Anomalous dispersion relations in the staggered flux state

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Abstract. We study the quasiparticle properties in the d-wave superconductivity, antiferromagnetism, and the staggered flux state within a renormalized mean-field theory based on the two-dimensional $t$-$J$ model. In particular, we focus on the anomalous quasiparticle dispersion relations around the antinodal region of the Brillouin zone argued in Hashimoto et al., Nature Phys. 6, 414 (2010). We obtain the qualitatively consistent results with their observations when we take account of the SF state. The present analysis shows that the SF order can be a possible candidate of symmetry-breaking pseudogap states coexisting with the dSC.

1. Introduction

Recent experimental studies have indicated that the pseudogap phase in underdoped high-Tc cuprates is accompanied by some phase transitions with the breaking of time-reversal [1, 2], rotational [3], or translational symmetry. These symmetry breakings imply that there can be nematic order, charge order, or other instabilities in the pseudogap phase[4, 5, 6, 7, 8]. It has also been suggested that the pseudogap order and d-wave superconductivity (dSC) can coexist within the superconducting dome of the cuprates at $p < 0.19$, where $p$ is the hole concentration.

One of the intriguing experimental evidences of the coexisting pseudogap phase with dSC is a gap-structure in the AREPES data opening with broken particle-hole symmetry found in Bi-2201 [9, 10]. They examined the quasi-particle dispersions along the Brillouin zone boundary, and claimed that the gap opens below the $T_c$ is distinct from dSC based on a phenomenological model calculation, and also that the gap can be understood by assuming the coexisting antiferromagnetic (AF) order with dSC. Soon after the that, Greco and Bejas [11] have carried out theoretical calculations of the quasiparticle properties in the pseudogap state incorporating the effects of $d$ charge-density-wave fluctuation, or the so-called staggered flux fluctuation) based on the $t$-$J$ model. They successfully described the anomalous dispersion relations along the zone-boundary without taking account of AF order or fluctuation.

Motivated by these backgrounds, we here study the quasiparticle properties in dSC, AF, and also the staggered flux (SF) states within the same theoretical framework. 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 [13, 14, 15, 16, 17, 18]. It was
considered firstly as a candidate of the ground state for the CuO$_2$ plain, then has been studied as a candidate for a non-superconducting state that causes the pseudogap found in underdoped cuprates. In this paper, we study the quasiparticle dispersions in the SF and dSC states by using the $t$-$J$ model within the Bogoliubov-de Gennes theory based on an extended version of the Gutzwiller approximation. We will see the SF state exhibits the qualitatively consistent dispersion relations with those observed in the ARPES experiments [9, 10].

2. model

In this study, we employ an advanced version of the renormalized mean-field theory for the $t$-$J$ model, the Hamiltonian of which is given as

$$\mathcal{H} = - \sum_{\langle i,j \rangle, \sigma} P_G(t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) P_G + J \sum_{\langle i,j \rangle} S_i \cdot S_j - \mu \sum_{i, \sigma} c_{i\sigma}^\dagger c_{i\sigma}$$

(1)

in the summation notation where $\langle i, j \rangle$ means the summation over nearest-neighbor pairs. The Gutzwiller’s projection operator $P_G$ is defined as $P_G = \Pi(1-n_{i\uparrow}n_{i\downarrow})$. The Bogoliubov-de Gennes (BdG) equation for a renormalized mean-field Hamiltonian based on an extended Gutzwiller approximation [19, 20, 21] is given as

$$\begin{pmatrix} H_{ij}^\uparrow & F_{ji}^\dagger \\ F_{ji} & -H_{ji}^\dagger \end{pmatrix} \begin{pmatrix} u_{ij}^\alpha \\ v_{ij}^\alpha \end{pmatrix} = E^\alpha \begin{pmatrix} u_{ij}^\alpha \\ v_{ij}^\alpha \end{pmatrix},$$

(2)

with

$$H_{ij}^\sigma = - \sum_\tau \left( t_{ij}^\text{eff} + J_{ij}^\text{eff} \chi_{ij} \right) \delta_{ij,i+\tau} - \sum_\nu t_{ij}^\text{eff} \delta_{ij,i+\nu} + \sigma \delta_{ij} \sum_\tau h_{ij,i+\tau}^\text{eff} - \mu \delta_{ij},$$

$$F_{ij}^\alpha = - \sum_\tau J_{ij}^\text{eff} \Delta_{ij} \delta_{ij,i+\tau},$$

(3)

where $\sigma = \pm 1$, $i + \tau$ represents the nearest neighbor sites of the site $i$, while $i + \nu$ the 2nd neighbor sites.

