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The coexisting state of the staggered flux and *d*-wave superconducting order in a *t-J* type model

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Abstract. We study the quasiparticle structures in the coexisting phase of the *d*-wave superconductivity (dSC) and the staggered flux state using the renormalized mean-field theory for the *t-J* type model with additional nearest-neighbor Coulomb repulsion V, based on the Gutzwiller approximation. We find that this coexisting state exhibits the dome-like behavior of dSC in the phase diagram and also the so-called two-gap structure found in ARPES experiments, both of which are quite consistent with the experimental results.

1. Introduction

A series of experimental studies over the recent decade has provided important information previously unexpected on the pseudogap (PG) state in cuprate superconductors: it is accompanied by some phase transitions with the broken rotational or translational symmetry, which implies that there can be nematic order or charge order. It has also been suggested that the PG phase and *d*-wave superconductivity (dSC) can coexist roughly in the first half of the superconducting dome. One of the experimental evidences of the coexisting pseudogap phase with dSC is a gap-structure in the ARPES data opening with broken particle-hole symmetry found in Bi-2201, which is consistent with the so-called two-gap structure in the quasiparticle excitation spectra [1, 2].

Quite recently, we have shown that the observed gap-structure can be well described if we assume that the staggered flux (SF) state exists in the PG phase [3]. We have also shown that the gap-structure cannot be described by assuming antiferromangetic order. The SF state is a normal, or non-superconducting state with broken symmetries, and has been studied by many groups since the early stage of research on cuprate superconductors [4, 5, 6, 7, 8, 9]. This state was proposed firstly as a candidate of the ground state for the CuO_2 plain, then has been studied in the context of the pseudogap phase. Theoretically, it has been known that the SF state has higher variational energy than that of dSC for all hole-doping $\delta > 0$ in the standard models, such as the *t-J* model and the Hubbard model [9, 10]. However, at least within a mean-field theory, the SF state can be stabilized by introducing the nearest-neighbor Coulomb repulsion V to the *t-J* model, and even can coexist with dSC [8] in the underdoped region of the phase diagram. Thus we can believe that the SF is still a possible candidate for the PG.

One prominent objection to the idea that the SF is the origin of the PG is that the SF gap opens always at the center of the tight-binding band due to the two-sublattice nature of the

SF state. The resulting gap structure in the quasiparticle densities of states (DOS) reported in previous studies [3, 7, 8] are highly electron-hole asymmetric even in the coexisting phase of SF and dSC, which has never been observed in STS experiments. Thus it is necessary to clarify if the coexisting phase of SF and dSC can exhibit a plausible quasiparticle spectra. In this paper, we carry out such a study using the renormalized mean-field theory for the t-J model with additional nearest-neighbor Coulomb repulsion V.

2. Model

We start with the t-J model with both the *next-nearest-neighbor* hopping term and the *nearest-neighbor* Coulomb interaction term, given as

$$
\begin{aligned}
\mathcal{H} &= -t \sum_{\langle i,j \rangle, \sigma} \left(c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.} \right) - t' \sum_{(i,j),\sigma} \left(c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.} \right) - \mu \sum_{i,\sigma} c_{i\sigma}^\dagger c_{i\sigma} \\
&\quad + J \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j + V \sum_{\langle i,j \rangle} n_i n_j
\end{aligned}
\tag{1}
$$

in the standard notation, where $n_j = \sum_\sigma c_{j\sigma}^\dagger c_{j\sigma}$, and $\langle i,j \rangle$ and (i,j) mean the summation over nearest-neighbor and next-nearest-neighbor pairs. Throughout this paper, we take $J/t = 0.2$, $t'/t = -0.3$, and $V/t = 0.1$. This Hamiltonian operates only in the subspace where there is no doubly occupied sites, which can be implemented by a Gutzwiller projection.

To deal with the projection effects, we can use the so-called renormalized mean-field theory in which the transfer integral t and the superexchange coupling J are renormalized as $t_{\text{eff}} = g_t t$ and $J_{\text{eff}} = \frac{3}{4} g_s J$ by using doping dependent factors

$$
g_t = \frac{2\delta}{1+\delta} \ , \ \ g_s = \frac{4}{(1+\delta)^2} \ ,
\tag{2}
$$

respectively [11]. Since we need further mean-field approximation to treat the renormalized Hamiltonian, we assume the particle-particle pairing amplitude

$$
\langle c_{\boldsymbol{k}\uparrow}^\dagger c_{-\boldsymbol{k}\downarrow}^\dagger \rangle = \Delta_d (\cos k_x - \cos k_y) \ ,
\tag{3}
$$

and also the particle-hole pairing amplitude

$$
\langle c_{\boldsymbol{k}\sigma}^\dagger c_{\boldsymbol{q}\sigma} \rangle = \xi_1 (\cos k_x + \cos k_y) \delta_{\boldsymbol{k},\boldsymbol{q}} + i\xi_2 (\cos k_x - \cos k_y) \delta_{\boldsymbol{k}+\boldsymbol{Q},\boldsymbol{q}} \ ,
\tag{4}
$$

