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Coexistence of $d_{x^2-y^2}$ superconductivity and antiferromagnetism in the two-dimensional t-J model and numerical estimation of Gutzwiller factors

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The coexisting phase of the d-wave superconducting and the antiferromagnetic order in the two-dimensional t-J model is reexamined using a variational Monte Carlo method in order to estimate the Gutzwiller factors. A trial wave function is used which is consistent with the mean-field solution. The Gutzwiller factors are determined by comparing the numerically obtained expectation values with the mean-field values. We find the z component of the Gutzwiller factor of exchange interaction is enhanced compared with the xy components. This effect does not appear in the conventional Gutzwiller approximation and is essential for the stabilization of the antiferromagnetic order in the presence of d-wave superconductivity. We discuss several applications of the present Gutzwiller factors to the problems with antiferromagnetism and d-wave superconductivity. [S0163-1829(99)51538-5]

I. INTRODUCTION

Since the discovery of high-T_c superconductivity (SC),[1] the ground states of these compounds are intensively investigated. Many experiments suggest that the ground state changes from the antiferromagnetic (AF) state to the $d_{x^2-y^2}$-wave (d-wave) SC as the carrier density increases.[2] Furthermore, the interplay between the AF and d-wave SC has recently attracted much attention because of the stripe phase[3] which is observed experimentally and a phenomenological SO(5) theory.[4] Thus it is urgent and important to develop a microscopic theory in which both the AF and d-wave SC are treated reasonably.

However, when we treat both the AF and the d-wave SC order parameters in simple mean-field theories for the two-dimensional (2D) t-J model, they lead to inconsistent results. In the slave boson mean-field approximation, the AF order is overestimated and extends to unphysical doping rates ($15 \sim 20\%$).[5] In this scheme, we are unable to discuss the stripe phase which is stablized near 12.5% hole doping. Another approximation on which we will focus is the Gutzwiller approximation (GA).[6] It has been shown that the GA gives a fairly reliable estimation for the variational energies for the pure d-wave SC state.[7] However if the AF order parameter is taken into account in the GA,[6] it can be shown that there is no region in the phase diagram where the AF state is stabilized. This is the opposite result compared with the slave boson mean-field approximation.

In this paper we solve this discrepancy by improving the GA for the coexistent state of the d-wave SC and the AF order using variational Monte Carlo (VMC) method where the double occupancy prohibition is rigorously treated. Our improved GA enables us to study the interplay between AF and d-wave SC in the stripe phase or around vortex cores and impurities.

Several works used the VMC method to discuss the phase diagram of the 2D t-J model.[7–9] It has been shown that the d-wave SC state is stabilized for finite doping range. As for the AF, Chen *et al.*[10] and Giamarchi and Lhuillier[11] proposed a coexisting wave function between the AF and d-wave SC order. The coexisting state has a lower energy than pure d-wave SC or AF state near half filling. However their wave function is slightly different from the mean-field solution. In order to determine the Gutzwiller factors in the GA, it is necessary to use a wave function which is consistent with the mean-field theory. It is shown that the coexistent state is stabilized up to the reasonable hole doping rate ($\sim 10\%$), which is similar to the previous results.[10,11]

Then, using these VMC results and comparing with the mean-field expectation values, we determined the Gutzwiller factors (g factors), which are coefficients used for the projection operator in the GA. By determining g factors numerically, we find that the anisotropy of g factors which was neglected before plays an essential role to stabilize the AF state. Our improved GA reproduces the variational energy obtained by the VMC calculation for the uniform case. We discuss the useful applications of the improved GA for the nonuniform states.

II. FORMULATION

A. Model and trial wave function

We use the 2D t-J model on a square lattice,

$$H = -t \sum_{\langle ij \rangle \sigma} P_G (c_{i\sigma}^{\dagger} c_{j\sigma} + \text{h.c.}) P_G + J \sum_{\langle ij \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j , \quad (2.1)$$

where $\langle ij \rangle$ represents the sum over the nearest-neighbor sites and $\boldsymbol{S} = c_{i\alpha}^{\dagger} (\frac{1}{2} \boldsymbol{\sigma})_{\alpha\beta} c_{i\beta}$. The Gutzwiller's projection operator P_G is defined as $P_G = \Pi_i (1 - \hat{n}_{i\uparrow} \hat{n}_{i\downarrow})$. For this Hamiltonian, we calculate the variational energy in the VMC method, using the following Gutzwiller projected trial wave function,

$$|\psi\rangle = P_G |\psi_0(\Delta_d, \Delta_{\text{af}}, \mu)\rangle, \quad (2.2)$$

where Δ_d, Δ_{af}, and μ are the variational parameters relating to d-wave SC, AF, and chemical potential, respectively.

