Band-renormalization effects on antiferromagnetism and d-wave superconductivity in two-dimensional t-J model

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Abstract. Recent studies reported that antiferromagnetic (AF) states become stable and d-wave superconducting (d-SC) states are almost excluded in underdoped strongly correlated Hubbard models in two dimensions. In a viewpoint of many-body variational theory, this result stems from a band-renormalization effect (BRE) in AF states. Here, using a variational Monte Carlo method, BRE on AF and d-SC states are studied in the t-t'-J model, in which d-SC (AF) states have been considered to be more stable (fragile) than in the Hubbard model. Many features are qualitatively similar to the Hubbard model including effectiveness of BRE and the existence of a Lifshitz transition in AF states. However, a d-SC state becomes more stable than an AF state widely in the underdoped regime for J/t=0.3, in contrast to the Hubbard model.

1. Introduction
Until a few years ago, it had been considered that the strongly correlated Hubbard model yields results consistent with the features of cuprate superconductors (SCs). However, recent studies using various refined methods [1], including ours [2], has argued that antiferromagnetic (AF) states (and phase separation) widely prevail in the underdoped regime of two-dimensional Hubbard (t-t'-U) model for U ≳ W (W: band width), and homogeneous d_x^2−y^2-wave superconductivity (d-SC) hardly appears. This outcome apparently disagrees with the features of cuprates. Thus, it is urgent to clarify the origin of this discrepancy.

In the preceding study [2], we showed using a variational Monte Carlo (VMC) method that the above results are reached by taking account of band-renormalization effects (BRE) in the AF state. Meanwhile, it has been reported in the t-J model, another reduced model of cuprate SCs, that AF states are rapidly destabilized by doping and d-SC states becomes stable in a wide range of doping rate (δ = 1 − N_e/N_s; N_e: number of electrons, N_s: number of sites) [3, 4, 5]. The t-J model seems more favorable for d-SC than the Hubbard model. However, in these VMC studies, BRE was not introduced. Thus, the purpose of this study is to check whether the t-J model preserves such features favorable to d-SC even by introducing BRE, and to grasp to what extent the properties of the t-J model are inherited from those of the Hubbard model.

2. Model and Method
We consider the t-J model on a square lattice with diagonal hopping,

\[ \mathcal{H} = \mathcal{H}_t + \mathcal{H}_{t'} + \mathcal{H} = -t \sum_{(i,j)\sigma} \left( \tilde{c}^\dagger_{i\sigma} \tilde{c}_{j\sigma} + \text{H. c.} \right) - t' \sum_{(i,j)\sigma} \left( \tilde{c}^\dagger_{i\sigma} \tilde{c}_{j\sigma} + \text{H. c.} \right) + J \sum_{(i,j)} \left( \mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} \tilde{n}_i \tilde{n}_j \right), \quad (1) \]
where \( c_{i\sigma} \) is an operator which annihilates an electron of spin \( \sigma \) at site \( i \), \( \tilde{c}_{i\sigma} = c_{i\sigma}(1 - n_{i-\sigma}) \) with \( n_{i\sigma} = \tilde{c}_{i\sigma}^\dagger \tilde{c}_{i\sigma} \), \( S_i = \frac{1}{2} \sum_{\alpha, \beta} c_{i\alpha}^\dagger c_{i\alpha} c_{i\beta}^\dagger c_{i\beta} \) (\( \alpha \): Pauli matrix), \( \tilde{n}_i = \sum_{\sigma} \tilde{c}_{i\sigma}^\dagger \tilde{c}_{i\sigma} \), and \( (i,j) \) and \( (i,j) \) indicate a nearest-neighbor and next-nearest-neighbor pair, respectively. We use \( t \) and the lattice spacing as the units of energy and length, respectively. As a value plausible to cuprates, we use \( J/t = 0.3 \) in this paper.

