Relationship between superconductivity and anisotropy in two-dimensional Hubbard model

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Abstract. In connection with the symmetry-breaking phenomena found in cuprate superconductors, we check whether an anisotropy spontaneously appears or not in strongly correlated electrons that exhibit superconductivity and/or antiferromagnetism. A variational Monte Carlo method is applied to the square-lattice Hubbard model ($U/t = 12$) with diagonal transfer $t'$. In the trial wave function used, we introduce band renormalization factors including adjustable parameters for the anisotropy corresponding to the fourfold rotational symmetry breaking. It is confirmed that the anisotropy appears in the overdoped regime, where the Fermi-liquid features are predominant. In the underdoped area, the anisotropy does not appear for $t'/t = 0$ and $+0.3$, whereas it possibly appears in the underdoped regime for $t'/t = -0.3$.

1. Introduction

Recently, symmetry-breaking phenomena have been successively found in cuprate superconductors; electronic nematic order breaking the rotational symmetry \cite{1} and charge density wave breaking the translational symmetry \cite{2} were experimentally discovered along with superconductivity (SC). These symmetry breakings attract much interests because they may provide important insights into the relationship between SC and the enigmatic pseudogap state. Pomeranchuk instability, a spontaneous breaking of fourfold rotational symmetry of the Fermi surface without lattice distortion in this case, is a noteworthy candidate for the nematicity observed in cuprate superconductors \cite{3, 4, 5}.

In this article, we will check whether the $x$-$y$ anisotropy spontaneously appears in the two-dimensional strongly correlated Hubbard model using a variational Monte Carlo (VMC) method, and clarify the relationship between the anisotropy and SC when the model parameters are varied. In order to accurately determine the $x$-$y$ anisotropy/isotropy in the electronic state, we employ the periodic boundary conditions in both $x$ and $y$ directions on a slightly tilted square lattice. In the trial wave function, we introduce the following features:

(i) We adopt a mixed state of antiferromagnetic (AF) and SC orders, by which we can treat a continuous description from their coexistence to the mutual exclusivity.

(ii) The band renormalization effect owing to electron correlation is independently introduced into AF and SC orders by adjusting the parameters of hopping integrals, some of which control the anisotropy in $x$ and $y$ directions.
(iii) As multi-body correlation factors, a doublon-holon binding factor important for Mott physics and an on-site Gutzwiller factor, are used to capture the essence of strong correlation.

By applying the VMC method with this wave function to a square Hubbard (t-t'-U) model, we will elucidate the relationship between SC and anisotropy in electronic states in the strongly correlated regime.

2. Method

We consider the Hubbard model on a square lattice with the next-nearest-neighbor transfer t', as shown in Fig. 1(a),

\[
\mathcal{H} = \mathcal{H}_t + \mathcal{H}_{t'} + \mathcal{H}_U = -t \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle, \sigma} \left( c^\dagger_{\mathbf{r}, \sigma} c_{\mathbf{r}', \sigma} + \text{h.c.} \right) - t' \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle, \sigma} \left( c^\dagger_{\mathbf{r}, \sigma} c_{\mathbf{r}', \sigma} + \text{h.c.} \right) + U \sum_{\mathbf{r}} n_{\mathbf{r}, \uparrow} n_{\mathbf{r}, \downarrow},
\]

(1)

where \(c^\dagger_{\mathbf{r}, \sigma}\) creates an electron of spin \(\sigma\) at site \(\mathbf{r}\), \(n_{\mathbf{r}, \sigma} = c^\dagger_{\mathbf{r}, \sigma} c_{\mathbf{r}, \sigma}\), and \(\langle \mathbf{r} \rangle\) and \(\langle \mathbf{r}' \rangle\) denote indices of nearest-neighbor and diagonal-neighbor pairs, respectively. In order to improve the accuracy in distinguishing between isotropy and anisotropy, we use periodic boundary conditions in both \(x\) and \(y\) directions. In addition, in order to increase the number of data points satisfying closed-shell conditions, under which VMC calculations are stabilized, we use a slightly tilted square lattice with edge vectors \(\mathbf{a}_1 = (m, n)\) and \(\mathbf{a}_2 = (-n, m)\) [Fig. 1(a)], where the unit of distance is the lattice constant. For this lattice, reciprocal primitive vectors are given by \(\mathbf{b}_1 = \frac{2\pi}{N_x} (m, n)\) and \(\mathbf{b}_2 = \frac{2\pi}{N_y} (-n, m)\), and the number of sites is \(N_s = m^2 + n^2\). Corresponding reciprocal lattice points in the first Brillouin zone are generated by Wigner-Seitz construction, as shown in Fig. 1(b). Note that this lattice has a slight Pomeranchuk instability because the rotational symmetry is strictly reduced from \(C_4\) to \(C_2\) in a finite system. Thus, VMC calculations are performed on the tilted square lattices of \(m = 9-13\) and \(n = 1\), and we compare results for different lattice sizes to distinguish between isotropy and anisotropy.

