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Renormalization of hopping integrals in coexistence phase of stripe and *d*-wave superconductivity in two-dimensional Hubbard model

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Abstract

We have performed a variational Monte Carlo simulation on a two-dimensional Hubbard model with first- and second-neighbor hopping terms in order to study the coexistence state of a static stripe state and a modulated *d*-wave superconductivity in the under-doped cuprates. In addition to a Gutzwiller, a Jastrow and a doublon-holon correlation effects, the band-renormalization effect was considered in the trial wave function. The condensation energies of an 8-period stripe state was computed as a function of a Coulomb energy under the hole-density x=1/8. Our results reveal that the renormalization of higher hopping parameters due to the strong correlation effect enhances the one-dimensional hole motion on a quarter-filled band in the stripe state, and brings quasi-Fermi surface close to the magnetic zone boundary in the coexistence state.

Keywords: variational Monte Carlo; Hubbard model; stripe; superconductivity; cuprate

1. Introduction

Recently, static incommensurate spin correlations have been observed by elastic neutron-scattering experiments on La-based cuprates [1,2]. These experimental results indicate that the striped spin- and charge-density modulation (stripe state) occurs in the under-doping region. The incommensurability δ, which corresponds to the inverse of the spin-stripe's period on the stripe order, is approximately proportional to x in the under-doped region (x<1/8) of La-214. This relation implies that the 1/4-filled charge-stripe (one hole per two Cu sites along stripe) is realized. In addition, by the angle-resolved photo-emission spectroscopy measurements, Zhou *et al.* have found that two sets of "1/4-filled one-dimensional" Fermi surface are formed near ($\pm\pi$, 0) or (0, $\pm\pi$) when x is close to 1/8 in LSCO [3].

The possible existence of the stripe state in a doped 2D Mott insulator has been theoretically investigated in both weak and strong correlations. A mean-field (MF) analysis [4] of the 2D Hubbard model with long-range hopping terms shows that an incommensurate spin-density-wave (ISDW) order with an incommensurate charge-density-wave (ICDW) is caused by the Fermi surface nesting for arbitrarily small doping, and that the linearity of δ with x is explained by choosing long-range hopping terms of holes. While, from a viewpoint of strong correlations, it is energetically expected that doped holes move freely along striped domain-wall without disturbing the antiferromagnetic (AF) ordered domains. It is predicted in the Hubbard model [5], the *d-p* model [6] and the *t-J* model [7] that the stripe state is stabilized in the under-doped region. However, the problem of why δ keeps a relationship of δ=x still remains controversial.

In this study, we take into account of a band-renormalization effect from moderate to strong coupling regions by using a variational Monte Carlo (VMC) method and apply it to the doped 2D *t-t'-U* Hubbard model (t and t' are first-

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and second-nearest neighbor transfer energies, respectively, and U is an on-site Coulomb energy). t' is introduced to describe the properties of cuprates. In order to compute more accurately the ground state energy in the under-doing region, a doublon-holon binding projection [8] is introduced to the Gutzwiller-Jastrow wave function. We will show that the renormalized t'/t makes stripe state stable, and the renormalized Fermi surface is formed in 1/4-filled one-dimensional band as U increases; the relation of $\delta=x$ is satisfied. Furthermore, it is shown that the spatially modulated *d*-wave superconductivity (SC) and the stripe state compete.

2. Methods

We start from the 2D *t-t'-U* Hubbard model,

$$H = -t\sum_{\langle ij\rangle\sigma}\left(\hat{c}^{+}_{i\sigma}\hat{c}_{j\sigma} + \text{h.c.}\right) - t'\sum_{\langle\langle ij\rangle\rangle\sigma}\left(\hat{c}^{+}_{i\sigma}\hat{c}_{j\sigma} + \text{h.c.}\right) + U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} \quad (1)$$