$|\psi_0(\Delta_d, \Delta_{\text{af}}, \mu)\rangle$ is a Hartree-Fock (HF) type wave function with the d-wave SC and AF orders. It is expressed as

$$|\psi_0(\Delta_d,\Delta_{\rm af},\mu)\rangle=\prod_{k,s(=\pm)}(u_k^{(s)}+v_k^{(s)}d_{k\uparrow}^{(s)\dagger}d_{-k\downarrow}^{(s)\dagger})|0\rangle \tag{2.3}$$

$$=\prod_{k,s}u_k^{(s)}\exp\left[\sum_{k,s}\frac{v_k^{(s)}}{u_k^{(s)}}d_{k\uparrow}^{(s)\dagger}d_{-k\downarrow}^{(s)\dagger}\right]|0\rangle, \tag{2.4}$$

where

$$\frac{v_k^{(\pm)}}{u_k^{(\pm)}}=\frac{\pm\Delta_d\gamma_k}{(\pm E_k-\mu)+\sqrt{(\pm E_k-\mu)^2+(\Delta_d\gamma_k)^2}}, \tag{2.5}$$

$$E_k=\sqrt{\epsilon_k^2+\Delta_{\rm af}^2}, \tag{2.6}$$

$\epsilon_k=-2(\cos k_x+\cos k_y)$ and $\gamma_k=2(\cos k_x-\cos k_y)$. The annihilation operators $d_{k\sigma}^{(s)}$ are related to the electron operators through the following unitary transformation,

$$\begin{pmatrix}d_{k\sigma}^{(+)}\\ d_{k\sigma}^{(-)}\end{pmatrix}=\begin{pmatrix}\alpha_{k\sigma} & -\beta_{k\sigma}\\ \beta_{k\sigma} & \alpha_{k\sigma}\end{pmatrix}\begin{pmatrix}c_{Ak\sigma}\\ c_{Bk\sigma}\end{pmatrix}, \tag{2.7}$$

with

$$\alpha_{k\sigma}=\sqrt{\frac{1}{2}\left(1-\frac{\sigma\Delta_{\rm af}}{E_k}\right)}$$
$$\beta_{k\sigma}=\sqrt{\frac{1}{2}\left(1+\frac{\sigma\Delta_{\rm af}}{E_k}\right)}. \tag{2.8}$$

Here $c_{Ak\sigma}(c_{Bk\sigma})$ are annihilation operators of an electron on the A(B) sublattice and σ represent $\uparrow(+1)$ and $\downarrow(-1)$. The wave vector $\boldsymbol{k}$ is limited to half of the Brillouin zone where $\epsilon_k<0$.

We can confirm that $|\psi_0\rangle$ is a vacuum of the annihilation operators which diagonalize

$$\sum_k\Bigg[\sum_\sigma\{\epsilon_k(c_{Ak\sigma}^\dagger c_{Bk\sigma}+\text{h.c.}) -(\mu+\sigma\Delta_{\rm af})c_{Ak\sigma}^\dagger c_{Ak\sigma}-(\mu-\sigma\Delta_{\rm af})c_{Bk\sigma}^\dagger c_{Bk\sigma}\} +\Delta_d\gamma_k(c_{A-k\downarrow}c_{Bk\uparrow}+c_{B-k\downarrow}c_{Ak\uparrow}+\text{h.c.})\Bigg]. \tag{2.9}$$

Thus, this wave function is a natural extension of the *d*-wave SC and of the AF order.

Chen *et al.*[10] and Giamarchi and Lhuillier[11] proposed a similar wave function with coexisting the *d*-wave SC and the AF orders. However, in their wave function, the $d_{k\sigma}^{(+)}$ operator is neglected and E_k in Eq. (2.5) is substituted for $|\epsilon_k|$. Therefore, in order to determine the Gutzwiller factors using the mean-field values, we have to use the state $|\psi_0\rangle$ with Eq. (2.5) which is consistent with the mean-field theory.

B. Gutzwiller factors

The Gutzwiller factor of an operator $\hat{O}$ is defined as

$$g_{\hat{O}}=\frac{\langle\psi_0|P_G\hat{O}P_G|\psi_0\rangle}{\langle\psi_0|\hat{O}|\psi_0\rangle}=\frac{\langle\hat{O}\rangle}{\langle\hat{O}\rangle_0}, \tag{2.10}$$

where $\langle\hat{O}\rangle_0$ is its mean-field expectation value. In the usual GA, g factors are estimated from the probabilities of the configurations that contribute to the expectation values. However, in this paper, we evaluate them using correct expectation values obtained numerically in the VMC calculation.

