Variational Monte Carlo simulation in hole-doped cuprate superconductors: Competition between antiferromagnetism and superconductivity

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Abstract

We present variational Monte Carlo (VMC) results for the Gutzwiller-projected coexisting state including both antiferromagnetic (AFM) order and superconducting (SC) order in the two-dimensional $t-t'-t''-J$ model. By further considering off-site spin correlation between electrons, in contrast to earlier VMC results [Phys. Rev. Lett. 102, 027002 (2009)], we find the apparent competition between AFM order and SC order near the underdoped regime instead of coexistence. The local ferromagnetic correlation introduced by spin-spin Jastrow correlators seem to be responsible for the disappearance of the coexisting state. We also demonstrate that the quasiparticle spectral weight from upper (lower) AFM band are strongly diminished (enhanced) by the spin-spin correlation. This result obviously leads to the loss of antinodal electron pockets and the appearance of nodal hole pockets as passing from the AFM phase to the SC phase in hole-doped cuprates, which is in consistent with the observation by angle-resolved photoemission spectroscopy.

Keywords: Variational Monte Carlo method; Strong electron correlation; Cuprate superconductor

1. Introduction

The doping phase diagram near the underdoped region is one of the important and long-debated issues with high-$T_c$ cuprates [1]. Since the parent compound is antiferromagnetic (AFM) Mott insulator, the AFM correlation plays...
a significant role in the emergence of superconductivity by doping charge carriers. The intrinsic proximity of the superconducting (SC) phase with the AFM phase is also shared by the phase diagrams of other SC materials, such as iron pnictides \[2\] and heavy fermion superconductors \[3\]. The multi-layered cuprate superconductors exhibit the coexistence of AFM and SC states at underdoping discovered by nuclear magnetic resonance measurements \[4, 5\]. However, the AFM phase and the SC phase never coexist in the phase diagram of single-layered cuprates such as La\(_{2-x}\)Sr\(_x\)CuO\(_4\) \[6\] and Bi\(_2\)Sr\(_2\)CuO\(_{6+\delta}\) \[7\]. In particular, Bi\(_2\)Sr\(_{2-x}\)La\(_x\)CuO\(_{6+\delta}\) systems shows that the three-dimensional AFM region, separated by the SC phase, even survives until a high underdoping level \[8\].

The existence of the coexisting state has been found by analytical and numerical approaches in Hubbard-type models \[9, 10, 11, 12, 13, 14, 15\] and \(t - J\)-type models \[16, 17, 18, 19, 20, 21, 22\]. They seem to contribute the underlying mechanism to the coexisting state observed in multi-layered cuprates. However, a proper mechanism to explain why these two phases do not like to coexist in single-layered cuprates remains needed. Interestingly, some previous studies proposed the spin-bag mechanism for superconductivity since two spin bags would attract each other to form a Cooper pair and lower the total energy \[23, 24, 25\]. As for doping more holes, therefore, it is necessary to re-examine how the local distortion of the AFM background around holes influences AFM order and SC order.

On the other hand, one of the most exciting experimental results is the observation of quantum oscillations in the hole-doped cuprates which pointed to electron pockets \[26, 27\]. In particular, they proposed that these electron pockets probably originate from the Fermi surface reconstruction caused by the onset of a density-wave phase, e.g. the AFM phase. Unfortunately the electron-like Fermi pockets have never been found in most of hole-doped cuprates using angle-resolved photoemission spectroscopy (ARPES) \[28, 29, 30\]. Thus, to comprehend the loss of the electron pocket observed by ARPES experiments, we inquire to what extent into the electronic correlations ignored in mean-field calculations.
In this work, we study Gutzwiller’s trial wave functions with the coexistence of AFM order and SC order by means of variational Monte Carlo (VMC) method. To improve the trial state, we further consider the off-site correlations between two electrons by applying suitable Jastrow correlators. Surprisingly, the long-range AFM order is strongly enhanced due to the local ferromagnetic (FM) Jastrow correlation, or precisely local AFM distortion, giving rise to the disappearance of the coexisting state near underdoping in the phase diagram. Besides, the spin-spin correlation in the non-coexisting state transfers the quasiparticle spectral weight from the antinodal electron pockets to the lower AFM band, and also the nodal hole pockets can remain until superconductivity occurs. Therefore, it is expected that the signal of the electron pockets around antinodes cannot be found in many hole-doped compounds by using ARPES.