where h.c. stands for Hermite conjugate and $\langle ij\rangle$ and $\langle\langle ij\rangle\rangle$ denote the first- and second-nearest-neighbor pairs, respectively. In the following, we consider t as the unit of energy. $\hat{c}^{+}_{i\sigma}(\hat{c}_{i\sigma})$ is the creation (annihilation) operator of the electron with spin $\sigma(\uparrow$ or $\downarrow)$ at site i (i=1~ N_{site}) and $\hat{n}_{i\sigma} = \hat{c}^{+}_{i\sigma}\hat{c}_{i\sigma}$. In the VMC calculation, the variational energy is written as $E_{\text{total}} = \langle\Psi_{\text{var}}|\hat{H}|\Psi_{\text{var}}\rangle/\langle\Psi_{\text{var}}|\Psi_{\text{var}}\rangle$. We use the trial wave function defined by $|\Psi_{\text{var}}\rangle = \hat{P}_{\text{G}}\hat{P}_{\text{J}}\hat{P}_{\text{Q}}|\phi\rangle$, where $\hat{P}_{\text{G}}$ is the Gutzwiller projection operator given by $\hat{P}_{\text{G}} = \prod_i(1-(1-g)\hat{n}_{i\uparrow}\hat{n}_{i\downarrow})$, where g is a variational parameter in the range from 0 to unity, which controls the on-site electron correlation. $\hat{P}_{\text{J}}$ is the Jastrow-type projection operator [9], $\hat{P}_{\text{J}} = \prod_{\langle ij\rangle} h^{\hat{n}_i\hat{n}_j}$, which allows the occupancy of the first-neighbor sites to be modified by adjusting h in the neighborhood of 1. $\hat{P}_{\text{Q}}$ is the doubon-holon correlation projection operator, $\hat{P}_{\text{Q}} = \prod_i(1-(1-\eta)\prod_\tau \hat{d}_i(1-\hat{e}_{i+\tau}))$, where $0 \le \eta \le 1$, $\hat{d}_i = \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$, $\hat{e}_i = (1-\hat{n}_{i\uparrow})(1-\hat{n}_{i\downarrow})$, and τ runs over all first-neighbor sites. η acts so as to avoid that double-occupied sites are surrounded by first-neighbor occupied sites, which are particularly important to describe the Mott transition in the 2D Hubbard model on a half-filled square lattice [8]. Regarding an one-body part $|\phi\rangle$, we employ the MF wave function for a striped ISDW-ICDW state, a commensurate SDW state and a Fermi sea represented by $|\phi^{\text{stripe}}_{\text{MF}}\rangle$, $|\phi^{\text{AF}}_{\text{MF}}\rangle$ and $|\phi^{\text{FS}}_{\text{MF}}\rangle$, respectively [5], and the MF wave function for the coexisting *d*-wave SC with a striped ISDW-ICDW state, $|\phi^{\text{coex}}_{\text{MF}}\rangle$, which is obtained from the effective MF Hamiltonian for the coexistence state [7,10],

$$H^{\text{coex}}_{MF} = \sum_{ij}\begin{pmatrix}\hat{c}^{+}_{i\uparrow} & \hat{c}_{i\downarrow}\end{pmatrix}\begin{pmatrix}H_{ij\uparrow} & F_{ij}\\ F^{*}_{ji} & -H_{ji\downarrow}\end{pmatrix}\begin{pmatrix}\hat{c}_{j\uparrow}\\ \hat{c}^{+}_{j\downarrow}\end{pmatrix} \quad (2)$$

where diagonal terms describe the MF due to ISDW-ICDW as

$$H_{ij\sigma} = -t\sum_{\mathbf{e}}\delta_{\mathbf{r}_j,\mathbf{r}_i+\mathbf{e}} - \tilde{t}'\sum_{\mathbf{e}'}\delta_{\mathbf{r}_j,\mathbf{r}_i+\mathbf{e}'} - \tilde{t}''\sum_{\mathbf{e}''}\delta_{\mathbf{r}_j,\mathbf{r}_i+\mathbf{e}''} + \left[-\mu + \rho_i + \text{sgn}(\sigma)(-1)^{x_i+y_i}m_i\right]\delta_{\mathbf{r}_j,\mathbf{r}_i} \quad (3)$$

with $\rho_i = \rho\cos(2\boldsymbol{q}\cdot\mathbf{r}_i)$ and $m_i = m\sin(\boldsymbol{q}\cdot\mathbf{r}_i)$, where **e**, **e'**, and **e''** are vectors toward first-, second- and third-neighbor sites, respectively. $\delta_{\mathbf{r}_i,\mathbf{r}_j}$ is Kronecker's delta. Variational parameters are chemical potential, μ, charge-amplitude, ρ, spin-amplitude, m, effective second- and third-neighbor transfer energies, $\tilde{t}'$ and $\tilde{t}''$ in $|\phi\rangle$. Note that Hamiltonian, eq. (1) does not contain the third-neighbor hopping term, t''. The vertical stripe state is defined with $\mathbf{q}=(0, 2\pi\delta)$ in which magnetic domains run along the x-direction. The charge-stripe period is one-half the spin-stripe period. On the other hand, the off-diagonal terms in eq. (2) are defined in terms of the spatially modulated *d*-wave SC gap as $F_{ij} = \sum_{\text{e}}\Delta_{ij}\delta_{\mathbf{r}_j,\mathbf{r}_i+\mathbf{e}}$ with $\Delta_{i,i+\hat{x}} = \Delta\cos(\boldsymbol{q}\cdot\mathbf{r}_i)$ and $\Delta_{i,i+\hat{y}} = -\Delta\cos(\boldsymbol{q}\cdot(\mathbf{r}_i + (0,1/2)))$, where Δ is another variational parameter in $|\phi\rangle$. The SC amplitude takes the maximum on the charge-stripes, and the sign of the SC gap is opposite between neighboring stripes. In the following, the system used is of $N_{\text{site}}=16\times16$ lattices with the periodic boundary conditions in both directions in order to avoid the influence due to the anisotropic condition. It is confirmed that there is no qualitative difference in the result with periodic-antiperiodic boundary condition. We assume δ=1/8 and total electron number N_{e}=224 (electron-density, $p=N_{\text{e}}/N_{\text{site}}$=0.875) in order to consider the 8-period stripe state observed at x=0.125 in La-214. The SC gap function is slightly modified to $F_{ij} = \sum_{\mathbf{e}}\Delta_{ij}\delta_{\mathbf{r}_j,\mathbf{r}_i+\mathbf{e}} + \varepsilon$ with $\varepsilon\sim10^{-6}$ to avoid divergence in computation. The variational energy is obtained as the average of the results of several Monte Carlo calculations run simultaneously each with 2.0×10^6 steps.