As a variational wave function, we use a Gutzwiller-Jastrow type, \(\Psi = \mathcal{P} \Phi\). For a many-body correlation factor \(\mathcal{P}\), we assume the form \(\mathcal{P} = \mathcal{P}_G \mathcal{P}_Q\), where \(\mathcal{P}_G\) is a usual on-site (Gutzwiller) projection [6], \(\mathcal{P}_G = \prod_{\mathbf{r}} [1 - (1 - g) n_{\mathbf{r}, \uparrow} n_{\mathbf{r}, \downarrow}]\), and \(\mathcal{P}_Q\) is an extended projection between a doubly occupied site (doublon, D) and an empty site (holon, H), which controls the probability weight of D-H binding classified by the surrounded configuration, namely, the number of H neighboring D and vice versa [7, 8].

For the one-body part \(\Phi\), we adopt a mixed state of \(d_{x^2-y^2}\)-wave SC (dSC) and AF orders for a continuous description of their interplay. For \(N_e\) electrons, \(d_{x^2-y^2}\)-wave singlet state \(\Phi\) with a nearest-neighbor-pairing gap \(\Delta_d\) is written as [9],

\[
\Phi = \left( \sum_{\mathbf{k}} \varphi_{\mathbf{k}} b^\dagger_{\mathbf{k} \uparrow} b^\dagger_{-\mathbf{k} \downarrow} \right) \frac{N_e}{2} |0\rangle, \quad (2)
\]

where

\[
\varphi_{\mathbf{k}} = \frac{\Delta(\mathbf{k})}{\varepsilon^{\text{SC}}(\mathbf{k}) - \zeta + \sqrt{(\varepsilon^{\text{SC}}(\mathbf{k}) - \zeta)^2 + \Delta(\mathbf{k})^2}},
\]

\[
\Delta(\mathbf{k}) = \Delta_d (\cos k_x - \cos k_y), \quad \text{and} \quad \zeta \text{ is a parameter corresponding to the chemical potential for } U/t \to 0. \quad \text{An AF gap } \Delta_{\text{AF}} \text{ is introduced through a quasi-particle operator } b_{\mathbf{k}\sigma} \text{ of a mean-field theory;}
\]
Figure 1. (a) Tilted square lattice, spanned by edge vectors $\mathbf{a}_1 = (m, n)$ and $\mathbf{a}_2 = (-n, m)$ with $m = 11$ and $n = 1$. (b) Corresponding reciprocal lattice in the first Brillouin zone by Wigner-Seitz construction with the periodic-periodic boundary conditions. Closed circles are reciprocal lattice points in the folded AF Brillouin zone.

$$b^\dagger_{k\sigma} = \alpha_{k^\dagger} c^\dagger_{k\sigma} + \lambda_{\sigma} \beta_{k^\dagger} c^\dagger_{k+Q\sigma}$$

and

$$b^\dagger_{k+Q\sigma} = -\lambda_{\sigma} \beta_{k^\dagger} c^\dagger_{k\sigma} + \alpha_{k^\dagger} c^\dagger_{k+Q\sigma},$$

where $\lambda_{\sigma} = +1(-1)$ for $\sigma = \uparrow(\downarrow)$, and

$$\alpha_{k} \ (\beta_{k}) = \left[ \frac{1}{2} \left( 1 - (+) \frac{\epsilon^{AF}(k)}{\sqrt{[\epsilon^{AF}(k)]^2 + |\Delta_{AF}|^2}} \right) \right]^{\frac{1}{2}},$$

with $Q = (\pi, \pi)$ and $k \in$ AF Brillouin zone.

