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Variational approach to strong correlation in the photoemission of electron-doped superconductors

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ABSTRACT

We use a variational approach with strictly strong-correlated constraint to gain insight into low-energy states of $t-t'-t''-J$ model in the electron-doped regime. Compared with the recent results on the electron-doped cuprates obtained by angle-resolved photoemission spectroscopy (ARPES), we show that based on the long-range ordered antiferromagnetic metallic state prohibiting vacant sites, our results lead to qualitatively similar trends in ARPES spectra and Fermi surface topology. Additionally, the results about the evolution of the energy gap and spectral weight as a function of doping will be discussed.

1. Introduction and overview

It has widely been accepted that high-T_c cuprates are Mott insulator before doping [1]. In generic phase diagram of the materials, the typical electron-doped cuprate $Nd_{2-x}Ce_xCuO_4$ (NCCO) remains an antiferromagnetic (AF) insulator up to doping of $x\sim0.13$ whereas in the hole-doped cuprate $La_{2-x}Sr_xCuO_4$ a small doping of $x\sim0.03$ is enough to destroy its AF correlation [2]. Theoretically it has been proposed that the asymmetry in the phase diagram can be modeled by adding intra-sublattice hopping terms to the $t-J$ model [3–5]. In the hole-doped cases, comparisons among the variational theories [6,7] and experiments have shown an overall semi-quantitative agreement on their doping dependence. So far there are few variational studies on the electron-doped systems [5]. Even so, various theoretical and numerical studies have confirmed that the electron-doped model has a robust AF order [8,9].

Recent angle-resolved photoemission spectroscopy (ARPES) experiments have revealed the evolution of the Fermi surface with doping in the electron-doped NCCO cuprate [10–13]. It was found by several groups [10,11,13] that with less than 0.13 doping a small pocket appears around $(\pi,0)$, in contrast to the hole-doped cuprates where the low-lying states are centered at $(\pi/2,\pi/2)$, which is consistent with the variational study [5] of the $t-J$ model by including appropriate intra-sublattice hoppings. Matsui et al. [13] have found near $(\pi,0)$ a gap-like structure below Fermi energy but not at $(\pi/2,\pi/2)$. They attributed it to the AF ordering and band folding. However the momentum dependence of this AF gap cannot be explained by this simple picture unless one assumes the strength of AF scattering has momentum dependence. Recently Ikeda et al. [14] have unearthed that the other electron-doped materials $Ln_{2-x}Ce_xCuO_4$ (Ln = Sm and Eu) at $x=0.15$ show the resembling Fermi surface topology as NCCO material and an energy gap at the Fermi level around the nodal point resulting from strong AF long-range order. These two materials either show a very weak superconductivity or none at all. Additionally, Park et al. [15] have also observed that there is no Fermi surface pocket near $(\pi/2,\pi/2)$ in $Sm_{1.86}Ce_{0.14}CuO_4$ material.

Contrary to the experimental situation, the theory in the electron-doped case is still highly contentious. First it has been proposed by Kusko et al. [16] that the Hubbard model is essential for studying the electron-doped cuprates. But in their theory the on-site U/t term is treated as a doping-dependent effective parameter. In addition, Kyung et al. [17,18] have shown that ARPES spectra [10,11] in the electron-doped cuprates can all be explained in detail within the Hubbard model in the weak to intermediate coupling regime. However, Millis et al. [19] have suggested that the electron-doped materials are approximately as strongly correlated as the hole-doped ones. The strong coupling $t-t'-t''-J$ model is adopted by [20,21] to construct the Fermi surface without any tuning parameter. Also Yuan et al. [22] have examined the electron-doped $t-t'-t''-J$ model in AF state by using the slave-boson mean-field theory. Their results in the strong coupling model are consistent with the experimental data.