3. Results

First, the condensation energy for the stripe state without SC is compared with that for the AF state. We compute the energy difference between the normal state and the stripe state defined as $\Delta E_{\text{stripe}}=(E(\Psi^{\text{FS}}_{\text{var}})-E(\Psi^{\text{stripe}}_{\text{var}}))/N_{\text{site}}$. ΔE_{AF}

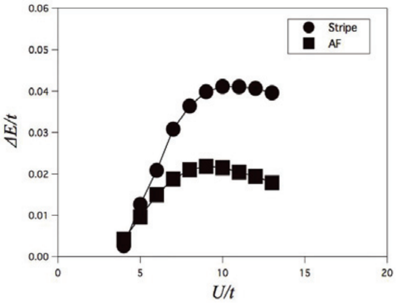

Fig. 1. Condensation energies of the 8-period stripe state and the AF state as a function of *U/t*. The system is a 16×16 lattice for the case of t'/t=−0.20, *p*=0.875. The statistical error-bars are smaller than the size of symbols.

for the AF state is obtained similarly. In Fig. 1, $\Delta E_{\rm stripe}$ and $\Delta E_{\rm AF}$ are plotted as a function of *U/t.* The stripe state is more stable than the AF state, which is the same as the calculation only using the Gutzwiller projection [5]. To see the renormalization of the Fermi surface due to the correlation effect, optimized values of $\tilde{t}'/t$ for $|\Psi_{\rm var}^{\rm stripe}\rangle$ are shown as a function of *U/t* in Fig. 2(a). For a comparison, values for $|\Psi_{\rm var}^{\rm FS}\rangle$ are also shown in Fig. 2(a). The $|\tilde{t}'|/t$ for the normal state decreases with *U/t* increases, which suggests that there is an energy gain due to the increase of the density of state because the Fermi surface close to the saddle point at (±π, 0) and (0, ±π) as $|\tilde{t}'|/t$ decreases. While, the *U*-dependence of $\tilde{t}'/t$ for the stripe state is opposite to that of the normal state. The $|\tilde{t}'|/t$ for $|\Psi_{\rm var}^{\rm stripe}\rangle$ increases as *U/t* increases (where note that the optimized $\tilde{t}''/t$ becomes almost zero). This result is quite different from that in the Mott insulating phase in the 2D Hubbard model with the half-filling where the large band renormalization with $\tilde{t}'/t$ ~0 occurrences [11]. Furthermore, it is similar to the result for VMC calculation in the *t-J* model [12], but its calculation was performed by using the Gutzwiller projected BCS wave function. In order to understand our result, the renormalized Fermi surface of $\tilde{t}'/t$ =−0.30, −0.40 and −0.50 are plotted in Fig. 2(b). In addition, the Fermi surface of one-dimensional electrons with 1/4-filling and the non-interacting Fermi surface with t'/t=−0.20 are plotted. As *U/t* increases, the renormalized Fermi surface near (0, ±π) approaches the one-dimensional electronic state with 1/4-filling. Our result indicates that the relation of *δ*=*x* depends not only on the Fermi surface nesting effect but also on the contribution of the electron correlation.

