Cuprate Superconductors in the Vicinity of a Pomeranchuk Instability

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Abstract

We propose that cuprate superconductors are in the vicinity of a spontaneous d-wave type Fermi surface symmetry breaking, often called a d-wave Pomeranchuk instability. This idea is explored by means of a comprehensive study of magnetic excitations within the slave-boson mean-field theory of the t-J model. We can naturally understand the pronounced xy anisotropy of magnetic excitations in untwinned $YBa_2Cu_3O_y$ and the sizable change of incommensurability of magnetic excitations at the transition temperature to the low-temperature tetragonal lattice structure in $La_{2-x}Ba_xCuO_4$. In addition, the present theoretical framework allows the understanding of the similarities and differences of magnetic excitations in Y-based and La-based cuprates.

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I. INTRODUCTION

Usually the symmetry of the Fermi surface (FS) satisfies the point-group symmetry of the underlying lattice structure. However, recently, symmetry breaking of the FS with the d-wave order parameter was discussed in the t-J[1] and Hubbard[2] models on a square lattice: the FS expands along the k_x direction and shrinks along the k_y direction, or vice versa. This d-wave type Fermi surface deformation (dFSD) is often called a d-wave Pomeranchuk instability, referring to Pomeranchuk's stability criteria of isotropic Fermi liquids.[3] But the dFSD occurs even without violating Pomeranchuk's criteria since the transition is usually of first order at low temperature,[4] and also occurs in strongly correlated electron systems such as those described by the t-J model.

The dFSD competes with superconductivity. In the slave-boson mean-field theory of the t-J model[1] superconductivity becomes more dominant and the dFSD instability does not occur, which was recently confirmed by a variational Monte Carlo calculation.[5] However, substantial correlations of the dFSD still remain and lead to a giant response to a small anisotropy, e.g. in a lattice.[1, 5]

Recently a pronounced anisotropy was reported in magnetic excitation spectra of un-twinned $YBa_2Cu_3O_y$ (YBCO).[6, 7] In the superconducting state[6] the peak of the imaginary part of the dynamical magnetic susceptibility $\chi(\mathbf{q}, \omega)$ at various frequencies appear at $\mathbf{q} = (\pi \pm 2\pi\eta_x, \pi)$ and $(\pi, \pi \pm 2\pi\eta_y)$ with $\eta_x \neq \eta_y$ and different peak intensity; $\eta_{x(y)}$ parameterizes the degree of incommensurability. In the pseudogap phase[7] the incommensurate (IC) peaks are smeared, and the spectral weight forms a broad distribution centered at (π, π), but with a strongly enhanced anisotropy characterized by an elliptic shape. In La-based cuprates, IC signals appear up to a temperature much higher than the superconducting transition temperature T_c. While the IC signals retain fourfold symmetry, namely $\eta_x = \eta_y = \eta$, the value of η turns out to show a sizable change when the lattice undergoes the structural phase transition from the low-temperature orthorhombic structure (LTO) to the low-temperature tetragonal structure (LTT) in $La_{2-x}Ba_xCuO_4$ (LBCO) with $x = 0.125$.[8]

In this paper, we show that the above experimental data are naturally understood in terms of dFSD correlations. While sizable dFSD correlations were found in the slave-boson,[1] exact diagonalization,[9] and variational Monte Carlo[5] techniques in the t-J model, and in various renormalization group analyses[2, 10–12] in the Hubbard model, we employ the t-J

model in the slave-boson mean-field theory, which has the advantage of dealing with both d-wave singlet pairing and dFSD correlations on an equal footing as well as performing a systematic calculation of magnetic excitations.

II.   MODEL AND FORMALISM

The t-J model

$$H = -\sum_{\mathbf{r},\mathbf{r}',\sigma} t_{\boldsymbol{\tau}}^{(l)} \tilde{c}_{\mathbf{r}\sigma}^{\dagger} \tilde{c}_{\mathbf{r}'\sigma} + \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} J_{\boldsymbol{\tau}} \mathbf{S}_{\mathbf{r}} \cdot \mathbf{S}_{\mathbf{r}'} \tag{1}$$

is defined in the Fock space with no doubly occupied sites. The operator $\tilde{c}_{\mathbf{r}\sigma}^{\dagger}$ $(\tilde{c}_{\mathbf{r}\sigma})$ creates (annihilates) an electron with spin σ on site $\mathbf{r}$, and $\mathbf{S}_{\mathbf{r}}$ is the spin operator; $J_{\boldsymbol{\tau}}(> 0)$ is a superexchange coupling between the nearest neighbor sites and $t_{\boldsymbol{\tau}}^{(l)}$ is a hopping amplitude between the lth nearest neighbors $(l \leq 3)$; $\boldsymbol{\tau} = \mathbf{r}' - \mathbf{r}$.