In this paper we shall focus on understanding the ARPES results [13–15] for the electron-doped system with AF long-range order metallic state. In previous studies of the extended $t-J$ model using the variational Monte-Carlo (VMC) method, we have proposed a wave function for this AF metallic (AFMM) state [5,23,24]. This AFMM state seems to be observed recently by NMR for hole-doped cuprates [25]. We have shown that for very low doping, the AFMM state explains many anomalous features of the

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results obtained by exact diagonalization [5]. This state originally proposed for the hole-doped system could be easily mapped to the electron-doped case. Based upon this AFMM trial wave function (TWF), low-energy excitation spectra, ARPES spectral weight and the corresponding Fermi surface are calculated. The general behavior of the ARPES gap observed by Matsui et al. [13] is obtained. The momentum dependence of this AF gap is purely an effect of strong correlation. The evolution of Fermi surface with doping as observed by experiments is also reproduced.

2. Model and trial wave function

The $t-t'-t''-J$ model for the electron-doped case is given by

$$H = H_t + H_J = -\sum_{ij} t_{ij}(\tilde{c}^{\dagger}_{i,\sigma}\tilde{c}_{j,\sigma} + h.c.) + J\sum_{\langle i,j\rangle}\left(\mathbf{S}_i\cdot S_j - \frac{1}{4}n_i n_j\right), \quad (1)$$

where $t_{ij} = t$, t', and t'' are for the nearest, second-nearest, and third-nearest neighbors i and j. $\langle i,j\rangle$ in H_J means the spin–spin interaction occurs only for the nearest neighbors and $\tilde{c}_{i,\sigma} = c_{i,\sigma}n_{i,-\sigma}$. Here $n_i = \sum_\sigma n_{i\sigma} = \sum_\sigma c^{\dagger}_{i\sigma}c_{i\sigma}$. Physical values $t'/t = -0.3$, $t''/t = 0.2$, and $J/t = 0.3$ are adopted.

There are several ways to construct the TWF [7,26]. We shall first follow the traditional mean-field theory by assuming two order parameters. The staggered magnetization is $m = \langle S^z_A\rangle = -\langle S^z_B\rangle$, where the lattice is divided into A and B sublattices, and d-wave resonating-valence-bond (d-RVB) order $\Delta = \langle c_{j\downarrow}c_{i\uparrow} - c_{j\uparrow}c_{i\downarrow}\rangle$ if i and j are nearest-neighbor sites in the x direction and $-\Delta$ for the y direction. Without d-RVB order, the mean-field Hamiltonian has the lower and upper spin-density-wave (SDW) bands with operators $a_{\mathbf{k}\sigma} = \alpha_{\mathbf{k}}c_{\mathbf{k}\sigma} + \sigma\beta_{\mathbf{k}}c_{\mathbf{k}+\mathbf{Q}\sigma}$ and $b_{\mathbf{k}\sigma} = -\sigma\beta_{\mathbf{k}}c_{\mathbf{k}\sigma} + \alpha_{\mathbf{k}}c_{\mathbf{k}+\mathbf{Q}\sigma}$, respectively. We set $\mathbf{Q} = (\pi,\pi)$ for commensurate SDW state with $\alpha^2_{\mathbf{k}} = \frac{1}{2}\{1 - \varepsilon_{\mathbf{k}}/\sqrt{\varepsilon^2_{\mathbf{k}} + m^2_v}\}$ and $\beta^2_{\mathbf{k}} = \frac{1}{2}\{1 + \varepsilon_{\mathbf{k}}/\sqrt{\varepsilon^2_{\mathbf{k}} + m^2_v}\}$, where $\varepsilon_{\mathbf{k}} = -(\cos\mathbf{k}_x + \cos\mathbf{k}_y)$ and $\xi^{\pm}_{\mathbf{k}} = \pm\sqrt{\varepsilon^2_{\mathbf{k}} + m^2_v} - \mu_v - t'_v\cos\mathbf{k}_x\cos\mathbf{k}_y - t''_v(\cos(2\mathbf{k}_x) + \cos(2\mathbf{k}_y))$. $\xi^{\pm}_{\mathbf{k}}$ are the dispersions for the upper and lower SDW bands. Including d-RVB order, the quasi-particle (QP) energy is $E^{\pm}_{\mathbf{k}} = \sqrt{{\xi^{\pm}_{\mathbf{k}}}^2 + \Delta^2_{\mathbf{k}}}$ with $\Delta_{\mathbf{k}} = \Delta_v(\cos\mathbf{k}_x - \cos\mathbf{k}_y)$.

