Interhole correlation and phase separation in $t$-$J$ model

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Abstract. Interhole and interelectron correlations as well as a transition to phase separation in the $t$-$J$ model near half filling are reconsidered using a variational Monte Carlo method. As a trial wave function, we use a state that can simultaneously represent a $d$-wave superconducting and antiferromagnetic (AF) orders and allows for nearest-neighbor hole-hole and spin-spin correlation factors and band renormalization effects. It is found that a transition occurs at $J = J_{PS} \sim 2.5t$ for the doping rates $\delta = 0.08$ and $0.20$ from a seemingly uniform state to phase separation ($J > J_{PS}$) of singly occupied sites and empty sites. For $J < J_{PS}$, where the values used for cuprate superconductors ($0.25 \lesssim J/t \lesssim 0.5$) are included, the interhole correlation is always repulsive. This result is negative to an intuitive picture for cuprates: Two holons coherently move in the background of AF orders.

1. Introduction

In early research on cuprate superconductors, it was often demonstrated that two holons (empty sites) can coherently move without destroying the background antiferromagnetic (AF) order, but a single holon cannot. A similar notion that the interhole correlation is attractive even for a small $J/t$ (plausible for cuprates) seems still alive. Furthermore, a problem as to the phase separation (PS) near half filling for small $J/t$ is still not settled [1, 2]. In such contexts, it is significant in the square-lattice $t$-$J$ model [3] to clarify at what values of $J/t$ the interhole correlation is switched from repulsive to attractive ($J_I/t$) and PS occurs ($J_{PS}/t$) when we fix the doping rate $\delta = 1 - N_e/N_s$ with $N_e$ and $N_s$ being number of electrons and number of sites, respectively. It is certain for $J/t \to 0$ that total energy ($E/t$) is lowered only by the hopping ($t$) term, so that the correlation should be repulsive to keep other holes away and the state should be uniform. For $J/t \to \infty$, because $E/t$ is reduced only by the superexchange ($J$) term, the correlation should be attractive and the state phase separates. For $\delta \to 1$, it is exactly known that $J_I/t = 2 [4, 5]$ and $J_{PS}/t = 3.4367 [4]$, whereas for a small $\delta$ of our interest, the problems are still unresolved; it remains unclear even whether $J_I/t$ and $J_{PS}/t$ differ or coincide.

In this study, we reconsider intersite correlation and PS in the $t$-$J$ model using a many-body variation theory with recently developed wave functions and procedures. As a first step, in the Jastrow-type trial wave function, we consider nearest-neighbor interhole and interspin correlation factors, which is simple but can cope with the present problem. In this trial state, we allow for $d$-wave superconducting ($d$-SC) and antiferromagnetic (AF) orders simultaneously, for both of which band renormalization effects (BRE) [6] are introduced. Using this wave function, we found $J_I = J_{PS}$ for underdoped ($\delta = 0.08$) and overdoped ($\delta = 0.20$) regimes. Then, we analyze the properties of PS arising for $J > J_{PS} \sim 2.5t$. 

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2. Model and Method
We consider the standard $t$-$J$ model [3] ($J/t \geq 0$) on the square lattice,

$$
H = \mathcal{H}_t + \mathcal{H}_J = -t \sum_{\langle i,j \rangle \sigma} \left( \hat{c}_{i \sigma}^\dagger \hat{c}_{j \sigma} + \text{h.c.} \right) + J \sum_{\langle i,j \rangle \sigma} \left( \mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} \tilde{n}_i \tilde{n}_j \right),
$$

(1)