2. Theory

Let us begin by the Hamiltonian on a square lattice of size $16 \times 16$,

$$H = -\sum_{i,j,\sigma} t_{ij} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + J \sum_{\langle i,j \rangle} \left( \mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j \right) ,$$  

(1)

where the hopping $t_{ij} = t, t', t''$ for sites $i$ and $j$ being the nearest, second-nearest, and third-nearest neighbors, respectively. Other notations are standard. We restrict the electron creation operators $\hat{c}_{i\sigma}^\dagger$ to the subspace without doubly-occupied sites. In the following, the bare parameters $(t', t'', J)/t$ in the Hamiltonian are set to be in the hole-doped regime: $(-0.3, 0.15, 0.3)$. In order to understand how AFM order and SC order compete in variational phase diagram, we choose the mean-field ground state including both AFM order and SC order (AFSC) as a starting point,

$$|\Psi_{AFSC}\rangle = \prod_{k,s=\{a,b\}} \gamma^a_{k}\gamma^s_{-k\downarrow} |0\rangle,$$

(2)

where the prime means the product only includes momenta inside the magnetic zone boundary (MZB). Note that $s$ represents the quasiparticle coming from the
upper AFM band \((s = b)\) or the lower AFM band \((s = a)\). The Bogoliubov’s quasiparticle operators \(\gamma_{ks}^{s}\) are defined as

\[
\gamma_{ks}^{s} = u_{ks}^{s}\hat{s}_{ks} - \sigma v_{ks}^{s}\hat{s}_{k}\bar{s}^{\dagger}.
\]  

(3)

The coefficients \(u_{ks}^{s}\) and \(v_{ks}^{s}\) are the BCS coherence factor of AFM quasiparticles corresponding to the \(s\) band,

\[
(u_{ks}^{s})^2 = \frac{1}{2} \left(1 + \frac{\epsilon_{k}^{s}}{\sqrt{\epsilon_{k}^{s}}^2 + \Delta_{k}^{s}}\right),
\]

\[
(v_{ks}^{s})^2 = 1 - (u_{ks}^{s})^2,
\]

(4)

where the AFM band dispersion \(\epsilon_{k}^{b/a} = \epsilon_{k}^{b} \pm \sqrt{(\epsilon_{k}^{b})^2 + m_{\text{AFM}}^2}\) and \(\epsilon_{k}^{s} \equiv (\epsilon_{k}^{s + Q_{k}}) / 2\).

Here \(\epsilon_{k}\) is the normal-state dispersion. \(\Delta_{k} = 2\Delta \cos k_{x} - \cos k_{y}\) is \(d\)-wave pairing amplitude and \(m\) AFM order parameter. The annihilation operators for AFM bands, \(\hat{s}_{ks}\), are given by

\[
\begin{pmatrix}
    a_{k\sigma} \\
    b_{k\sigma}
\end{pmatrix} = \begin{pmatrix}
    \alpha_{k} & \sigma \beta_{k} \\
    -\sigma \beta_{k} & \alpha_{k}
\end{pmatrix} \begin{pmatrix}
    c_{k\sigma} \\
    c_{k + Q\sigma}
\end{pmatrix},
\]

(5)

with \(Q = (\pi, \pi)\) and the coefficients

\[
\begin{align*}
\alpha_{k}^2 &= \frac{1}{2} \left(1 - \frac{\epsilon_{k}^{-}}{\sqrt{\epsilon_{k}^{-}}^2 + m_{\text{AFM}}^2}\right), \\
\beta_{k}^2 &= 1 - \alpha_{k}^2.
\end{align*}
\]

(6)

In order to introduce more correlations in the mean-field wave function, we first formulate the trial wave function fixing the number of electrons \(\hat{P}_{N_{e}}\) with on-site Gutzwiller projector \(\hat{P}_{G}(= \prod_{i} (1 - \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}))\) and charge-charge Jastrow correlator \((\hat{P}_{j}^{CC})\) [31, 32],

\[|\Psi_{CC}\rangle = \hat{P}_{N_{e}} \hat{P}_{G} \hat{P}_{j}^{CC} |\Psi_{AFSC}\rangle.\]