To this model, we apply a VMC method, in which variational expectation values with respect to many-body trial wave functions are computed in a virtually exact manner, using a Monte Carlo algorithm; local correlation factors are treated exactly. As a trial wave function, we adopt Jastrow-type ones [6]: \( |\Psi\rangle \equiv \mathcal{P} \mathcal{P} \Phi \), where \( \Phi \) is a Hartree-Fock-type one-body state and \( \mathcal{P} \) and \( \mathcal{P} = \prod (1 - n_{j_1} n_{j_2}) \) are intersite and onsite correlation factors, respectively. For \( \mathcal{P} \), we consider both charge density and spin correlations between nearest-neighbor sites: \( \mathcal{P} = \mathcal{P}_h \mathcal{P}_s \), where

\[
\mathcal{P}_h = \prod_{(i,j)} [1 - (1 - \alpha) h_i h_j] \tag{2}
\]

which \( h_j = (1 - n_{j_1})(1 - n_{j_2}) \), and

\[
\mathcal{P}_s = \prod_{(i,j)} [1 - (1 - \beta_1) (n_{i_1} n_{j_1} + n_{i_2} n_{j_2})] [1 - (1 - \beta_2) (n_{i_3} n_{j_3} + n_{i_4} n_{j_4})] \tag{3}
\]

In Eqs. (2) and (3), \( \alpha, \beta_1, \) and \( \beta_2 \) are variational parameters. Using \( \mathcal{P}_h \) and \( \mathcal{P}_s \), we can assign distinct weights to all different nearest-neighbor bond configurations. \( \mathcal{P}_s \) plays a corrective role for the (often overestimated) AF order in \( \Phi_{AF} \) discussed below.

For the one-body part \( |\Phi\rangle \), we consider states with \( d \)-wave SC and AF orders independently similar to those used in Ref. [2]. A mixed state of the two orders will be discussed elsewhere. As a \( d \)-SC wave function, we use a canonical BCS wave function with fixed electron number \( N_e \):

\[
|\Phi_{d-SC}\rangle = \left( \sum_k A(k) c_{k\uparrow}^\dagger c_{k\downarrow} \right)^{N_e/2} |0\rangle, \tag{4}
\]

\[
A(k) = \frac{\Delta_d}{\varepsilon_k^{SC} - \xi + \sqrt{\varepsilon_k^{SC} \xi - \xi^2 + (\Delta_d)^2}}, \tag{5}
\]

where we assume a \( d_{x^2-y^2} \) symmetry SC gap \( \Delta_d = \Delta_{SC}(\cos k_x - \cos k_y) \). \( \Delta_{SC} \) and \( \xi \) are variational parameters that correspond to the singlet gap and chemical potential, respectively, for \( U/t \to 0 \). We will explain BRE owing to \( \varepsilon_k^{SC} \) shortly. As an AF state, we use

\[
|\Phi_{AF}\rangle = \prod_{k \in \{k_{occ}\}} a_{k\sigma}^\dagger a_{k\sigma}^\dagger |0\rangle \tag{6}
\]

with AF Hartree-Fock quasi-particle operators

\[
a_{k\sigma}^\dagger = \alpha_{k\sigma} c_{k\sigma}^\dagger + \text{sgn}(\sigma) \beta_{k\sigma} c_{k+Q,\sigma}^\dagger \quad (k \in \text{magnetic BZ}) \tag{7}
\]

\[
a_{k+Q,\sigma}^\dagger = -\text{sgn}(\sigma) \beta_{k\sigma} c_{k\sigma}^\dagger + \alpha_{k\sigma} c_{k+Q,\sigma}^\dagger \quad (k + Q \notin \text{magnetic BZ}), \tag{8}
\]

where \( Q = (\pi, \pi) \), \( \text{sgn}(\sigma) = 1(-1) \) for \( \sigma = \uparrow (\downarrow) \), and
\[ \alpha_k(\beta_k) = \frac{1}{\sqrt{2}} \left[ 1 - (+) \frac{\epsilon_{k}^{\text{AF}}} {\sqrt{(\epsilon_{k}^{\text{AF}})^2 + (\Delta_{\text{AF}})^2}} \right]. \] (9)