The renormalized parameters $t_{ij}^\text{eff}$, $J_{ij}^\text{eff}$, $h_{ij}^\text{eff}$ and $\Delta_{ij}$ have somewhat complicated forms depending on the local expectation values $\Delta_{ij} = \frac{1}{2} \langle c_{j\uparrow}^\dagger c_{i\downarrow}^\dagger - c_{j\downarrow}^\dagger c_{i\uparrow} \rangle$, $\chi_{ij} = \langle c_{j\sigma}^\dagger c_{i\sigma} \rangle$, and $m_i = \frac{1}{2} (n_{i\uparrow} - n_{i\downarrow})$ [19, 20, 21]. These parameters are determined from cluster calculations to reproduce the variational Monte Carlo results [19]. Thus the present renormalized mean-field theory can give more reliable results than theories based on the conventional slave boson or Gutzwiller approximation [22]. In particular, the overestimation of AF commonly seen in the conventional mean-field theories is improved in the present theoretical treatment. Since the detailed derivation of these parameters are given in ref. [19], here we only show in Table 1 the self-consistently obtained numerical values of them for the $t$-$J$ model with $J/t = 0.3$, $t'/t = -0.3$, and the hole doping $\delta = 0.09$. In the present calculation, we regard the 2×2 square lattice as a unit cell to solve the BdG equation numerically.

3. Results and discussion

Let us look at firstly the quasiparticle states of dSC and SF states. Figure 1 shows the density of states (DOS) per each site for dSC and SF states. Here the DOS is given as

$$N_j(E) = \frac{1}{N_c} \sum_{\mathbf{k}, \alpha} \left[ |v_{ij}^\alpha(\mathbf{k})|^2 \delta(E^\alpha(\mathbf{k}) - E) + |v_{ij}^\dagger(\mathbf{k})|^2 \delta(E^\alpha(\mathbf{k}) + E) \right]$$

(4)
Table 1. Renormalized model parameters for the \(t\)-\(J\) model with \(J/t = 0.3\), \(t'/t = -0.3\), and \(\delta = 0.09\). Here we omit the site indices \(i\) and \(j\) because we are studying homogeneous electronic states.

| state          | \(t_{\text{eff}}\) | \(t'_{\text{eff}}\) | \(J_{\text{eff}}\) | \(\tilde{\Delta}_{\text{eff}}\) | \(\tilde{\chi}_{\text{eff}}\) | \(h_{\text{eff}}\) | \(\mu\)  |
|----------------|--------------------|--------------------|--------------------|-------------------|-----------------|----------------|-------|
| normal state   | 0.1445             | -0.0495            | 0                  | 0.0805            | 0               | -0.161        |       |
| dSC            | 0.1403             | -0.0494            | 0.032              | 0.0642            | 0               | -0.143        |       |
| SF             | 0.1416             | -0.0497            | 0                  | 0.067±0.0332       | 0               | -0.165        |       |
| dSC+AF         | 0.1384             | -0.0491            | 0.030              | 0.062             | 0.0285          | -0.144        |       |

where \(j\) represents a site where the local density of states is calculated, \(\alpha\) is the eigenstate index, and \(k\) is the Bloch wave number of the present unit cells. The blue line in Fig. 1 represents the DOS for dSC, and the red one for SF states. The form of the FS implies that the DOS at zero-energy is nonzero, in contrast to the results for dSC, as previously found by Morr [16]. In particular, we can see that the DOS for the SF state is shifted downwards in energy, in comparison to the case of dSC. Thus we can expect the quasiparticle excitation energy for the SF is larger than that of dSC around the antinodal region of the Brillouin zone.

![Figure 1](image.png)

Figure 1. The density of states (DOS) per each site for dSC (blue) and SF (red) states.