To improve accuracy of the wave function, a band-renormalization effect owing to electron correlation is individually introduced into the $d$SC and AF orders by adjusting the parameters of hopping integrals. To this end, we assume that $\epsilon^{SC}(k)$ in Eq. (3) and $\epsilon^{AF}(k)$ in Eq. (6) are separately fitted by a tight-binding band composed of transfers up to fifth-neighbor sites as shown in Fig. 2,

$$\epsilon^{X}(k) = -2(t_{1x}^X \cos k_x + t_{1y}^X \cos k_y) -2t_{2x}^X \cos(k_x + k_y) -2t_{2m}^X \cos(k_x - k_y) -2t_{3}^X [\cos(2k_x) + \cos(2k_y)] -4t_4^X [\cos(2k_x) \cos(k_y) + \cos(k_x) \cos(2k_y)] -2t_5^X [\cos(3k_x) + \cos(3k_y)].$$
Figure 2. Band parameters $t^X_\ell$ for fitting $\varepsilon^X(k)$ with $X = \text{SC or AF}$, which are optimized to adjust the band-renormalization effect owing to electron correlation.

with $X = \text{SC or AF}$, where asymmetries in $t^X_1$ between $x$ and $y$ directions and $t^X_2$ between upward and downward diagonals are also introduced to deal with the Pomeranchuk instability. Here, $t^X_1 (X = \text{SC, AF})$ is fixed to $t$ in Eq. (1) as the unit of energy.

As a result, variational parameters to be optimized in $\Phi$ amount to $\Delta_d$, $\Delta_{AF}$, $\zeta$, $t^X_1$, $t^X_2$, $t^X_3$, $t^X_5$ with $X = \text{SC, AF}$. Besides these fifteen in $\Phi$, variational parameters in the correlation factors are $g$ in $P_G$ and 10 parameters of for the nearest-neighbor D-H binding in $P_Q$. According to a standard procedure of VMC using the correlated measurement for efficient optimization [10], we obtain the optimal set of the 26 parameters by minimizing the energy. Using the optimized wave functions, we calculate various quantities. Among them, we mainly discuss the following quantities, here. As an order parameter of $d$SC, we use the real-space $d$SC correlation function for the nearest-neighbor pairing defined by,

$$P_d(r) = \frac{1}{N_s} \sum_{r'} \sum_{\tau,\tau'} \lambda_{xy}(\tau) \lambda_{xy}(\tau') \langle \Delta^1(r' + r, \tau) \Delta(r', \tau') \rangle ,$$

with

$$\Delta(r, \tau) = \frac{1}{\sqrt{2}} (c_{r\uparrow} c_{r+\tau\downarrow} - c_{r\downarrow} c_{r+\tau\uparrow}) ,$$

$$\lambda_{xy}(\tau) = +1 \text{ for } \tau = (\pm 1, 0), \text{ and } \lambda_{xy}(\tau) = -1 \text{ for } \tau = (0, \pm 1).$$

Actually, we show $P_d(r)$ at the farthest distance $r_{\text{max}}$ as a measure of $d$SC order. The staggered magnetization,

$$m_s = \frac{1}{N_s} \left| \sum_r e^{iQ \cdot r} \langle S^z_r \rangle \right| ,$$

with $Q = (\pi, \pi)$ is also calculated as an order parameter of AF state.

To check whether the $x$-$y$ anisotropy spontaneously appears, we will calculate a discrepancy between electron-transfers in different directions, $A_\ell$ for the $\ell$-th neighbor hoppings, defined by

$$A_1 = |h(1, 0) + h(-1, 0) - h(0, 1) - h(0, -1)| ,$$

$$A_2 = |h(1, 1) + h(-1, -1) - h(1, -1) - h(-1, 1)| ,$$

where

$$h(\tau) = \frac{1}{N_s} \sum_{r,\sigma} \langle c^\dagger_{r,\sigma} c_{r+\tau,\sigma} + \text{h.c.} \rangle$$
is the expectation value of bare electron-hoppings without hamiltonian parameters, and $\tau$ is a vector connecting neighbor sites; $\tau = \pm(1,0), \pm(0,1)$ for the nearest-neighbors, or $\tau = \pm(1,1), \pm(1,-1)$ for the second-nearest-neighbors. For $A_\ell \sim 0$, hoppings are isotropic whereas for finite values of $A_\ell$, hoppings become anisotropic between the orthogonal directions. In addition, we discuss the anisotropy using the momentum distribution function,

$$n(k) = \frac{1}{2} \sum_\sigma \langle c_{k,\sigma}^\dagger c_{k,\sigma} \rangle.$$ (13)

As pilot calculations, we have fixed the value of $U/t$ at 12 as a typical case of strongly correlated regime, and compare the results of $t'/t = 0$ and $t'/t = \pm 0.30$ for the tilted square lattices of $m = 9$–13 and $n = 1$ ($N_s = 82$–170) with periodic-periodic boundary conditions.

![Figure 3](image-url)

**Figure 3.** Anisotropy indicator $A_1$ (in $x$–$y$ directions) and $A_2$ (lattice-diagonal directions) defined in Eq. (11) as functions of $\delta$. The lattice size is $N_s = 82$ ($m = 9$) in the first row [(a)–(c)], $N_s = 122$ ($m = 11$) in the second row [(d)–(f)], and $N_s = 170$ ($m = 13$) in the last row [(g)–(i)], with $n = 1$. From left to right, the value of $t'/t$ is varied: $t'/t = 0$, +0.3, and -0.3.