As emphasized in Ref. [2], it is vital, especially for \( \Phi_{\text{AF}} \), to take account of BRE owing to electron correlation, namely, energy dispersions \( \epsilon_k^\Lambda \) (\( \Lambda = \text{AF} \) or \( \text{d-SC} \)) in \( |\Phi_{\text{AF}}\rangle \) and \( |\Phi_{\text{d-SC}}\rangle \) should be also optimized. To this end, we fit \( \epsilon_k^\Lambda \) to a form of tight-binding bands up to the three-step distance as

\[ \epsilon_k^\Lambda = -2t(\cos k_x + \cos k_y) - 4t_1^\Lambda \cos k_x \cos k_y - 2t_2^\Lambda (\cos 2k_x + \cos 2k_y) \]
\[ - 4t_3^\Lambda (\cos 2k_x \cos k_y + \cos k_x \cos 2k_y) - 2t_4^\Lambda (\cos 3k_x + \cos 3k_y). \] (10)

Here, four hopping integrals \( t_j^\Lambda (j = 1 - 4) \) work as band-adjusting parameters that are optimized with the other variational parameters at the same time. The reason why almost all previous studies have not treated the optimization of \( \epsilon_k^\Lambda \) lies in the difficulty in the minimization of \( E/t : E/t \) is not only extremely slowly changing but also discontinuous as a function of \( t_j^\Lambda \) for finite-size systems. This discontinuous behavior originates in discontinuous changes of occupied \( \mathbf{k} \) points (or Fermi surface) as \( t_j^\Lambda \) change. Therefore, in this paper, we optimize the parameters with a fixed occupied \( \mathbf{k} \)-point set \( \{ \mathbf{k}_{\text{occ}} \} \) and find the global energy minimum among various \( \{ \mathbf{k}_{\text{occ}} \} \)'s. Here, for simplicity, we create \( \{ \mathbf{k}_{\text{occ}} \} \)'s according to

\[ \epsilon_k = -2t(\cos k_x + \cos k_y) - 4t_p \cos k_x \cos k_y, \] (11)

where \( t_p \) is varied in a moderate range [see Fig. 1 for instance]; note that \( t_p \) is used only for creating \( \{ \mathbf{k}_{\text{occ}} \} \) and is independent of \( t_1 \) in Eq. (10) as well as \( t' \) in Eq. (1). We confirmed that the optimized result \( \{ \mathbf{k}_{\text{occ}} \} \) using \( \epsilon_k \) in Eq. (11) becomes identical to that using a type of \( \epsilon_k^{\text{AF}} \) in Eq. (10) within the range of the system size and model parameters used in this paper.

Thus, because the variational energy \( E/t \) becomes a smooth function of variational parameters, optimization methods using differentiation become applicable such as the quasi-Newton method [7] and the stochastic reconfiguration method [8]. We mainly used the latter. The VMC calculations were performed on \( N_{\text{s}} (= L \times L) \)-site lattices with \( L = 10 - 16 \) and the periodic-antiperiodic boundary conditions. Typically, \( 2.5 \times 10^5 \) samples are used in estimating various physical quantities.