It has been shown [7,26] that the TWF constructed with the method discussed above have a substantial superconductivity coexistent with AF order. A simple generalization of the wave function above to a TWF with much weaker superconductivity, or for the AFMM state, could be easily carried out by following the work by Lee and Shih [5,23]. The TWF that we shall use in the electron-doped cuprates is constructed by adding electrons to the half-filled wave functions. The parameters μ_v, t'_v, and t''_v are all set to zero. We only have two variational parameters m_v and Δ_v to be optimized. Then charge excitations are created by adding electrons. Its Fermi surface determined by the wave vectors of the added electrons has the shape of small pockets [9]. As shown before [5] the lowest energy states are obtained by adding electrons with momenta $(\pi,0)$ or $(0,\pi)$ and their neighboring wave vectors. We shall denote these wave vectors as the set **S**. Specifically for the ground state doped with n electrons, the TWF is

$$|\Psi_n\rangle = \hat{P}\prod_{\mathbf{k}_i\in\mathbf{S}}^{n/2} c^{\dagger}_{\mathbf{k}_i\uparrow}c^{\dagger}_{-\mathbf{k}_i\downarrow}c^{\dagger}_{\mathbf{k}_i+\mathbf{Q}\uparrow}c^{\dagger}_{-\mathbf{k}_i+\mathbf{Q}\downarrow} \times\left(\sum_{\mathbf{q}\neq\mathbf{k}_i}{}' A_{\mathbf{q}}a^{\dagger}_{\mathbf{q}\uparrow}a^{\dagger}_{-\mathbf{q}\downarrow} + B_{\mathbf{q}}b^{\dagger}_{\mathbf{q}\uparrow}b^{\dagger}_{-\mathbf{q}\downarrow}\right)^{(N-n)/2}|0\rangle, \quad (2)$$

where N is the lattice size and n is even number for ground state. The coefficients $A_{\mathbf{k}} = (E^-_{\mathbf{k}} - \xi^-_{\mathbf{k}})/\Delta_{\mathbf{k}}$ and $B_{\mathbf{k}} = (-E^+_{\mathbf{k}} + \xi^+_{\mathbf{k}})/\Delta_{\mathbf{k}}$. The summation of $\mathbf{q}$ is within magnetic Brillouin zone (MBZ). The prime on the summation symbol indicates that the momentum $\mathbf{k}_i$ is excluded from the sum if $\mathbf{k}_i$ is within the MBZ; otherwise, $\mathbf{k}_i - \mathbf{Q}$ is excluded. $\mathbf{k}_i$ belong to set **S**. The projection operator $\hat{P}$ enforces the constraint of no vacant site for cases with finite electron doping. Noted that there are no more electrons could be added to the system with momentum inside the set **S**. Hence the momenta in **S** are fully occupied.

For $n-1$ doped electrons, we have two possibilities to construct the excitations by starting from Eq. (2). One of these is taking one electron away with a momentum inside the set **S**. The electron left unpaired behaves like a QP [5]. The TWF is of the form

$$|\Psi^{QP}_{n-1}(\mathbf{k})\rangle = \hat{P}c^{\dagger}_{\mathbf{k}\uparrow}c^{\dagger}_{\mathbf{k}+\mathbf{Q}\uparrow}c^{\dagger}_{-\mathbf{k}+\mathbf{Q}\downarrow}\prod_{\mathbf{k}_i\in\mathbf{S}}^{n/2-1} c^{\dagger}_{\mathbf{k}_i\uparrow}c^{\dagger}_{-\mathbf{k}_i\downarrow}c^{\dagger}_{\mathbf{k}_i+\mathbf{Q}\uparrow}c^{\dagger}_{-\mathbf{k}_i+\mathbf{Q}\downarrow} \times\left(\sum_{\mathbf{q}\neq\mathbf{k},\mathbf{k}_i}{}' A_{\mathbf{q}}a^{\dagger}_{\mathbf{q}\uparrow}a^{\dagger}_{-\mathbf{q}\downarrow} + B_{\mathbf{q}}b^{\dagger}_{\mathbf{q}\uparrow}b^{\dagger}_{-\mathbf{q}\downarrow}\right)^{(N-n)/2}|0\rangle. \quad (3)$$

