Delta/t$ large statistical fluctuations are observed, and the results of two trials are depicted for some values of $n$.

Fig. 19. Optimized value of $\Delta/t$ for some values of $J^{(3)}/J$ as a function of $J/t$. Solid lines are guides for eyes. The wave function has the $d_{x^2-y^2}$-wave pairing symmetry.

Fig. 20. Comparison of total energies among three variational states obtained in the Gutzwiller approximation as a function of $n$ near the half filling ($J^{(3)} = 0$).

Fig. 21. Phase diagram obtained in the Gutzwiller approximation for the ground state of the 2D $t$-$J$-type model.

Fig. 22. Total variational energy for 2D Hubbard model as a function of electron density near the half filling, with respect to the Gutzwiller wave function. Used lattice sizes are indicated by the same symbols with Fig. 1. Lines are a guide for the eyes. $3 \times 10^4$ samples are used.
Table I. Differences of energy components from the GWF for $J/t = 0.5$ in the high electron density. The values of the GWF are given as the references. The system with $L = 10$ is used. The last digit for each value includes some error.

| n   | State | $E_i/t$ | $(S,S_j)$ | $\langle -\frac{\delta n_i}{n_j} \rangle$ | Total     |
|-----|-------|---------|------------|----------------------------------|-----------|
| GWF | 0.0   | -0.2706 | -0.25      | -0.5206                          |           |
| TLL | 0.0   | 0.0     | 0.0        | 0.0                              |           |
| 1.00| AF    | -0.0500 | -0.0      | -0.0500                          |           |
|     | $d_{xy}$ | 0.0    | -0.0493   | 0.0                              | -0.0493   |
|     | Exact  | -0.0641 | 0.0       | -0.0641                          |           |
| GWF | -0.1080 | -0.2216 | -0.2302   | -0.5597                          |           |
| TLL | ~ 0   | ~ 0     | ~ 0       | ~ 0                              | -0.0001   |
| 0.96| AF    | +0.0098 | -0.0543   | -0.0000                          | -0.0447   |
|     | $d_{xy}$ | +0.0053 | -0.0004  | -0.0004                          | -0.0555   |
|     | s+i$d$ | +0.0075 | -0.0568   | -0.0004                          | -0.0497   |
|     | Ext.s | +0.0037 | -0.0001   | -0.0000                          | +0.0048   |
| GWF | -0.3089 | -0.1746 | -0.1925   | -0.6755                          |           |
| TLL | -0.0004 | +0.0001 | +0.0002   | -0.0005                          |           |
| 0.88| AF    | +0.0173 | -0.0268   | -0.0000                          | -0.0100   |
|     | $d_{xy}$ | +0.0149 | -0.0499   | -0.0012                          | -0.0367   |
|     | s+i$d$ | +0.0203 | -0.0435   | -0.0011                          | -0.0242   |
|     | Ext.s | +0.0212 | +0.0007   | -0.0003                          | +0.0216   |
| GWF | -0.4834 | -0.1426 | -0.1575   | -0.7834                          |           |
| TLL | -0.0022 | +0.0005 | +0.0005   | -0.0012                          |           |
| 0.80| AF    | 0.0     | 0.0       | 0.0                              | 0.0       |
|     | $d_{xy}$ | +0.0195 | -0.0357   | -0.0017                          | -0.0179   |
|     | s+i$d$ | +0.0232 | -0.0273   | -0.0014                          | -0.0055   |
|     | Ext.s | +0.0297 | -0.0005   | -0.0005                          | +0.0288   |
| GWF | -0.6290 | -0.1193 | -0.1257   | -0.8743                          |           |
| TLL | -0.0042 | +0.0009 | +0.0010   | -0.0021                          |           |
| 0.72| AF    | 0.0     | 0.0       | 0.0                              | 0.0       |
|     | $d_{xy}$ | +0.0102 | -0.0143   | -0.0010                          | -0.0050   |
|     | s+i$d$ | +0.0168 | -0.0118   | -0.0009                          | +0.0040   |
|     | Ext.s | +0.0226 | -0.0002   | -0.0004                          | +0.0219   |

Table II. Critical values of $J/t$ of the phase boundary between homogeneous and separated phases for the low electron density. The exact value for $n = 0$ is by Hellberg and Manousakis. The last digit for each value includes some errors.

| n   | $N/N_a$ | $J_c/t$ | State   |
|-----|---------|---------|---------|
| 0.0 | 2/$\infty$ | 3.4367  | Exact   |
| 0.0059 | 4/676   | 3.432   | Ext.s   |
| 0.01 | 4/400   | 3.429   | Ext.s   |
| 0.0156 | 4/256   | 3.423   | Ext.s   |
| 0.0204 | 4/196   | 3.418   | Ext.s   |
| 0.03 | 12/400  | 3.389   | Ext.s   |
| 0.0612 | 12/196  | 3.345   | TLL     |
| 0.0816 | 16/196  | 3.313   | TLL     |
| 0.0938 | 24/256  | 3.284   | TLL     |