3. Results and discussions

To begin with, we discuss the optimization of AF state. Figure 1 shows the total energy per site \( E/t \) as a function of \( \{ \mathbf{k}_{\text{occ}} \} \)-determining parameter \( t_p \) for two values of doping rate \( \delta \). \( E/t \) discontinuously changes when \( \{ \mathbf{k}_{\text{occ}} \} \) changes. Because \( t_p \) determines only \( \{ \mathbf{k}_{\text{occ}} \} \), \( E/t \) is constant in a range of the same \( \{ \mathbf{k}_{\text{occ}} \} \). The other parameters are optimized in each at range of \( t_p \). For each \( \delta \), data for seven values of \( t'/t (-0.3 \leq t'/t \leq 0.3) \) are shown. The solid (open) arrows indicate the optimal range of \( t_p/t \) for positive (negative) values of \( t'/t \). The range of \( t_p \) or \( \{ \mathbf{k}_{\text{occ}} \} \) that gives the lowest energy is primarily determined by the sign of \( t'/t \) and not by the absolute value of \( t'/t \). For a negative \( t'/t \), the minimal \( E/t \) is given in narrow ranges of \( -0.2 \leq t_p/t \leq -0.1 \) for both doping rates. On the other hand, for a positive \( t'/t \), the minimal \( E/t \) is given in relatively wide ranges including \( t'/t = 0 \). Thus, the renormalized \( \{ \mathbf{k}_{\text{occ}} \} \) is distinct between the two cases. \( E/t \) is greatly improved compared to the energy without BR at \( t_p = t' \), especially for a large \(| t'/t | (\Delta E \sim 0.01) \).
Figure 1. Variational energy per site of the AF state is plotted as a function of the $\{k_{\text{occ}}\}$-determining parameter $t_p$ for two doping rates. The scale for $\delta = 0.0278$ (0.00833) is given in the left (right) axis. In each $\delta$, data for seven values of a model parameter $t'/t$ are compared. Empty (solid) arrows show the lowest energy region of $t_p/t$ for negative (positive) values of $t'$.

Figure 2. The momentum distribution functions along the path $(0,0)-(\pi,0)-(\pi,\pi)-(0,0)$ are compared between $t'/t = -0.3$ (red, type II) and 0.3 (blue, type I). A Lifshitz transition occurs at $t'/t \sim 0$. For each value of $t'/t$, data of three values of doping rate are plotted. The arrows indicate the centers of pocket Fermi surfaces for the two $t'/t$ values $J/t = 0.3$.

This different behavior according to the sign of $t'/t$ is probably related to the Lifshitz transition found in strongly correlated AF states for the Hubbard model[2]. Next, we discuss this point. As mentioned in Ref. [2], in the Hubbard model, a pocket-like Fermi surface centered at $(\pi/2, \pi/2)$ for $t' < t'_L$ (we called it type II AF) in doped AF states is switched to a one centered at $(\pi,0)$ (similarly type I AF) at $t'_L/t \sim -0.05$ as $t'/t$ increases. Actually, a corresponding difference in the position of pocket Fermi surface is observed between hole-doped and electron-doped cuprates by angle resolved photoemission spectroscopy experiments [9]. We find a corresponding Lifshitz transition in the $t-J$ model at $t'_L/t \sim 0$, where various quantities exhibit anomalous behavior (not shown). In Fig. 2, we show a momentum distribution function $n(k)$ along the path $(0,0)-(\pi,0)-(\pi,\pi)-(0,0)$ for $t'/t = 0.3(-0.3)$ as a typical case of the type I (II) AF state. It shows that a pocket Fermi surface centered at $(\pi/2, \pi/2)$ [(\pi,0)] appears for a negative [positive] value of $t'/t$, irrespective of the doping rate. This aspect already arises in theories for weak correlations [2], but the sharpness of the transition becomes conspicuous for strongly correlated cases. The present result in the $t-J$ model is consistent with that of the Hubbard model. Strictly speaking, the Lifshitz transition point in the $t-J$ model is situated at $t'/t \sim 0$ rather than $\sim -0.05$; for $t'/t = 0$, the position of Fermi surface depends on the system size and doping rate. Anyway, a type I (II) AF state is realized for $t'/t > 0$ ($t'/t < 0$) in the $t-J$ model.