where $c_{j \sigma}$ is an operator which annihilates an electron of spin $\sigma$ at site $j$, $\hat{c}_{i \sigma} = c_{i \sigma} (1 - n_{i-\sigma})$ with $n_{i\sigma} = c_{i \sigma}^\dagger c_{i \sigma}$, $\mathbf{S}_j = \frac{1}{2} \sum_{\alpha,\beta} \epsilon_{j \alpha}^\dagger \sigma_{\alpha\beta} c_{j \beta}$ ( $\sigma$: Pauli matrix), $\tilde{n}_j = \sum_{\sigma} \hat{c}_{j \sigma}^\dagger \hat{c}_{j \sigma}$. $\langle i, j \rangle$ in the summations indicates a pair of nearest-neighbor sites. We use $t$ and the lattice spacing as the units of energy and length, respectively. This model was derived from a more realistic $d$-$p$ model, but it is also connected to the Hubbard model near half filling through a strong-coupling expansion for $J/t \to 0$ and $t/U \to 0$ with $J = 4t^2/U$. The parameters of this model are the ratio of interaction strength $J/t$ and doping rate $\delta$. As values plausible to cuprates, $J/t = 0.25 - 0.5$ are often used in literatures; this model becomes unrelated to the Hubbard model for $J/t \gtrsim 1$.

To this model, we apply a VMC method, which enables us to exactly compute variational expectation values with respect to many-body trial wave functions. As a trial wave function, we adopt a Jastrow type: $|\Psi\rangle = P_j P_G |\Phi\rangle$. In the correlation factors, the complete exclusion of doubly occupied sites by $P_G = \prod_j (1 - n_{j\uparrow} n_{j\downarrow})$ is inevitable for the $t$-$J$ model. The choice of intersite correlation factor $P_j$ is important to the present subject. As a first step, we restrict it to between the nearest-neighbor sites, but take account of both charge density and spin correlations: $P_j = P_h P_s$. The charge part is written as an interhole correlation:

$$
P_h = \prod_{\langle i,j \rangle} \left[ 1 - (1 - \xi_{h-h}) h_i h_j \right],
$$

(2)

with $h_j = (1 - n_{j\uparrow})(1 - n_{j\downarrow})$, and the spin-dependent part is given by

$$
P_s = \prod_{\langle i,j \rangle} \left[ 1 - (1 - \xi_{\uparrow-\uparrow}) (n_{i\uparrow} n_{j\uparrow} + n_{i\downarrow} n_{j\downarrow}) \right] \left[ 1 - (1 - \xi_{\downarrow-\downarrow}) (n_{i\uparrow} n_{j\downarrow} + n_{i\downarrow} n_{j\uparrow}) \right],
$$

(3)

where $\xi_{h-h}$, $\xi_{\uparrow-\uparrow}$ and $\xi_{\downarrow-\downarrow}$ are variational parameters. If the optimized value is $1/\xi_{h-h} > 1$ ($0 \leq 1/\xi_{h-h} < 1$), the interhole correlation is repulsive (attractive). This is also the case for $\xi_{\uparrow-\uparrow}$ and $\xi_{\downarrow-\downarrow}$. Using $P_h$ and $P_s$, we can assign distinct weights to all different nearest-neighbor bond configurations. $P_s$ plays a corrective role for the (often overestimated) AF order in $\Phi_{AF}$ discussed below.

Now, we turn to the one-body state $|\Phi\rangle$ in $|\Psi\rangle$. To construct a mixed state of $d$-wave SC and AF orders, we first mention pure states of each order [6]. For a $d$-SC wave function, we use a BCS state with the electron number fixed:

$$
|\Phi_{d-SC}\rangle = \left( \sum_{\mathbf{k}} A(\mathbf{k}) c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\downarrow}^\dagger \right)^{\frac{N_e}{2}} |0\rangle,
$$

(4)

$$
A(\mathbf{k}) = \frac{\Delta_d}{\epsilon^{SC}_k - \zeta + \sqrt{(\epsilon^{SC}_k - \zeta)^2 + (\Delta_d)^2}},
$$

(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 $\zeta$ are variational parameters, which correspond to the SC gap and chemical potential, respectively, for $U/t \to 0$. BRE explained below is introduced into $\epsilon^{SC}_k$. For an AF state, we employ a Hartree-Fock type at half filling,

$$
|\Phi_{AF}\rangle = \prod_{\mathbf{k} \in \{\text{k_{occ}\} }} a_{\mathbf{k}\uparrow}^\dagger a_{\mathbf{k}\downarrow}^\dagger |0\rangle
$$

(6)
with AF quasi-particle operators

\[ a_{k,\sigma}^\dagger = \alpha_k c_{k,\sigma}^\dagger + \text{sgn}(\sigma) \beta_k c_{k+Q,\sigma}^\dagger \] \quad (k \in \text{magnetic BZ}),