(7)

More importantly, we also consider the correlation between spins by using spin-spin Jastrow correlator \((\hat{P}_{j}^{SS})\),

\[|\Psi_{CCSS}\rangle = \hat{P}_{j}^{SS} |\Psi_{CC}\rangle.\]

(8)
The Jastrow correlator is constructed by classical Boltzmann operator, \( \hat{P}_j = e^{\hat{H}_j} \), encoding the intersite correlations. For the sake of simplicity, \( \hat{H}_i \) depicting charge \((i = CC)\) and spin \((i = SS)\) parts are chosen to be diagonal in real-space configuration. The charge-charge Jastrow correlator describes the short- and long-range correlations between holes in the lattice system. Thus,

\[
\hat{H}_{CC} = \sum_{i<j} \eta_{ij} \hat{n}_{ih} \hat{n}_{hj},
\]

with \( \eta_{ij} \equiv \ln(r_{ij}^{\alpha} v_{i+\gamma}) \). Here \( r_{ij} \) is the chord length of \(|\mathbf{r}_i - \mathbf{r}_j|\) and \( \hat{n}_{ih} = 1 - \sum_{\sigma} \hat{n}_{i\sigma} \). We consider three parameters \( v_\gamma \), the nearest \((\gamma = 1)\), second-nearest \((\gamma = 2)\) and third-nearest \((\gamma = 3)\) neighbors, standing for short-range hole-hole repulsion if \( v_\gamma < 1 \). The factor \( r_{ij}^{\alpha} \) denotes attractive long-range \((r_{ij} > 1)\) and repulsive short-range \((r_{ij} < 1)\) correlations between holes if \( \alpha > 0 \).

A similar formalism to the spin-spin correlation has been considered at half-filling \[33\]. We further imitate the formalism described above to write down the spin-spin Jastrow correlator,

\[
\hat{H}_{SS} = \sum_{i<j} \kappa_{ij} \hat{S}_{iz} \hat{S}_{jz},
\]

where \( \kappa_{ij} \equiv \ln(r_{ij}^{\beta} w_{i+\gamma}^{\delta}) \) and \( \hat{S}_{iz} \) the spin operator along \( z \) direction at site \( i \). The only difference from the charge counterpart is that the sign of \( \hat{S}_{iz} \hat{S}_{jz} \) determines the type of magnetic correlations. In other words, it will be the FM (AFM) correlation if \( \hat{S}_{iz} \hat{S}_{jz} > 0 \ (< 0) \). In addition to the parameter \( \beta \) controlling the long-range spin correlations, we consider the other three parameters \( w_{\gamma=1,2,3} \) for the neighboring spin-spin correlations. For example of the FM case, the short-range correlation would be suppressed when \( w_\gamma < 1 \). On the other hand, the factor \( r_{ij}^{\beta} \) control the long-range \((r_{ij} > 1)\) and short-range \((r_{ij} < 1)\) correlations. In the long-range case of \( \beta < 0 \), for instance, \( r_{ij}^{\beta} \) would decrease the FM correlation but conversely increase the AFM correlation.

In addition to the ground state, we also propose a trial wave function for the low-lying excitation of the Gutzwiller-projected coexisting state simply gener-
ated by Gutzwiller projecting the mean-field excited state

\[ |\psi_{AFSC}^{k \sigma s} \rangle = (\gamma_{k \sigma}^s)^\dagger |\psi_{AFSC} \rangle. \]  

(11)

Here we have applied the particle-hole transformation \[34, 35\] into Eq. (11) to avoid the divergence from the nodes of the mean-field wave function. The Gutzwiller-projected excited state with both AFM order and SC order fixing to \(N_e - 1\) electrons is written as

\[ |\psi_{k \sigma}^{s} \rangle = \hat{P}_{N_e - 1} \hat{P}_{G} \hat{P}_{j} \hat{P}_{j} \hat{P}_{SS} |\psi_{AFSC}^{k \sigma s} \rangle. \]  