### 3. Results and discussion

Let us begin with the $x$–$y$ anisotropies of hoppings. In Fig. 3, the anisotropy indicator $A_\ell$ [Eq. (11)] is plotted as a function of doping rate $\delta$ for $N_s = 82, 122, 170$ and for $t'/t = 0, \pm 0.3$. The $\delta$ dependence of $A_1$ and $A_2$ often exhibits zigzag behavior in every panel. We find that at most data points where $A_1$ and $A_2$ have an appreciable finite value, the one-body state becomes a degenerate (open-shell) state. Therefore, whether or not the state becomes anisotropic is a subtle problem that sensitively depends on the system size and the boundary conditions. In such a premise, we argue that $x$–$y$ anisotropy hardly appears in the underdoped regime ($\delta \lesssim 0.16$) where the AF order develops, for $t'/t = 0$, and +0.3 (the first and second
columns of panels), but the anisotropy appreciably appears in the overdoped regime, where the Fermi-liquid (metallic) behavior becomes marked. This is consistent with the previous study [5]. In contrast, for $t' / t = -0.3$ (the last column in Fig. 3), the anisotropy appears even in the underdoped regime. In this case, however, the magnitude of $A_1$ and $A_2$ tends to decrease as $N_s$ increases. Thus, we would like to leave the conclusion as to the underdoped regime for future studies.

Plotted in Fig. 4 are the expectation values of $P_d(r_{\text{max}})$ and $m_s$ estimated with the optimized $\Psi$ for the systems corresponding to Fig. 3. Comparing $P_d(r_{\text{max}})$ and $m_s$ in Fig. 4 with those previously obtained in the periodic-antiperiodic boundary conditions [11, 12], the data of $P_d(r_{\text{max}})$ largely fluctuate, suggesting that $d$SC is sensitive to the underlying Fermi surface. Comparing Figs. 3 and 4, we find that if the orders (AF or SC), especially both, are robust, the anisotropy is suppressed. We will discuss the competition between each order and the anisotropy again in a coming publication.

Lastly, we show contour maps of the momentum distribution function $n(k)$ for $N_s = 122$ in Fig. 5. For clarity, the axes of the wave vector $k$ in the reciprocal space are reversely rotated by $-\theta$, where $\theta = \tan^{-1}(n/m)$ is a tilt angle for tilted square lattice with edge vectors $a_1 = (m, n)$ and $a_2 = (-n, m)$. Panels in the first column [Figs. 5(a), 5(e), and 5(i)] show the cases at half filling for $t' / t = 0$, and $\pm 0.3$. In fact, the fourfold rotational symmetry in the occupied $k$ points is subtly broken even at half filling for finite $N_s$. This weak anisotropy will disappear as $m$ increases. Anyway, the symmetricity seems broadly preserved at half filling. However, the Pomeranchuk instability becomes marked in some cases, for example in Fig. 5(k), corresponding to the large values of $A_4$ in Fig. 3. We will check the size dependence again in a future study.

Figure 4. $\delta$ dependence of order parameters, namely, $P_d(r_{\text{max}})$ for dSC (diamonds, right axis) and $m_s$ for AF (triangles, left axis). The system sizes and values of $t' / t$ are the same as those in Fig. 3.
Figure 5. Contour plots of the momentum distribution function $n(k)$. From left to right, the doping rate is increased: $\delta = 0$ (half-filling), 0.066, 0.131, and 0.197. The values of $t'/t$ are 0 [first row, (a)–(d)], +0.3 [second row, (e)–(h)], and −0.3 [third row, (i)–(l)]. The lattice size is $N_s = 11^2 + 1^2 = 122$, and $U/t = 12$. The thick pink line in each panel indicates Fermi-level line drawn by connecting the points that take the half of electron density, $(1 - \delta)/2$.

4. Summary
We have studied the spontaneous appearance of the fourfold rotational anisotropy in the two-dimensional strongly correlated $t$-$t'$-$U$ model on the bases of VMC calculations. Using an improved wave function on a lattice with the fourfold rotational symmetry, we confirmed that the anisotropy appears in the overdoped area, where the state is almost Fermi liquid [5]. In the underdoped regime, the anisotropy is suppressed in the cases of type-I AF ($t'/t = 0, +0.3$), whereas in the case of the type-II AF ($t'/t = -0.3$) the anisotropy possibly appear. More
systematic calculations are left for future studies.

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