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

where \( Q = (\pi, \pi) \), \( \text{sgn}(\sigma) = 1 (-1) \) for \( \sigma = \uparrow (\downarrow) \), and

\[ \alpha_k(\beta_k) = \frac{1}{\sqrt{2}} \sqrt{1 - (+)} \frac{\epsilon_k^{AF}}{(\epsilon_k^{AF})^2 + (\Delta_{\Lambda k})^2}. \] \quad (9)

BRE is also introduced into \( \epsilon_k^{AF} \). A mixed state actually used is obtained by replacing the bare electron operators \( c_{\sigma}^\dagger \) in Eq. (4) by the AF quasiparticle operators \( a_{\sigma}^\dagger \) in Eqs. (7) and (8) [7]:

\[ |\Phi_{\text{Mixed}}\rangle = \left( \sum_k A(k) a_{k,\uparrow}^\dagger a_{-k,\downarrow}^\dagger \right)^{\frac{N}{2}} |0\rangle. \] \quad (10)

It is vital, especially for the AF order, to take account of BRE [6]. To this end, we fit \( \epsilon_k^A (\Lambda = \text{AF or } d\text{-SC}) \) in \( |\Phi_\Lambda\rangle \) to a form of tight-binding bands up to the three-step distance as,

\[ \epsilon_k^A = -2t(\cos k_x + \cos k_y) - 4t_1^A \cos k_x \cos k_y - 2t_2^A (\cos 2k_x + \cos 2k_y) \]
\[ -4t_3^A (\cos k_x \cos k_y + \cos k_x \cos 2k_y) - 2t_4^A (\cos 3k_x + \cos 3k_y). \] \quad (11)

Here, four hopping integrals \( t_j^A \) (\( j = 1-4 \)) for each \( \Lambda \) work as band-adjusting parameters, which are simultaneously optimized with the other variational parameters. Note that it is important to optimize \( t_j^{d\text{-SC}} \) and \( t_j^{AF} \) in \(|\Phi_{\text{Mixed}}\rangle\) independently.

In optimization, the stochastic reconfiguration method [8] is used. The VMC calculations were performed on the \( N_{\text{seg}} (= L \times L) \)-site lattice with \( L = 10 \), and the periodic-antiperiodic boundary conditions are imposed. Typically, \( 2.5 \times 10^5 \) samples are used for estimating physical quantities.

3. Results

We start with the character of intersite correlation. Figure 1 shows the evolution of the optimized inverse correlation parameters (1/\( \xi \)) as \( J/t \) increases. The interhole correlation preserves 1/\( \xi_{\text{h-h}} > 0 \) up to \( J/t = J_{PS}/t \sim 2.5 \) and tends to rise for \( J \sim J_{PS} \), especially, in the underdoped regime in (b). That is, the interhole correlation is repulsive and becomes stronger as \( J/t \) increases. In contrast, the electron correlations both for parallel and antiparallel spins are attractive (1/\( \xi_{\uparrow-\uparrow}, 1/\xi_{\downarrow-\downarrow} < 1 \)) and become strong as \( J/t \) increases. Because a repulsive (attractive) correlation between holes (electrons) encourages the hopping (exchange) term, the two terms compete with each other in this regime of \( J/t \). In Fig. 1, all 1/\( \xi \) suddenly drop to small values (1/\( \xi \ll 1 \)) at \( J = J_{PS} \); all intersite correlations become strongly attractive for \( J > J_{PS} \). As expected and as we will confirm below, this anomaly indicates a transition to PS. To sum up, the interelectron correlations are always attractive and become strong as \( J/t \) increases, whereas the interhole correlation is repulsive up to \( J = J_{PS} \) far above the plausible range of cuprates (0.25 \( \lesssim J/t \lesssim 0.5 \)). The interhole correlation becomes attractive only when PS is arising (\( J > J_{PS} \)). Incidentally, the value of \( J_{PS}/t \) is \( \sim 2.5 \) both for \( \delta = 0.08 \) and 0.20. This probably originates in the short-range Jastrow factor used. We would like to check such points using long-range factors in future.
Figure 1. \( J/t \) dependence of optimized inverse intersite correlation parameters for (a) overdoped (\( \delta = 0.20 \)) and (b) underdoped (\( \delta = 0.08 \)) cases. The dashed lines indicate \( \xi = 1 \), which is the boundary of whether the intersite correlation is attractive (\( 1/\xi < 1 \)) or repulsive (\( 1/\xi > 1 \)).