(12)

Hence we can compute the excitation energies \(E_k (\equiv \langle \psi_{k \sigma}^{s} | H | \psi_{k \sigma}^{s} \rangle - \langle \psi_0 | H | \psi_0 \rangle)\) for either upper \((s = b)\) or lower \((s = a)\) AFM quasiparticles. Furthermore, the quasiparticle spectral weight measured from ARPES can be obtained by calculating

\[ Z_k = \frac{|\langle \psi_{k \sigma}^{s} | c_{-k \bar{\sigma}} | \psi_0 \rangle|^2}{\langle \psi_{k \sigma}^{s} | \psi_{k \sigma}^{s} \rangle \langle \psi_0 | \psi_0 \rangle}. \]  

(13)

Some details in the VMC calculation should be noticed. The boundary condition we use is periodic along both directions. In order to achieve a reasonable acceptance ratio, the simulation consists of a combination of one-particle moves and two-particle moves. The variational parameters of the Gutzwiller-projected coexisting state are optimized by using the stochastic reconfiguration method \[36\]. All physical quantities are evaluated using the optimized parameters. We also take a sufficient number of samples \((= 2 \times 10^5)\) to reduce the statistical errors, and keep the sampling interval \((\sim 40)\) long enough to ensure statistical independence between samples.

### 3. Results

We first consider the trial state with only the charge-charge Jastrow correlator to better demonstrate the variational phase diagram. Then we further include the spin-spin Jastrow correlator to see how the phase diagram changes.
Figure 1: (a) Variational phase diagram plotted by staggered magnetization $M_s$ (squares) and superconducting order parameter $\Delta_{SC}$ (circles). Filled and empty symbols represent $|\Psi_{CC}\rangle$ and $|\Psi_{CSS}\rangle$, respectively. (b) The difference of the energy components between $|\Psi_{CSS}\rangle$ and $|\Psi_{CC}\rangle$ as a function of hole doping $\delta$ in $16 \times 16$ lattice.

Order parameters shown in the phase diagram are determined by the staggered magnetization

$$M_s = \frac{1}{N} \sum_i \langle \hat{S}_z^i \rangle e^{iQ \cdot R_i}$$

and the long-range pair-pair correlation function

$$C_{PP}(R) = \frac{1}{N} \sum_{i,\alpha,\alpha'} \lambda_{\alpha,\alpha'} \langle \Delta^\dagger_{i,\alpha} \Delta_{i+R,\alpha'} \rangle.$$ 

The creation operator $\Delta^\dagger_{i,\alpha} (= \hat{c}^\dagger_{i,\alpha} \hat{c}^\dagger_{i+\alpha,\downarrow} - \hat{c}^\dagger_{i,\alpha} \hat{c}^\dagger_{i+\alpha,\uparrow})$ creates a singlet on the bond $(i, i+\alpha)$, $\alpha = x,y$. The factor $\lambda_{\alpha,\alpha'}$ describes $d$-wave symmetry: $\lambda_{\alpha,\alpha'} = 1 (-1)$ as $\alpha = \alpha' (\alpha \neq \alpha')$.

In Fig.1(a), without the spin-spin Jastrow correlators as indicated by $|\Psi_{CC}\rangle$,
there exists a region showing the coexistence of AFM order and SC order within
doping $\delta \lesssim 0.125$ in the phase diagram $[20, 21, 22]$, where $M_s$ and $\Delta_{SC}(\equiv \sqrt{C_{PP}(R > 2)})$ are finite. Let us turn to the case with both charge-charge and spin-spin Jastrow correlators denoted by $|\Psi_{CCSS}\rangle$. Obviously the coexisting region disappears and a clear boundary separating the AFM phase and the SC phase shows up at doping $\delta = 0.156$. Note that near the boundary the spin-spin Jastrow correlator can greatly improve the ground-state energies from 0.3% to 0.7%. From the numerical optimization, we find the spin-spin Jastrow correlator can provide a conduit to vary the mean-field AFM order in $|\Psi_{AFSC}\rangle$. Surprisingly, the optimized spin-spin Jastrow parameters slightly display short-range FM correlations in the AFM background (e.g. at $\delta = 0.156$ the spin-spin Jastrow weights $w_\gamma$ for $\gamma = 1, 2$ and 3 would be increased to 1.12, 1.02 and 1.01, respectively). The local FM correlation introduced by the Jastrow factors is harmful to the mean-field AFM order. To make them balance, it is inevitable to largely enhance the AFM background in $|\Psi_{AFSC}\rangle$. The surprising competition between AFM order and SC order near the phase boundary is mainly due to the hugely enhanced AFM order further leading to the diminished SC order.