Next, we show the antinodal quasiparticle dispersions \(E_{\text{dSC}}(k)\) for dSC (blue) and \(E_{\text{SF}}(k)\) for SF (red) [23] along the Brillouin zone boundary \(k_x = \pi\) in Fig. 2. We also plot the normal state dispersion relation (green) for comparison. As expected, the dSC state shows the superconducting energy gap \(\Delta E_{\text{dSC}} \sim 0.12\) around \(k_y/\pi \sim \pm 0.08\) as indicated by blue arrows. This momenta with the gap minima is slightly different from the Fermi wave number in the normal state due to the chemical potential shift accompanying the superconducting phase transition, as shown in Table 1. The SF state exhibits the larger excitation energy gap \(\Delta E_{\text{SF}} \sim 0.14\) around \(k_y/\pi \sim \pm 1.1\), which is markedly away from those for the dSC state, as indicated by red arrows in Fig. 2. Since the chemical potential in the SF state is almost the same as the normal state (Table 1), the marked difference of the momenta with the gap minima from the Fermi wave number is due to the broken particle-hole symmetry in the SF state. These results are consistent with the recent ARPES observations [9, 10] in which an anomalous dispersion relation has been found at \(T < T_c\) in an optimally doped Bi-2201 cuprate.
superconductor. Thus the SF state can be a possible candidate of symmetry-breaking pseudogap states coexisting with the dSC. We note here that, in the present calculation, the SF state does not have a lower energy than the dSC, and also that the coexisting state of these two (dSC+SF) has not been found. We can expect, however, that the SF or the SF+dSC state may be stabilized when we consider finite temperature effects, or intersite Coulomb repulsion [17].

![Figure 2](image)

**Figure 2.** Quasiparticle dispersion relation for dSC (blue), SF (red), and the normal state (green) along the Brillouin zone boundary $k_x = \pi$.

Finally, let us mention the effects of antiferromagnetic (AF) order on the anomalous dispersion relation found in the zone boundary shown in Fig. 2. If the AF order is taken into account in our calculation, we find a small expectation value of $\langle S_j^z \rangle \sim \pm 0.05$ coexisting with the dSC state for the hole doping $\delta = 0.09$. Thus the antiferromagnetic gap is also very small, and we confirm that the DOS for this coexisting state is almost similar with that of the dSC, as shown in Fig. 3 (a). A small gap-like structure can be found around $E/t \sim 0.1$. In order to clarify the effect of this small gap structure in the DOS, we calculate the momentum distribution function $n(k)$ for the coexisting state (dSC+AF) and the dSC state. Figure 3 (b) shows the difference of the $n(k)$ between these two states in the full Brillouin zone. We can clearly see that the effects of the coexisting AF order is concentrated around the AF hot spots, and does not have a significant effect around the antinodal region of the Brillouin zone. Thus we speculate that the anomalous dispersion relation found in the ARPES experiments [9, 10] is not due to AF.

### 4. Summary

We have studied the quasiparticle dispersion relation around the antinodal region of the full Brillouin zone in the dSC and SF states within the renormalized mean-field theory based on the $t$-$J$ model. The present analysis has shown that the SF order can be a possible candidate of symmetry-breaking pseudogap states coexisting with the dSC.

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### References

[1] A. Kaminski, S. Rosenkranz, H. M. Fretwell, J. C. Campuzano, Z. Li, H. Raffy, W. G. Cullen, H. You, C. G. Olsonk, C. M. Varma, and H. Höchst, Nature **416**, 610 (2002).
Figure 3. (a) The DOS for the dSC state coexisting with AF order. (b) The difference of the momentum distribution functions between the dSC and the coexisting state.