Figure 2. The two elements of energy per site (left axis) and the order parameters of \( d \)-SC (\( P_d \)) and AF (\( m \)) orders (right axis) are plotted as functions of \( J/t \). The doping rates are (a) 0.20 and (b) 0.08. For ease of eyes, \( P_d \) is shown by 15 magnifications. The dashed lines indicate (1 − \( \delta \))\( m_0 \) [red] and (1 − \( \delta \))\( E_{\text{Heis}}/J \) [green] with \( m_0 \) and \( E_{\text{Heis}} \) being \( m \) and \( E_J \) at half filling, respectively.

Next, let us consider the \( d \)-SC and AF orders. In Fig. 2, \( J/t \) dependence of the order parameters for both orders are shown; \( m \) is the staggered magnetization defined as

\[
m = \frac{2}{N_a} \left| \sum_j e^{iQ_{xy}} \langle S_j^z \rangle \right|,
\]

(12)
and $P_d$ is the $d$-SC correlation function for nearest-neighbor singlet pairs given as

$$P_d(\mathbf{r}) = \frac{1}{N_s} \sum_i \sum_{\tau, \tau'} (-1)^{1-\delta, \delta'} \left\langle \Delta_0^\dagger(\mathbf{R}_i) \Delta_0(\mathbf{R}_i + \mathbf{r}) \right\rangle,$$

where $\mathbf{x}$ ($\mathbf{y}$) denotes the lattice vector in $x$ ($y$) direction and $\Delta_0^\dagger(\mathbf{R}_i)$ is the creation operator of a nearest-neighbor singlet pair around site $\mathbf{R}_i$: $\Delta_0^\dagger(\mathbf{R}_i) = (c_{i\uparrow}^\dagger c_{i+\tau\uparrow}^\dagger + c_{i+\tau\downarrow}^\dagger c_{i\downarrow}^\dagger)/\sqrt{2}$. For $P_d(\mathbf{r})$, we will plot the value at the farthest point $\mathbf{r} = (L/2, L/2)$ as $P_d$. We find that the $d$-SC order appears for any $J/t < J_{PS}$ in both doping rates, whereas the AF order vanishes for $J/t < 1.5$ in the overdoped case. This tendency is consistent with that for the Hubbard model with moderate values of $U/t$ (e.g. $=12$) [6]; the $d$-SC order is somewhat more favored in the $t$-$J$ model. Both order parameters monotonically become large as $J/t$ increases, indicating that the driving force of both orders is, in common, magnetic interaction. When the present-type PS occurs, $P_d$ vanishes. In contrast, AF orders become more robust and almost constant $m = m_0(1-\delta)$ for $J > J_{PS}$, where $m_0$ is the value of $m$ at half filling 0.737 (Heisenberg model). The subtle difference between this value (dashed lines) and the corresponding VMC data for $J > J_{PS}$ stem from finite-size effects.

Now, we consider the state for $J > J_{PS}$. The above behavior of $m$ suggests that the state phase separates into two domains: the domain of half-filled Heisenberg model and the domain of holons (empty sites). In Fig. 2, we also show the $J/t$ dependence of energy elements ($E_t = \langle \mathcal{H}_t \rangle$, $E_J = \langle \mathcal{H}_J \rangle$) per site. For $J > J_{PS}$, the hopping energy vanishes, whereas the exchange energy becomes almost constant $E_J = E_{\text{Heis}}(1-\delta)$ with $E_{\text{Heis}} = -1.165J$ being the energy of the Heisenberg model ($\delta = 0$). This behavior also supports the above PS. In Fig. 3, snapshots of typical electron configurations taken in VMC sweeps for $J/t = 0.3$ and 3.0 ($\delta = 0.20$) are shown to corroborate PS of the present type. In the former ($J < J_{PS}$), electrons are uniformly distributed. In the latter ($J > J_{PS}$), however, the electron configuration is composed of a holon island ($\delta = 0$) and a Heisenberg sea ($\delta = 1$).