To further demonstrate the energy competition, we analyze the difference of the energy components in the Hamiltonian between $|\Psi_{CCSS}\rangle$ and $|\Psi_{CC}\rangle$ shown in Fig.1(b). Our data clearly show that within $0.04 < \delta < 0.2$ the spin Jastrow correlator helps the trial mean-field state gain much more energy from the second-nearest-neighbor hopping term. On the other hand, the competing energy primarily comes from the spin-spin superexchange interaction. From real-space point of view, holes prefer to move along diagonal direction in strong AFM background so that the hopping energy from the second nearest neighbors ($t'$) is likely to compete with the superexchange energy ($J$).

In momentum space, it is apparent that the $t'$ energy gain would influence how the band dispersion evolves from Fermi pocket to Fermi surface as increasing doping. In Fig.2(a)-(c), the difference of the momentum distribution function between $|\Psi_{CCSS}\rangle$ and $|\Psi_{CC}\rangle$ shows how electrons distribute in the band structure. At $\delta = 0.125$ (Fig.2(a)), obviously electrons in the system would
Figure 2: The difference of the momentum distribution function between $|\Psi_{CCSS}\rangle$ and $|\Psi_{CC}\rangle$ for doping (a) $\delta = 0.125$, (b) $\delta = 0.156$ and (c) $\delta = 0.188$ plotted in the first Brillouin zone. (d) The next-nearest-neighbor energy component, $-4t' \cos(k_x) \cos(k_y)$. The black diamond is the half-filled Fermi surface. White (Purple) regions present the positive (negative) values. Red lines mean zero.

prefer to stay around "hot spots" rather than living near nodes and antinodes, which hole pockets and electron pockets seem to be observed as well. The hot spot is defined as the momenta along the MZB that can be connected by $(\pi, \pi)$ momentum scattering. Once doping is increased to 0.156 which is the phase boundary (Fig.2(b)), hole pockets become larger and electron pockets slightly shrink. Now that electrons like to circle just outside the electron pockets, they attempt to form a large Fermi surface. Indeed, as further increasing doping to 0.188 where the long-range AFM order almost disappears (Fig.2(c)), a clear Fermi surface in which electrons cluster together can be seen. So far, we also understand the reason why the system gain much energy from $t'$ term since the hot spots are located right at the purple region shown in Fig.2(d).

In Fig.3 we compute the spin-spin, hole-hole and pair-pair correlation functions (already shown in Eq.(15)) defined as,

$$C_{CC}(R) = \frac{1}{N} \sum_i \langle \hat{n}_i^h \hat{n}_{i+R}^h \rangle,$$

(16)
Figure 3: (a) Spin-spin, (b) hole-hole and (c) pair-pair correlation functions for the optimized state |Ψ_{CCSS}⟩ (|Ψ_{CC}⟩), denoted by red circle (black square) symbols. There are 40 doped holes in 16 × 16 lattice (δ = 0.156).

\[
C_{SS}(\mathbf{R}) = \frac{1}{N} \sum_i \langle \hat{S}_i^z \hat{S}_{i+\mathbf{R}}^z \rangle e^{iQ\cdot \mathbf{R}}.
\]  

(17)

The doping density we choose to present is 0.156. Figure 3(a) illustrates that the spin-spin Jastrow correlators indirectly induce the stronger AFM background showing a constant tail in the staggered spin-spin correlation function which implies a clear AFM order. Note that The enhancement of the AFM order mainly arises from the mean-field wave function |Ψ_{AFSC}⟩. Furthermore, we find in Fig.3(b) that the hole-hole correlation function makes no difference even if including the spin-spin Jastrow correlators, except that the short-range part becomes less staggered. For spin and charge, there is no correlation for their long-range behavior. Finally, we can also see in Fig.3(c) that as considering
the pair-pair correlation almost vanishes at large distances so that the SC properties is not available.