We introduce the slave particles, $f_{\mathbf{r}\sigma}$ and $b_{\mathbf{r}}$, as $\tilde{c}_{\mathbf{r}\sigma} = b_{\mathbf{r}}^{\dagger} f_{\mathbf{r}\sigma}$, where $f_{\mathbf{r}\sigma}$ $(b_{\mathbf{r}})$ is a fermion (boson) operator that carries spin σ (charge e), and $\mathbf{S}_{\mathbf{r}} = \frac{1}{2} f_{\mathbf{r}\alpha}^{\dagger} \boldsymbol{\sigma}_{\alpha\beta} f_{\mathbf{r}\beta}$ with the Pauli matrices $\boldsymbol{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$. The slave bosons and fermions are linked by the local constraint $b_{\mathbf{r}}^{\dagger} b_{\mathbf{r}} + \sum_{\sigma} f_{\mathbf{r}\sigma}^{\dagger} f_{\mathbf{r}\sigma} = 1$. This is an exact transformation known as the slave-boson formalism. We then decouple the interaction with the so-called resonating-valence-bond (RVB) mean fields: $\chi_{\boldsymbol{\tau}} \equiv \langle \sum_{\sigma} f_{\mathbf{r}\sigma}^{\dagger} f_{\mathbf{r}'\sigma} \rangle$, $\langle b_{\mathbf{r}}^{\dagger} b_{\mathbf{r}'} \rangle$, and $\Delta_{\boldsymbol{\tau}} \equiv \langle f_{\mathbf{r}\uparrow} f_{\mathbf{r}'\downarrow} - f_{\mathbf{r}\downarrow} f_{\mathbf{r}'\uparrow} \rangle$. These mean fields are assumed to be real constants independent of site $\mathbf{r}$. We approximate the bosons to condense at the bottom of the band, which leads to $\langle b_{\mathbf{r}}^{\dagger} b_{\mathbf{r}'} \rangle = \delta$, where δ is the hole density. The order parameter of the dFSD is defined as $\phi = (\chi_y - \chi_x)/2$ and d-wave singlet pairing is given by $\Delta = |\Delta_x - \Delta_y|/2$; both orders are generated by the second term in the Hamiltonian (1). After determining the RVB mean fields by minimizing the free energy, we compute the dynamical magnetic susceptibility $\chi(\mathbf{q}, \omega)$ numerically in the renormalized random phase approximation (RPA).[13, 14]

The material dependence of high-T_c cuprates is taken into account mainly by different choices of band parameters. While the parameters $t_{\boldsymbol{\tau}}^{(l)}$ and $J_{\boldsymbol{\tau}}$ are considered on a square lattice for La-based cuprates, the bilayer coupling is included to perform a more realistic calculation for Y-based cuprates. The details of our formalism are presented in Refs. 15 and 16 for Y-based and La-based cuprates, respectively. We show results for $\delta = 0.12$, which may be complement to those references.

III.   RESULTS FOR UNTWINNED Y-BASED CUPRATES

The crystal structure of untwinned YBCO is orthorhombic in the carrier doping region where superconductivity is realized at low T, yielding a small xy anisotropy to the electronic band structure. We introduce 5% anisotropy to hopping integrals between the x and y direction, and 10% anisotropy between J_x and J_y, twice as large, as imposed by the superexchange mechanism. Since CuO chains run along the y direction, we assume the band parameters are enhanced more along the y direction.

The order parameter of the dFSD ϕ is plotted in Fig. 1(a) together with the d-wave singlet pairing Δ. ϕ increases with decreasing T and exhibits a cusp at the onset of Δ, which is denoted as T_{RVB}; T_{RVB} is interpreted as pseudogap crossover temperature T^* in the underdoped regime and as T_c in the overdoped regime of high-T_c cuprates. Below T_{RVB}, ϕ is suppressed because of competition with singlet pairing but still enhanced compared with the value of ϕ at high T.

The FSs at low T are shown in Fig. 1(b). The inner (outer) FS is formed by the antibonding (bonding) band due to the bilayer coupling. The inner FS can easily open in the presence of an anisotropy while the outer FS is still holelike.