In the next section, we calculate the g factors for the following operators: $\Sigma_{\langle ij\rangle\sigma}c_{i\sigma}^\dagger c_{j\sigma}$, $\Sigma_{\langle ij\rangle}(S_i^xS_j^x+S_i^yS_j^y)$, and $\Sigma_{\langle ij\rangle}S_i^zS_j^z$, corresponding to g_t, g_s^{xy}, and g_s^z, respectively. The values of g factors depend on the trial wave function via the variational parameters. To compare with previous works on the GA,[6] it is convenient to treat the g factors as functions of expectation values $\overline{\Delta}$, $\overline{m}$, and $\overline{n}$ in the wave function $|\psi_0\rangle$, which are defined as,

$$\overline{\Delta}_\tau\equiv\frac{1}{4N}\sum_{i,\delta=\pm\tau}\langle c_{i\uparrow}^\dagger c_{i+\delta,\downarrow}^\dagger-c_{i\downarrow}^\dagger c_{i+\delta,\uparrow}^\dagger\rangle_0$$

$$\overline{\Delta}\equiv(\overline{\Delta}_x-\overline{\Delta}_y)/2 =\frac{1}{8N}\sum_{k,\pm}\frac{\Delta_d\gamma_k^2}{\sqrt{(\pm E_k-\mu)^2+(\Delta_d\gamma_k)^2}}, \tag{2.11}$$

$$\overline{m}\equiv\frac{1}{N}\sum_i(-1)^i\langle c_{i\uparrow}^\dagger c_{i\uparrow}-c_{i\downarrow}^\dagger c_{i\downarrow}\rangle_0 =\frac{1}{N}\sum_{k,\pm}\frac{\Delta_{\rm af}(\pm E_k-\mu)}{\pm E_k\sqrt{(\pm E_k-\mu)^2+(\Delta_d\gamma_k)^2}}, \tag{2.12}$$

$$\overline{n}\equiv\frac{1}{N}\sum_{i\sigma}\langle c_{i\sigma}^\dagger c_{i\sigma}\rangle_0 =1-\frac{1}{N}\sum_{k,\pm}\frac{(\pm E_k-\mu)}{\sqrt{(\pm E_k-\mu)^2+(\Delta_d\gamma_k)^2}}, \tag{2.13}$$

where N is the number of sites. Note that the values $\overline{\Delta}$, $\overline{m}$, and $\overline{n}$ are uniquely determined from the variational parameters Δ_d, $\Delta_{\rm af}$, and μ.

III. NUMERICAL RESULTS

A. Variational Monte Carlo

We use the VMC method by fixing the electron number N_e (Refs. 7 and 9) on a square lattice, whose size N is from 8×8 up to 14×14. The distribution of the wave vectors $\boldsymbol{k}$ is determined by a periodic-antiperiodic boundary condition as to avoid the degeneracy of the Fermi surface and the gap node of *d*-wave SC. We set the parameter of the *t*-*J* model as $J/t=0.3$. All data are calculated with more than 10^4 Monte Carlo samples. Though we should calculate in the whole three-dimensional parameter space $(\Delta_d,\Delta_{\rm af},\mu)$, the parameter μ is replaced by the value without Gutzwiller projection. This implies that $N_e/N=\overline{n}$ (i.e., $\langle n_i\rangle=\langle n_i\rangle_0$).

Figure 1 shows the Δ_d, $\Delta_{\rm af}$ dependence of the expectation value $2\langle\boldsymbol{S}_i\cdot\boldsymbol{S}_j\rangle$ per site at half filling. In the following, we use t as an energy unit. The number of the sites is 10×10. When $\Delta_{\rm af}\sim0$, there are two degenerated minima at $\log_{10}\Delta_d\sim\pm0.6$ as found by Yokoyama and Shiba.[8] On the

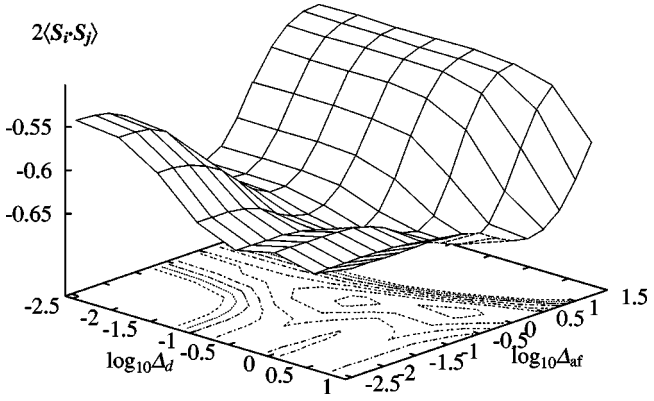

FIG. 1. Variational parameter dependence of the energy at half filling. The number of sites is 10×10 and the number of the Monte Carlo samples is 1×10^4.