$$\delta=0.20 \quad L=10$$

\begin{align*}
+ + + + 0 + + + + & + + + + + + + + \\
+ + 0 + + 0 + 0 + & + + + + + + + \\
+ + + + 0 + 0 + 0 + & + + 0 0 0 0 + + + \\
+ + + 0 0 + + + + & + + 0 0 0 0 + + + \\
+ + + 0 + + + + & + + 0 0 0 0 + + + \\
+ + + 0 + + + + & + + 0 0 0 0 + + + \\
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+ + + 0 + + + + & + + 0 0 0 0 + + + \\
+ + + 0 + + + + & + + 0 0 0 0 + + + \\
J/t=0.3 & J/t=3.0
\end{align*}

**Figure 3.** Snapshots of typical electron configurations in VMC sweeps with the optimized states are compared between $J/t = 0.3$ and 3.0. The characters ‘+’, ‘-’, and ‘0’ indicate up- and down-spin sites, and empty site, respectively. For $J/t \geq 2.5$, phase separation occurs with an AF order. The AF order vanishes for $J/t \lesssim 1.5$ at $\delta = 0.20$.

$$L=10, \ \delta=0.08$$

**Figure 4.** Real-space charge density correlation function for various values of $J/t$. Cold (warm) colors are used for $J < J_{PS}$ ($J > J_{PS}$).
In Fig. 4, we show the charge density correlation function,

\[ N(r_i) = \frac{1}{N_s} \sum_j \langle n_j n_{j+i} \rangle - n^2 = \frac{1}{N_s} \sum_j \langle h_j h_{j+i} \rangle - h^2. \]

(14)

where \( n_j = \sum_\sigma n_{j\sigma}, \) \( n = N_e/N_s, \) and \( h = 1 - n. \) For \( J > J_{PS}, \) reflecting PS, \( N(r_i) \) exhibits appreciable values for \( |r_i| \leq R, \) compared to the value in the long-distance limit \( N(\sqrt{2L}/2), \) where \( R \) is the longest intersite distance possible in the holon island: \( R = \sqrt{10} \) \((4 \times 2 \text{ island})\) in the present case. \( R \) depends on the system size. On the other hand for \( J < J_{PS}, \) \( N(r_i) \) converges to the long-distance value for \( |r_i| > D, \) where \( D \) is determined by the length of correlation factors: \( D = 1 \) (nearest neighbors) in the present case. \( D \) will not be varied even if \( L \) is varied. It means that the system is uniform for \( J < J_{PS}. \)

4. Summary and discussions

We studied interhole and interelectron correlations, as well as the phase separation, by applying a VMC method with a wave function that can exhibit AF and \( d-\text{SC} \) orders to the square-lattice \( t-J \) model. In this report, the intersite correlation factor is restricted to that between nearest-neighbor sites. It is found that (i) the interhole correlation remains repulsive up to the transition point to PS \( J = J_{PS} \approx 2.5t \) both for \( \delta = 0.08 \) and \( 0.20. \) This contrasts with an early intuitive argument of SC in cuprates by coherent motion of hole pairs. In this regime, both AF and \( d-\text{SC} \) order become robust as \( J/t \) increases. (ii) A transition to PS is observed within a single wave function. For \( J > J_{PS}, \) the state separates into the domains of \( \delta = 0 \) and 1 (Fig. 3).

In previous VMC studies \([5, 9], \) the transition point to PS was estimated by comparing the variational energy of the uniform state with the exact estimation of the separated phase. Therefore, the transition point tends to be underestimated e.g. \( J/t \approx 2 \) for \( \delta = 0.20. \) There has been intensive debate as to whether the transition point to PS for \( \delta = 0 \) is \( J/t = 0 \) or a finite small value, e.g. \( J/t = 0.7 \) \([10]. \) In many related studies \([11], \) charge compressibility becomes zero in appreciable ranges of \( \delta \) near half filling, meaning that arbitrary electron densities in these ranges are allowed as separated phases. It is an important remaining problem whether or not these separated phases continue to what we treated in this report as \( J/t \) is increased.

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