Next, it would be interesting to examine the low-lying single-particle excitation spectra near the phase boundary. In Fig.4 by applying the ansatz (Eq.(12)) to the single-particle excitation, we calculate two quasiparticle band dispersions \( (s = a, b) \) and their corresponding spectral weight for removing one particle defined by Eq.(13). In order to compare with the excitations with/without spin-spin Jastrow correlators \( \hat{P}^{SS}_J \), we plot their excitation energy \( E_k \) along the high symmetric momenta in Fig.4(a). In the case where the trial state only includes the charge-charge Jastrow factors, its optimized mean-field parameters \( \Delta \gg m \). Due to large \( d \)-wave BCS pairing contribution, the dispersions thus show convex around the antinodes and almost zero gap between the two bands at nodes. Especially, the upper AFM band is beneath the lower AFM band near the antinodal regions, and hence there is a clear signal of electron pockets arising from the upper AFM band shown in Fig.4(c).

When further considering spin-spin Jastrow correlators, the optimized mean-field parameters \( m \gg \Delta \). Such a huge AFM parameter \( m \) gives rise to a typical AFM band dispersion and opens a AFM gap between these two bands at nodes, as indicated by red circles in Fig.4(a). Interestingly, Fig.4(c) shows that near antinodes the quasiparticle spectral weight of the upper AFM band disappear and transfer to almost entire lower AFM band (see Fig.4(b)). In particular, a clear hole pocket of the lower AFM band centering around \( Q/2 \) is also observed in Fig.4(b). The Gutzwiller and Jastrow correlators arising from electronic correlation firmly influence the low-lying quasiparticle excitation spectra of the mean-field state \( |\Psi_{AFSC}\rangle \). Therefore, the loss of the electron pockets due to electron correlations provides a route to figure out why electron pockets have never been found in most of hole-doped cuprates measured by ARPES.
Figure 4: (a) The quasi-particle excitation dispersion $E_k$ for different optimized states (denoted in the legend of (c)) along high symmetric momenta at $\delta = 0.156$. Empty (Filled) symbols represent the upper (lower) AFM band and squares (circles) the trial state $|\Psi_{CC}\rangle$ ($|\Psi_{CCSS}\rangle$). Due to much smaller $\Delta$ than $m$ for the trial state $|\Psi_{CCSS}\rangle$, we simply plot the lower AFM band (red circles) below the Fermi level (pink line) except the nodal regions for clear demonstration. The quasiparticle spectral weight $Z_k^{-}$ are obtained from (b) the lower AFM band and (c) the upper AFM band.

4. Conclusions

Summing up, by using VMC approach we have studied the coexisting state with both AFM order and SC order simultaneously underneath the Gutzwiller’s projection and Jastrow correlators. We have thereby re-examined the variational ground-state phase diagram and found that the AFM phase competes with the SC phase as further considering off-site spin correlations. The reasoning for the competition is that the mean-field AFM order is considerably enhanced due to short-range FM correlation introduced by the spin-spin Jastrow factors, further leading to the vanished SC order. As well, we have first investigated the Gutzwiller-projected quasiparticle excitations of the coexisting state. Based on the Gutzwiller ansatz, passing through the boundary between AFM and SC phases, we have observed the loss of electron pockets near antinodes coming from the upper AFM band and the occurrence of hole pockets near nodes arising from the lower AFM band as long as the spin-spin Jastrow correlators are
included. Therefore, such a strongly correlated electron system needs to be carefully inspected in the explanation for the low-lying quasiparticle excitations observed by ARPES experiments.

5. Acknowledgments

Greatly thanks S.-M. Huang, W. Ku and T.-K. Lee for helpful discussions. This work is supported by the Postdoctoral Research Abroad Program sponsored by National Science Council in Taiwan with Grant No. NSC 101-2917-I-564-010 and by CAEP and MST. All calculations are performed in the National Center for High-performance Computing in Taiwan.

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