We turn to the behavior of order parameters in the AF and $d$-SC states: the staggered magnetization...
\[ m = \frac{2}{N_s} \sum_j e^{i \mathbf{Q} \cdot \mathbf{r}_j} \langle S_j^z \rangle \]  \hspace{1cm} (12)

and \( P_d \), the nearest-neighbor pair correlation function at the farthestmost distance \( \mathbf{r} = (L/2, L/2) \) (for the definition of \( P_d \), see Ref. [10]). In Fig. 3, we show \( \delta \) dependence of \( m \) and \( P_d \) calculated using \( \Psi_{\text{AF}} \) and \( \Psi_{d-\text{SC}} \), respectively, for some values of \( t'/t \). The SC order parameter exhibits a domelike shape [3] and its area extends as \( t'/t \) decreases [5]. This \( t'/t \) dependence is understood as loss in kinetic energy (not shown). Note that the behavior of \( P_d \) changes only a little even if BRE is introduced, as seen for \( t'/t = -0.3 \) in Fig. 3. On the other hand, \( m \) is greatly affected by BRE. In previous studies (without BRE) [3], AF state is rapidly vanished as \( \delta \) increases, as shown by solid symbols in Fig. 3. When BRE is introduced, however, the range of \( m \) greatly extends to the overdoped regime. The tendencies of \( d \)-SC and AF orders are basically consistent with those in the Hubbard model [2]. In both models, BRE is vital to stabilize, especially, AF states.

**Figure 3.** AF and \( d \)-SC order parameters, namely, the SC correlation function of nearest-neighbor singlet pairs at the farthestmost distant point \( P_d \) (blue) and staggered magnetization \( m \) (red) are shown as functions of doping rate for several values of \( t'/t \). Solid symbols indicate the data for cases without BR for \( t'/t = -0.3 \), where we set \( t_1/t = t_2/t = -0.3 \) and \( t_3 = t_4 = 0 \). The system size is \( L = 12 \).

Finally, we consider the energy difference between the AF and \( d \)-SC states:

\[ \Delta E = E_{d-\text{SC}} - E_{\text{AF}}, \]  \hspace{1cm} (13)

If \( \Delta E/t < 0 (\Delta E/t > 0) \), the \( d \)-SC (AF) state is more stable. Figure 4 shows the \( \delta \) dependence of \( \Delta E/t \). As mentioned, in the Hubbard model, the area in the model parameter space where the \( d \)-SC state is more stable than the AF state is limited to a narrow range in the overdoped density [2]. However, in the \( t-J \) model with \( J/t = 0.3 \), \( \Psi_{d-\text{SC}} \) is more stable than \( \Psi_{\text{AF}} \) in a much wider range of \( \delta \) for small values of \( |t'/t| \). This tendency is consistent with many previous studies. Thus, a phase

**Figure 4.** Energy difference between SC and AF states is shown as a function of doping rate. For \( \Delta E > 0 \), the AF state is more stable than the \( d \)-SC state. Data of four values of \( t'/t \) are plotted; for each \( t'/t \), date of two system sizes (\( L = 10,12 \)) are compared.
diagram in the $t$-$J$ model for $j/t = 0.3$ will be at least quantitatively different from that obtained for the Hubbard model with $U/t = 12$.

4. Summary
In this paper, we studied properties of an AF and $d$-SC states independently in the $t$-$J$ model, for comparing with those in the Hubbard model [2]. We use a VMC method which takes account of BRE. The AF ($d$-SC) state is markedly (a little) stabilized by BRE. In the AF state, a Lifshitz transition was found at $t'/t \sim 0$, corresponding to that in the Hubbard model. In contrast to the Hubbard model with $U/t = 12$, the $d$-SC state becomes more stable in a wide area in the underdoped regime for $j/t = 0.3$. It is important to pursue the origin of this stability of $d$-SC state. In future publications, we would like to consider $j/t$ dependence, treat a mixed state of AF and SC orders, and check the stability against inhomogeneous phases in the $t$-$J$ model.

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