with $\boldsymbol{Q} = (\pi, \pi)$. It should be noted here that ξ_2 in (4) is the order parameter of SF. Then we obtain the set of the self-consistent equations, with $s = \pm 1$, as follows:

$$
\xi_1 = \frac{1}{2N_s} \sum_{\boldsymbol{k},s} \tanh\left(\frac{E_{\boldsymbol{k}s}}{2T} \right) \frac{A_{\boldsymbol{k}} \gamma_{\boldsymbol{k}}}{E_{\boldsymbol{k}s}} \left[1 + s \frac{4g_t t' \varphi_{\boldsymbol{k}} + \tilde{\mu}}{\varepsilon_{\boldsymbol{k}}} \right] \ ,
\tag{5}
$$

$$
\xi_2 = \frac{1}{2N_s} \sum_{\boldsymbol{k},s} \tanh\left(\frac{E_{\boldsymbol{k}s}}{2T} \right) \frac{B_{\boldsymbol{k}} \eta_{\boldsymbol{k}}}{E_{\boldsymbol{k}s}} \left[1 + s \frac{4g_t t' \varphi_{\boldsymbol{k}} + \tilde{\mu}}{\varepsilon_{\boldsymbol{k}}} \right] \ ,
\tag{6}
$$

$$
\Delta_d = \frac{1}{2N_s} \sum_{\boldsymbol{k},s} \tanh\left(\frac{E_{\boldsymbol{k}s}}{2T} \right) \frac{D_{\boldsymbol{k}} \eta_{\boldsymbol{k}}}{E_{\boldsymbol{k}s}} \ ,
\tag{7}
$$

$$
\delta = -\frac{1}{N_s} \sum_{\boldsymbol{k},s} \tanh\left(\frac{E_{\boldsymbol{k}s}}{2T} \right) \frac{s \left[\varepsilon_{\boldsymbol{k}} + s \left(4g_t t' \varphi_{\boldsymbol{k}} + \tilde{\mu} \right) \right]}{E_{\boldsymbol{k}s}} \ ,
\tag{8}
$$

where

$$A_{\boldsymbol{k}} = \left(2g_t t + J_{\text{eff}}^{+}\xi_1\right)\gamma_{\boldsymbol{k}} \ , \ \ B_{\boldsymbol{k}} = J_{\text{eff}}^{+}\xi_2\eta_{\boldsymbol{k}} \ , \ \ D_{\boldsymbol{k}} = J_{\text{eff}}^{-}\Delta_d\eta_{\boldsymbol{k}} \ , \tag{9}$$

with

$$\varepsilon_{\boldsymbol{k}} = \sqrt{A_{\boldsymbol{k}}^2 + B_{\boldsymbol{k}}^2} \ , \ \ E_{\boldsymbol{k}s} = \sqrt{\left(s\varepsilon_{\boldsymbol{k}} + 4g_t t'\varphi_{\boldsymbol{k}} + \tilde{\mu}\right)^2 + D_{\boldsymbol{k}}^2} \ , \tag{10}$$

and

$$\gamma_{\boldsymbol{k}} = \cos k_x + \cos k_y \ , \ \ \eta_{\boldsymbol{k}} = \cos k_x - \cos k_y \ , \ \ \varphi_{\boldsymbol{k}} = \cos k_x \cos k_y \ . \tag{11}$$

The additional renormalized parameter $J_{\text{eff}}^{\pm}$ in the above equations is given as

$$J_{\text{eff}}^{\pm} = J_{\text{eff}} \pm V \ . \tag{12}$$

We note here that Δ_d and ξ_2 are the order parameters of dSC and SF, respectively. Thus, the effective coupling constant for dSC is $J_{\text{eff}}^{-} = J_{\text{eff}} - V$, while that for SF is $J_{\text{eff}}^{+} = J_{\text{eff}} + V$. This implies that the nearest-neighbor Coulomb repulsion V enhances SF, but suppresses dSC.