Momentum space maps of $\mathrm{Im}\chi(\mathbf{q}, \omega)$ for a sequence of temperatures are shown in Fig. 2 for $\omega = 0.30J$ and $\delta = 0.12$ in the odd channel; a similar result is obtained in the even channel.[15] The strong intensity region forms a deformed diamond shape at low T [Fig. 2(a)], and the spectral weight inside the diamond gradually increases with T [Fig. 2(b)]. The spectral weight around $\mathbf{q} = (\pi, \pi)$ becomes dominant at temperature slightly below $T_{\mathrm{RVB}} = 0.124J$ and an enhanced anisotropy appears with an elliptic-shape distribution as shown in Fig. 2(c). When T increases further, however, the anisotropy is reduced [Fig. 2(d)]. This strong T dependence is characteristic of the effect of dFSD correlations.

IV.   RESULTS FOR LA-BASED CUPRATES

Three different crystal structures are realized in La-based high-T_c cuprates, depending on temperature and carrier doping: high-temperature tetragonal structure (HTT), LTO, and LTT. In the former two structures, the lattice does not produce a xy anisotropy and thus not couple to the underlying dFSD tendency. We expect an electronlike FS for $\delta = 0.12$ as

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shown in Fig. 3(a). The LTT, however, yields a small xy anisotropy, the direction of which alternates along the z axis. Such a small anisotropy is then strongly enhanced by dFSD correlations as we have seen in Fig. 1(a). Through a coupling to the LTT, therefore, we expect a strongly deformed FS as shown by solid lines in Fig. 3(b); the FS is deformed in the opposite direction (gray lines) in neighboring CuO_2 planes and thus the superimposed FS recovers fourfold symmetry. A weak interlayer coupling then leads to two FSs, an inner electronlike FS and an outer holelike FS as shown in Fig. 3(c). Note that dynamical fluctuations of the dFSD are expected in the presence of the soft phonon mode toward the LTT phase transition even in the LTO phase.[17]

For simplicity we do not consider the interlayer coupling, although it is important in the sense that it can yield a one-dimensional-like incommensurate peak along the direction $\mathbf{q} = \frac{1}{\sqrt{2}}(q, q)$.[18] We compute $Im\chi(\mathbf{q}, \omega)$ for the FSs shown in Figs. 3(a) and (b). We find that similar magnetic excitations are obtained for both FSs.[16] The spectral weight distribution has fourfold symmetry around $\mathbf{q} = (\pi, \pi)$. At low T, the strong intensity region forms a diamond shape as shown in Fig. 2(a), and pronounced IC signals appear at $(\pi \pm 2\pi\eta, \pi)$ and $(\pi, \pi \pm 2\pi\eta)$. With increasing T, the spectral weight around $\mathbf{q} = (\pi, \pi)$ increases and the IC signals become less clear, but they are still discernible even at high temperature ($\sim 0.15J$),[16] different from the result in Fig. 2(d). Since dFSD correlations produce a distinct change of the FS shape from Fig. 3(a) to (b) when the lattice undergoes a phase transition to the LTT, such a FS change in general leads to a sizable change of η at the LTT transition. This features the underlying dFSD correlations in La-based cuprates.

V. DISCUSSION AND CONCLUSION

dFSD correlations lead to a strong anisotropy of magnetic excitations at relatively high T [Fig. 2(c)], which accounts for the recent observation in the pseudogap phase in untwinned $YB_2Cu_3O_{6.6}$.[7] In La-based cuprates, dFSD correlations are expected to lead to a change of the FS (Fig. 3) through the LTT phase transition, which is in general accompanied by a sizable change of incommensurability of magnetic excitations; the FS shown in Fig. 3(b) tends to favor a larger η. Such a change was recently observed in LBCO with $x = 0.125$,[8] although the authors[8] interpreted the data differently as due to a charge stripe formation.

Magnetic excitations in high-T_c cuprates, especially in La-based cuprates, are frequently

discussed in terms of charge stripes or electronic nematic order envisaged as a partial stripe order.[19] Although the state with a d-wave deformed FS has the same symmetry as the nematic order, dFSD correlations originate from forward scattering processes of quasiparticles[1, 2] and do not require charge stripe correlations. An interesting open question is whether the dFSD state can have an instability toward a charge ordered state such as stripes. Even if it were the case, our calculation shows that many salient features of magnetic excitations observed in La-based cuprates are already well-captured without stripes. Observations of weak charge order signals[20] do not necessarily mean that charge stripes are crucial to magnetic excitations. The effect of charge order on magnetic excitations can be higher order corrections beyond the present renormalized RPA.