other hand, in the case of $\Delta_d \sim 0$, the minimum energy exists at $\log_{10}\Delta_{af} \sim -0.6$. However, we can see that the lowest energy states locate at $(\log_{10}\Delta_d, \log_{10}\Delta_{af}) = (-0.6, -0.6)$ and $(0.6, -0.1)$ and these states almost degenerate at the value $2\langle \boldsymbol{S}_i \cdot \boldsymbol{S}_j \rangle = 0.6645 \pm 0.0005$.

For the various hole dopings, we determine the ground-state energy and the staggered magnetization at $J/t = 0.3$ (Fig. 2). The AF and d-wave SC coexisting state has a lower energy than the pure d-wave SC state up to about 10% doping. At half filling, the energy is -0.1994, which is close to the best estimated value -0.20076 in the Green's function Monte Carlo method.[12] The staggered magnetization at half filling is 0.75, which is also close to reliable studies on the Heisenberg model.[13] If we use the pure AF state, the staggered magnetization is 0.9 (Ref. 14), which is too large. As the doping increases, the staggered magnetization reduces and disappears around the reasonable hole doping ($\delta \sim 0.1$).

B. Gutzwiller factors

We calculate the g factors defined in Eq. (2.10) using the VMC results. At first, we discuss the g factors for the $J\boldsymbol{S}\cdot\boldsymbol{S}$ term. The $\bar{m}$ dependence of the g factors at half filling with $\bar{\Delta}$ being fixed at 0.02 and 0.18 is shown in Fig. 3. g_s^{xy} and g_s^z correspond to the enhancement factors for $S^xS^x + S^yS^y$ and S^zS^z, respectively. The most important feature is that the z component of the enhancement factor g_s^z has a maxima at $\bar{m} \sim 0.15$. On the other hand, the xy component does not have this feature and decreases monotonically as $\bar{m}$ increases. The size dependences of the maxima are found in the region of $0 < \bar{\Delta} < 0.12$, but we think that the qualitative features do not change. For $\bar{\Delta} > 0.12$ the small system already gives a fairly good result. For comparison, the g factor obtained in the simple GA,[6] $g_s^{\mathrm{GA}} = 4/(1+\bar{m}^2)^2$, is shown by a broken line in Fig. 3. It is readily seen that $g_s(\bar{m}=0) \sim 4$ is fairly consistent with the GA. Furthermore it is shown that g_s^{xy} is very close to g_s^{GA} except for the small $\bar{\Delta}$ dependence. On the contrary, the enhancement of g_s^z near $\bar{m} \sim 0.15$ was not expected in the simple GA. This enhancement is the main reason for the stabilization of the AF order.

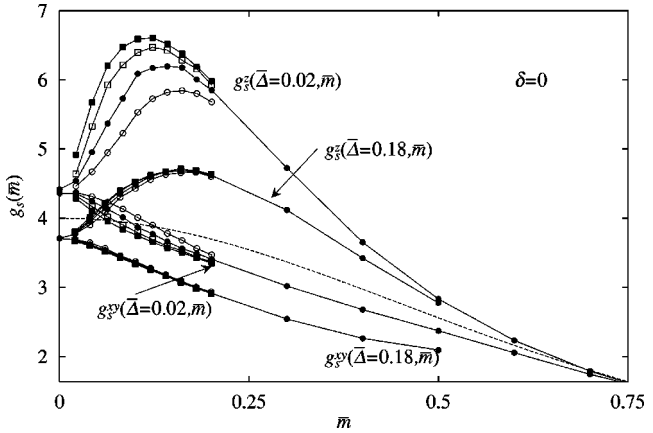

FIG. 3. $\bar{m}$ dependence of g_s^{xy} and g_s^z with fixing $\bar{\Delta} = 0.02$, 0.18. Sizes are 8×8 (open circles), 10×10 (filled circles), 12×12 (open squares), and 14×14 (filled squares). (The broken line is g_s^{GA}.)