3. Results and Discussion

First we show the doping dependences of the order parameters Δ_d and ξ_2 given in eqs. (3) and (4) in Fig. 1. The dSC gradually emerges only when $\delta \gtrsim 0.05$ by hole doping, while the SF state monotonically decreases and vanishes at $\delta \simeq 0.2$. Here we can clearly see that these two states coexist within the region of $0.05 \lesssim \delta \lesssim 0.2$. It is worth emphasizing here that dSC does not appear between $\delta = 0$ and 0.05, which is consistent with the typical experimental phase diagram, and at the same time, cannot be captured within the previous mean-field or variational scenario. For example, when we consider the coexisting phase of dSC and antiferromagnetism, it is known that the dSC order parameter appears even at half-filling [12]. Thus the dome-like behavior of the dSC order parameter shown in Fig. 1 can be a peculiarity of the coexisting phase of SF and dSC.
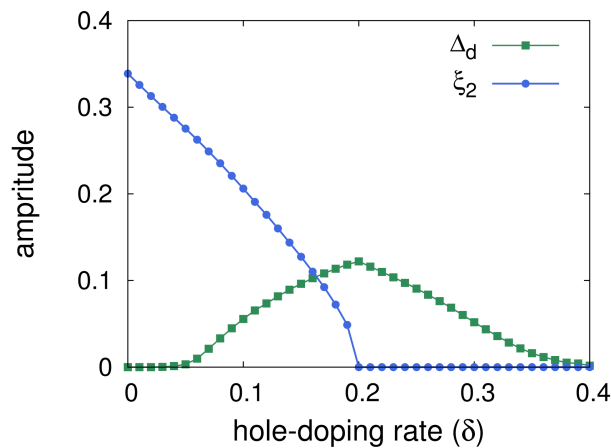
Figure 1. The order parameters Δ_d and ξ_2 versus hole doping at $T = 0$.

Next, let us look at the quasiparticle states in the coexisting state. Figure 2 shows the density of states (DOS) for the coexisting state (the red line) and the pure SF state (the blue line). The pure SF state shows a highly electron-hole asymmetric spectra, which is consistent with previous studies [3, 7]. In the coexisting state, however, the DOS exhibits two different gap-structures, one is highly asymmetric and another is symmetric around the Fermi energy ($E/t = 0$), as

seen in Fig. 2. Comparing this DOS with that for pure SF state, we easily notice that the larger asymmetric gap is due to SF state, and the smaller symmetric gap is a consequence of the coexisting dSC. We note here that the gap amplitudes found in the DOS roughly correspond to $J_{\text{eff}}^{+}\xi_2$ and $J_{\text{eff}}^{-}\Delta_d$. In this situation, we find that the dSC gap is formed using the residual quasiparticle states around the Fermi energy in the SF state.
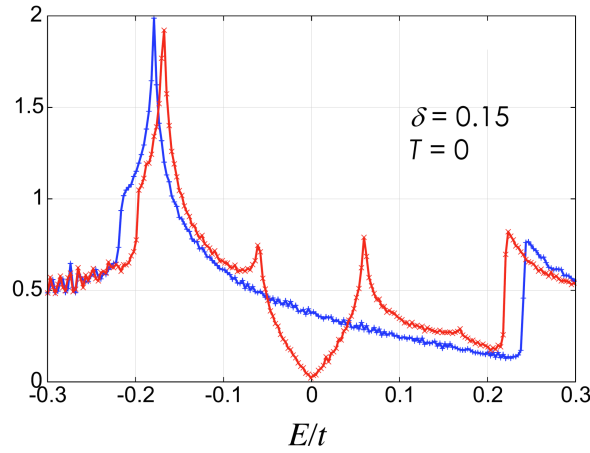
Figure 2. The density of states (DOS) for pure SF state (blue), and the coexisting phase of SF and dSC (red).

Finally, let us discuss the doubly gapped structure found in Fig. 2 in some more detail. Since the $\boldsymbol{k}$-dependences of the quasiparticle states are integrated out in the DOS, it is interesting to see here the angle resolved gap structure in the coexisting state. Fig. 3 shows the gap functions for the coexisting state, and also the pure dSC state as functions of the so-called Fermi angle. Here, $\theta = \pi/4$ corresponds to the nodal direction of the dSC gap in $\boldsymbol{k}$-space. We can clearly see the two-gap structure which is quite consistent with the ARPES experimental data [13]. Therefore, we can conclude that the coexisting state of SF and dSC can be a possible candidate of the pseudogap phase.
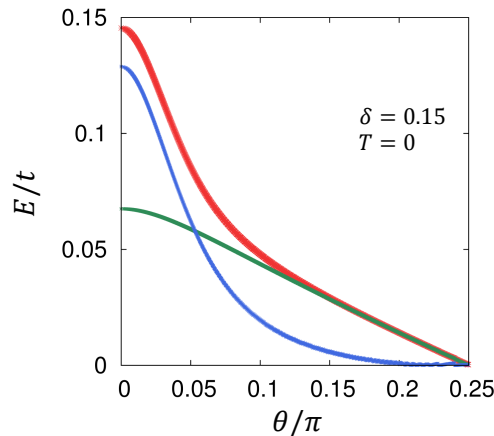
Figure 3. Gap functions for the coexisting phase of SF and dSC (red),pure SF state (blue) and pure dSC state (green) as functions of the Fermi angle.

4. Summary

We have studied the quasiparticle states in the coexisting phase of dSC and SF states within the renormalized mean-field theory based on the *t-J* model. The present analysis has shown that the dome-like structure of dSC in the phase diagram and the two-gap structure can be well described by the coexisting state, and thus also shown that the SF phase can be a possible candidate of symmetry-breaking pseudogap states coexisting with the dSC.

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