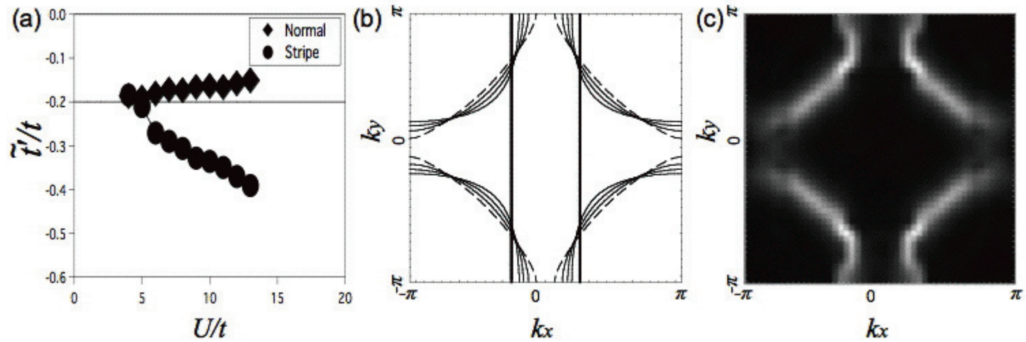

Fig. 2. (a) Optimized effective second-neighbor transfer energies, $\tilde{t}'/t$, for $|\Psi_{\rm var}^{\rm Stripe}\rangle$ and $|\Psi_{\rm var}^{\rm FS}\rangle$ as a function of *U/t*. The system is a 16×16 lattice for the case of t'/t=−0.20 and *p*=0.875. (b) Renormalized quasi-Fermi surfaces for $\tilde{t}'/t$ = −0.30, −0.40 and −0.50. As a reference, the non-interaction Fermi surface for t'/t=−0.20 (dashed line) and the 1D Fermi surface at 1/4-filling (thickness line) are plotted. (c) Contour Plot of $|\nabla n_{\boldsymbol{k}}|$ measured by $|\Psi_{\rm var}^{\rm Stripe}\rangle$ with 24×24 lattice. Note that the optimized variational parameters are employed in the case of 16×16 lattice with t'/t=−0.20, *p*=0.875 and *U/t*=8. $|\nabla n_{\boldsymbol{k}}|$ is larger in brighter areas.

Here, we check the visualized Fermi surface represented by the gradient of the momentum distribution function, $|\nabla n_{\boldsymbol{k}}|$, calculated in the optimized $|\Psi_{\rm var}^{\rm stripe}\rangle$. In order to increase the resolution of $\boldsymbol{k}$-space, we calculate on the 24×24 lattice by using optimized variational parameters on the 16×16 lattice since the change of optimized parameters due to the size effect is small. In Fig. 2(c), brighter areas coincide with the renormalized Fermi surface with $\tilde{t}'/t$=−0.31 and $\tilde{t}''/t$=0.0 with *U/t*=8, except around (0, ±π) and (±π, 0) where the 1/4-filled one-dimensional structure appears, and it seems that the reconstructed Fermi surface is smeared related to the opening the striped ISDW gap.

Next, the modulated *d*-wave SC coexisting with the stripe state is considered. The condensation energy of SC, $\Delta E_{\rm SC}$=($E(\Psi_{\rm var}^{\rm stripe})$−$E(\Psi_{\rm var}^{\rm coex})$)/$N_{\rm site}$, is almost zero with *U/t*=8 and *p*=0.875 although the finite optimized *d*-wave SC gap (*Δ*~0.018) is obtained. This result is in contrast to the homogeneous *d*-wave SC without SDW state in the optimal

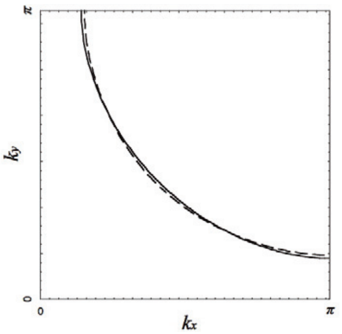

Fig. 3. Renormalized quasi-Fermi surfaces with U/t=12 and p=0.875. Solid line is for the coexistence state with optimized values, $\tilde{t}'/t$ =−0.29 and $\tilde{t}''/t$ =0.025. Dashed line is for the stripe state with optimized values, $\tilde{t}'/t$ =−0.37 and $\tilde{t}''/t$ =0.0.

doping [13]. Furthermore, Figure 3 shows the renormalized Fermi surface in the coexistence state with U/t=12 and p=0.875, where the optimized $|\tilde{t}'|/t$ decreases and $|\tilde{t}''|/t$ increases in comparison with those of the stripe state; the renormalized Fermi surface approaches to the AF Brillouin zone, which indicates that the AF spin-fluctuation enhances. The similar tendency was explained by the study on the bases of the fluctuation-exchange-approximation [14]. Our results reveal that the modulated d-wave SC competes with stripes in the coexistence state.

4. Conclusions

In summary, we study the renormalization effect of $\tilde{t}'/t$ and $\tilde{t}''/t$ due to the strong correlation in the stripe state and in the SC coexisting with the stripes in the 2D Hubbard model by using VMC method. We found that the effective second-neighbor transfer energy increases in the stripe state, but decreases accompanied with the increase of the effective third-neighbor transfer energy in the coexistence state. At the 1/8-doping, the static 8-period stripes and d-wave SC compete. The condensation energy of the SC is very small even if they coexist.

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