The second possibility is to take one electron outside **S** by breaking one of the $(N-n)/2$ electron pairs in Eq. (2). These states are denoted as the spin-bag (SB) states [24]:

$$|\Psi^{SB}_{n-1}(\mathbf{k})\rangle = \hat{P}c^{\dagger}_{\mathbf{k}\uparrow}\prod_{\mathbf{k}_i\in\mathbf{S}}^{n/2} c^{\dagger}_{\mathbf{k}_i\uparrow}c^{\dagger}_{-\mathbf{k}_i\downarrow}c^{\dagger}_{\mathbf{k}_i+\mathbf{Q}\uparrow}c^{\dagger}_{-\mathbf{k}_i+\mathbf{Q}\downarrow} \times\left(\sum_{\mathbf{q}\neq\mathbf{k},\mathbf{k}_i}{}' A_{\mathbf{q}}a^{\dagger}_{\mathbf{q}\uparrow}a^{\dagger}_{-\mathbf{q}\downarrow} + B_{\mathbf{q}}b^{\dagger}_{\mathbf{q}\uparrow}b^{\dagger}_{-\mathbf{q}\downarrow}\right)^{(N-n-2)/2}|0\rangle. \quad (4)$$

It should be noted that the SB state given by Eq. (4) is only one of the many possibilities for this kind of states. As discussed in [24], in addition to the QP state, the QP excitations expressed by the SB state involves excitation of a spin wave. Hence it has a continuum of excitations and Eq. (4) represents the lowest energy SB state. Since the detail has been discussed in [24], we will not discuss it further here.

There is another similar wave function which replaces $\mathbf{k}$ by $\mathbf{k}+\mathbf{Q}$ in Eqs. (3) and (4). Since we are considering the case with AF long-range order, the $\mathbf{k}$ and $\mathbf{k}+\mathbf{Q}$ states are coupled. And these two coupled states may not be orthogonal, we must orthogonalize them by using Gram–Schmidt method firstly. After diagonalizing QP and SB states we obtain the new eigenstates:

$$|\Psi^{U/L}_{QP}(\mathbf{k})\rangle = C^{U/L}_{1,\mathbf{k}}|\Psi^{QP}_{n-1}(\mathbf{k})\rangle + C^{U/L}_{2,\mathbf{k}}|\Psi^{QP}_{n-1}(\mathbf{k}+\mathbf{Q})\rangle, \quad (5)$$

$$|\Psi^{U/L}_{SB}(\mathbf{k})\rangle = D^{U/L}_{1,\mathbf{k}}|\Psi^{SB}_{n-1}(\mathbf{k})\rangle + D^{U/L}_{2,\mathbf{k}}|\Psi^{SB}_{n-1}(\mathbf{k}+\mathbf{Q})\rangle, \quad (6)$$

which correspond to the upper (U) and lower (L) eigenenergies of QP and SB states, respectively. The variational energy of the U (L) state is closer to (further away from) the ground-state energy. In other words, the U and L states could be regarded as states in upper and lower SDW bands, respectively. The coefficients $C^{U/L}_{1/2,\mathbf{k}}$ and $D^{U/L}_{1/2,\mathbf{k}}$ are determined from the orthonormal condition.

3. Result and discussion

Before presenting the VMC results we shall briefly discuss about what is expected from a simple mean-field SDW theory. Based on the SDW bands $\xi^{\pm}_{\mathbf{k}}$, the energy gap between the two separated bands has the same size along the MBZ boundary, as shown in the inset of Fig. 1(b). However, it is inconsistent with the experiment [13] that there is an indication of non-uniform AF gap which becomes larger as bands approaching $(\pi/2,\pi/2)$.