[2] Y. Li, G. Yu, M. K. Chan, V. Balédent, Y. Li, N. Barisić, X. Zhao, K. Kradil, R. A. Mole, Y. Sidis, P. Steffens, P. Bourges, and M. Greven, Nature Phys. 8, 404 (2012).
[3] M. Fujita, H. Hiraka, M. Matsuda, M. Matsuura, J. M. Tranquada, S. Wakimoto, G. Xu, and K. Yamada, J. Phys. Soc. Jpn. 81, 011007 (2012).
[4] G. Ghiringhelli, M. Le Tacon, M. Minola, S. Blanco-Canosa, C. Mazzoli, N. B. Brookes, B. M. De Luca, A. Frano, D. G. Hawthorn, F. He, T. Loew, M. M. Sala, D. C. Peets, M. Salluzzo, E. Schierle, R. Sutarto, G. A. Sawatzky, E. Wescieke, B. Keimer, and L. Brivio, Science 337, 821 (2012).
[5] K. Nakayama, T. Sato, T. Dobashi, K. Terashima, S. Souma, H. Matsui, T. Takahashi, J. C. Campuzano, K. Kudo, T. Sasaki, N. Kobayashi, T. Kondo, T. Takeuchi, K. Kadowaki, M. Kofu, and K. Hirota, Phys. Rev. B 74, 054505 (2006).
[6] S. E. Sebastian, N. Harrison, E. Palm, T. P. Murphy, C. H. Mielke, R. Liang, D. A. Bonn, W. N. Hardy, and G. G. Lonzarich, Nature 454, 200 (2008).
[7] E. Razzoli, Y. Sassa, G. Drachuck, M. Mansson, A. Keren, M. Shay, M. H. Berntsen, O. Tjernberg, M. Radovic, J. Chang, S. Pailhes, N. Momono, M. Oda, M. Ido, O. J. Lipson, S. M. Hayden, L. Pattthey, J. Mesot, and M. Shih, New J. Phys. 12, 125003 (2010).
[8] R.-H. He, X. J. Zhou, M. Hashimoto, T. Yoshida, K. Tanaka, S.-K. Mo, T. Sasagawa, N. Mannella, W. Meevasana, H. Yao, M. Fujita, T. Adachi, S. Komiyama, S. Uchida, Y. Ando, F. Zhou, Z. X. Zhao, A. Fujimori, Y. Koike, K. Yamada, Z. Hussain, and Z.-X. Shen, New J. Phys. 13, 013031 (2011).
[9] M. Hashimoto, R.-H. He, K. Tanaka, J.-P. Testaud, W. Meevasana, R. G. Moore, D. Lu, H. Yao, Y. Yoshida, H. Eisaki, T. P. Devereaux, Z. Hussain, and Z.-X. Shen, Nature Phys. 6, 414 (2010).
[10] M. Hashimoto, I. M. Vishik, R.-H. He, T. P. Devereaux, and Z.-X. Shen, Nature Phys. 10, 483 (2014).
[11] A. Greco and M. Bejas, Phys. Rev. B 83, 212503 (2011).
[12] K. Fujita, A. R. Schmidt, E.-A. Kim, M. J. Lawler, D. H. Lee, J. C. Davis, H. Eisaki, and S. Uchida, J. Phys. Soc. Jpn. 81, 011005 (2012).
[13] I. Affleck and J. B. Marston, Phys. Rev. B 37, 3774 (1988).
[14] P. A. Lee and X.-G. Wen, Phys. Rev. B 63, 224517 (2001).
[15] S. Chakravarty, R. B. Laughlin, D. K. Morr, and C. Nayak, Phys. Rev. B 63, 094503 (2001).
[16] D. K. Morr, Phys. Rev. Lett. 89, 106401 (2002).
[17] S. Zhou and Z. Wang, Phys. Rev. B 70, 020501(R) (2004).
[18] H. Yokoyama, S. Tamura, and M. Ogata, J. Phys. Soc. Jpn. 85, 124707 (2016).
[19] M. Ogata and A. Himeida, J. Phys. Soc. Jpn. 72, 374 (2003).
[20] H. Tsuchiura, Y. Tanaka, M. Ogata, and S. Kashiwaya, Phys. Rev. B 64, 140501(R) (2001).
[21] H. Tsuchiura, M. Ogata, Y. Tanaka, and S. Kashiwaya, Phys. Rev. B 68, 012509 (2003).
[22] F. C. Zhang, C. Gros, T. M. Rice, and H. Shiba, Supercond. Sci. Technol. 1, 36 (1988).
[23] A detailed derivation of the dispersion relation $E_{SF}(k)$ is given, for example, in the Appendix A of [18].