A well-known distinction of magnetic excitations between La-based and Y-based cuprates is that low-energy IC signals are realized up to a temperature much higher than T_c in the former,[21, 22] while they are realized only below T_c or possibly below pseudogap temperature T^* in the latter.[23] This difference comes from a FS difference in the present theory. For the FSs shown in Figs. 3(a) and (b), there are no particle-hole scattering processes with $\mathbf{q} = (\pi, \pi)$ for low energy, yielding a robust incommensurate structure even in the normal state, while the FS shown in Fig. 1(b) allows such scattering processes, smearing incommensurate signals in the normal state. The FS geometry is essential for the material dependence of magnetic excitations, the same insight as the early proposal,[24, 25] although we have extended the early studies in the t-J model[26–28] by introducing an idea of the dFSD. More detailed comparisons of magnetic excitations between Y-based and La-based cuprates are presented in Ref. 16.

We have shown that many salient features of magnetic excitations in high-T_c cuprates are well-captured in terms of particle-hole excitations. In particular, dFSD correlations are essential for the pronounced anisotropy observed in untwinned YBCO[6, 7] and the sizable change of incommensurability at the onset temperature of the LTT phase transition in LBCO.[8] Cuprate superconductors are expected to be in the vicinity of the dFSD instability, the so-called d-wave Pomeranchuk instability, leading to a giant response to a small external xy anisotropy.

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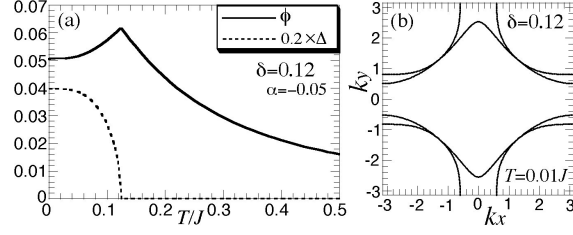[28] J. Brinckmann and P. A. Lee, Phys. Rev. B **65**, 014502 (2002).

FIG. 1: The mean-field solution in the presence of an anisotropy for $\delta = 0.12$. (a) T dependence of ϕ and Δ. (b) Fermi surface at low T.
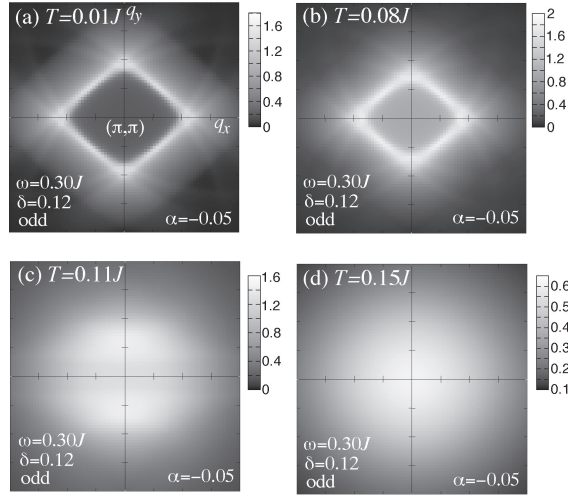

FIG. 2: $\mathbf{q}$ maps of $\mathrm{Im}\chi(\mathbf{q}, \omega)$ for a sequence of T in $0.6\pi \leq q_x, q_y \leq 1.4\pi$ for $\omega = 0.30J$ and $\delta = 0.12$ in the odd channel; here $T_{\mathrm{RVB}} = 0.124J$.
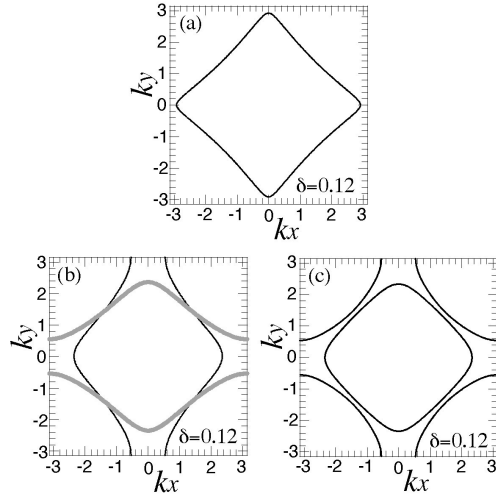
FIG. 3: (a) Fermi surface expected in the HTT and LTO phases for $\delta = 0.12$. (b) and (c) Fermi surface expected in the LTT phase; a weak interlayer coupling is considered in (c) but not in (b).