The doping rate ($\delta = 1 - \bar{n}$) dependence of g_s^z is shown in Fig. 4. $\bar{\Delta}$ is fixed at 0.18 to avoid the size dependence. The maximum exists for every doping rate, but the enhancement becomes weaker as we increase the number of holes. Actually, the ratio of the values between $\bar{m} = 0.15$ and $\bar{m} = 0$, $g_s^z(\bar{m}=0.15)/g_s^z(\bar{m}=0)$, decreases from 1.28 ($\delta = 0$) to 1.13

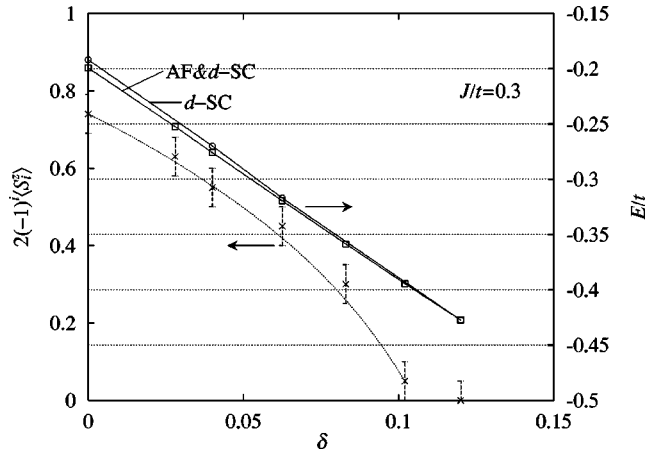

FIG. 2. Doping dependence of the ground-state energy and staggered magnetization at $J/t = 0.3$. The lines are guide to eyes.

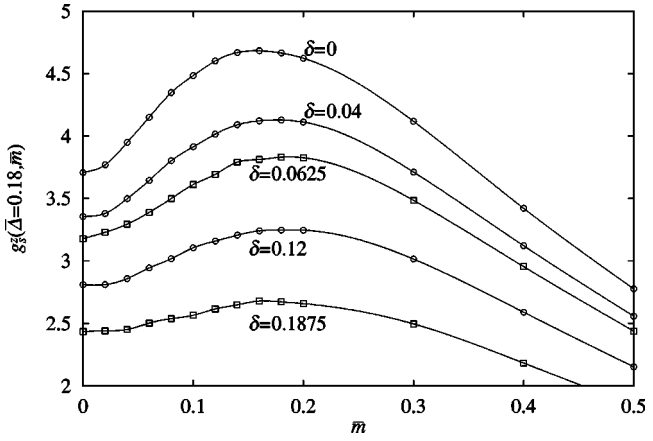

FIG. 4. $\bar{m}$ dependence of g_s^z for various hole doping with fixing $\bar{\Delta} = 0.18$.

($\delta=0.18$). This effect results in the disappearance of the AF order around the 10% doping rate.

Next let us briefly discuss the dependence on $\bar{\Delta}$ with m and δ fixed. Even if we change $\bar{\Delta}$, g_s^{xx} and g_s^z do not change so much. Only for the low doping cases ($\delta<5\%$), there is a small minima (less than 10% reduction) at $\bar{\Delta}\sim 0.17$ compared with $\bar{\Delta}=0$.

The g factor for the hopping term, $g_t(\bar{m})$, is also obtained numerically. We find that, on the contrary to g_s^z, g_t is very close to the GA, $g_t^{\mathrm{GA}}=2\delta/\{(1+\delta)(1+\bar{m}^2/(1-\delta^2))\}$. At $\bar{m}=0$, the obtained g_t is independent of $\bar{\Delta}$.

IV. SUMMARY

We use the VMC method to investigate the coexisting state of the AF and the d-wave SC order in the 2D t-J model. The ground-state energy is slightly lower than the pure d-wave SC state up to 10% hole doping.

We also study the g factors taking into account the full effect of the double occupancy prohibition. We find that the g_s^z has a peak around $\bar{m}\sim 0.15$. This property results in the stablization of the AF order and is not deduced from the conventional GA. On the other hand, g_s^{xy} and g_t show qualitatively the similar behavior to the GA in terms of $\bar{m}$.

These results offer important information to improve the GA and can be used in studies of the spatial variation of the order parameters as far as the variation is slow. For example, we can apply our g factors to the problem of vortex cores in the t-J model. It has been argued that an AF correlation can be induced around vortex cores or impurities. In such cases, the conventional mean-field approximation or GA will give wrong answers because the coexistence between the AF and d-wave SC is not treated reasonably. The modified GA obtained in this paper can be applied to these cases assuming that the g factors depend on the local values of order parameters. The stripe state which is experimentally observed is another important application.

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