Breakdown of Fourfold Symmetry of Fermi Surface and Magnetic Excitation Spectrum

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Performing the slave-boson mean-field approximation to the two-dimensional t–J model under the assumption of the uniform charge density, we find two mechanisms that lead to the breaking of fourfold symmetry of the Fermi surface (FS) and the magnetic excitation spectrum. One mechanism originates from the J-term, which has an intrinsic instability toward the formation of a quasi-one-dimensional FS. The other mechanism comes from the inclusion of the small interlayer hopping $t_{\perp}$, which can lead to the drastic breaking of fourfold symmetry in the diagonal incommensurate magnetic peaks around (π, π). These findings are discussed with emphasis on possible relevance to $La_{2-x}Sr_xCuO_4$ systems.

KEYWORDS: A. oxides; D. superconductors; D. Fermi surface; D. magnetic properties

1. Introduction

Elastic neutron scattering in Nd-doped $La_{2-x}Sr_xCuO_4$ (LSCO) around $x \approx 0.12$[1,2] has revealed some charge density modulation (CDM), which is accompanied by incommensurate antiferromagnetic long-range order at lower temperature; the wavevector of the CDM is just twice larger than that of the magnetic order. On the basis of this data, the so-called 'spin-charge stripes' scenario has been proposed:[1] there may exist an intrinsic instability toward one-dimensional (1d) charge ordering, namely 'charge stripes', in each CuO_2 plane, by which 1d incommensurate magnetic order (or fluctuations) may be realized. Recent finding of '1d-like' *diagonal* incommensurate magnetic order in LSCO with $0.02 \lesssim x \lesssim 0.05$[3,4] is often discussed as a strong support of this scenario, where the direction of 'charge stripes' is assumed to be rotated by 45° from the Cu-O bond direction. The CDM, however, has not been detected in such low doping region. On the theoretical side, the possible formation of the 'spin-charge stripes' has been argued in different contexts,[5,6] but remains to be clarified.

On the other hand, leaving a possible formation of some CDM to a future study and assuming the uniform charge density, we analyze the two-dimensional (2d) t–J model within the slave-boson mean-field scheme. We find two mechanisms that lead to the breaking of fourfold symmetry of the Fermi surface (FS) and the magnetic excitation spectrum. (i) One mechanism originates from the J-term, which has an intrinsic instability toward the formation of a quasi-one-dimensional (q-1d) FS. The incommensurate (IC-) peaks at $(\pi,\, \pi \mp 2\pi\eta_a)$ (tetragonal notation) and $(\pi \mp 2\pi\eta_b,\, \pi)$ lack the fourfold symmetry around $(\pi,\, \pi)$, but the degree of the symmetry breaking is not so strong that an 1d magnetic structure is realized. The diagonal IC (DIC-) peaks at $(\pi \mp 2\pi\eta_c,\, \pi \mp 2\pi\eta_c)$ and $(\pi \pm 2\pi\eta_d,\, \pi \mp 2\pi\eta_d)$, on the other hand, retain the fourfold symmetry around $(\pi,\, \pi)$. (ii) The other mechanism comes from the inclusion of the small interlayer hopping $t_\perp$, which can lead to the drastic breaking of fourfold symmetry in the DIC-peaks. We point out that these mechanisms may give another scenario in discussing LSCO systems.

2. Model and Formalism

As a theoretical model for high-T_c cuprates, we use the 2d t–J model defined on a square lattice

$$H = -\sum_{i,\, j,\, \sigma} t_\tau^{(l)} f_{i\,\sigma}^\dagger b_i b_j^\dagger f_{j\,\sigma} + \sum_{\langle i,j\rangle} J_\tau \boldsymbol{S}_i \cdot \boldsymbol{S}_j, \tag{1}$$

$$\sum_\sigma f_{i\,\sigma}^\dagger f_{i\,\sigma} + b_i^\dagger b_i = 1 \quad \text{at each site } i, \tag{2}$$

where $f_{i\,\sigma}$ (b_i) is a fermion (a boson) operator that carries spin σ (charge e), namely the slave-boson scheme. $t_\tau^{(l)} = t^{(l)}$ is a hopping integral between the l-th nearest neighbor (n.n.) sites i and j ($l \le 3$) with τ being the bond direction $\boldsymbol{\tau} = \boldsymbol{r}_j - \boldsymbol{r}_i$. $J_\tau = J > 0$ is the superexchange coupling between the n.n. spins, and $\boldsymbol{S}_i = \frac{1}{2}\sum_{\alpha,\beta} f_{i\,\alpha}^\dagger \boldsymbol{\sigma}_{\alpha\,\beta} f_{i\,\beta}$ with Pauli matrix $\boldsymbol{\sigma}$. The constraint eq. (2) excludes double occupations at every site.

Following the previous procedure,[7,8] we introduce mean fields: $\chi_\tau^{(l)} \equiv \left\langle \sum_\sigma f_{i\,\sigma}^\dagger f_{i+\tau\,\sigma} \right\rangle$, $\left\langle b_i^\dagger b_{i+\tau} \right\rangle$ and $\Delta_\tau^{(1)} \equiv \langle f_{i\uparrow} f_{i+\tau\downarrow} - f_{i\downarrow} f_{i+\tau\uparrow} \rangle$, where each is taken to be a real constant independent of lattice coordinates, but is allowed to depend on $\boldsymbol{\tau}$. (Note that the fourfold symmetry, $\chi_x^{(1)} = \chi_y^{(1)}$ and $\left|\Delta_x^{(1)}\right| = \left|\Delta_y^{(1)}\right|$, was assumed in the previous study.[7,8]) Also, the local constraint eq. (2) is loosened to a global one, $\sum_i \left(\sum_\sigma f_{i\,\sigma}^\dagger f_{i\,\sigma} + b_i^\dagger b_i \right) = N$ with N being the total number of lattice sites. We then decouple the Hamiltonian eq. (1) to obtain the mean-field Hamiltonian. We approximate the boson to be condensed at the bottom of its band, and determine the mean fields by minimizing the free energy. This approximation will be reasonable at low temperature and leads to $\left\langle b_i^\dagger b_{i+\tau} \right\rangle = \delta$ where δ is the hole density.

Using the mean-field Hamiltonian, we calculate the 'RPA' dynamical magnetic susceptibility

$$\chi(\boldsymbol{q},\, \omega) = \frac{\chi_0(\boldsymbol{q},\, \omega)}{1 + 2rJ(\boldsymbol{q})\chi_0(\boldsymbol{q},\, \omega)}\ , \tag{3}$$

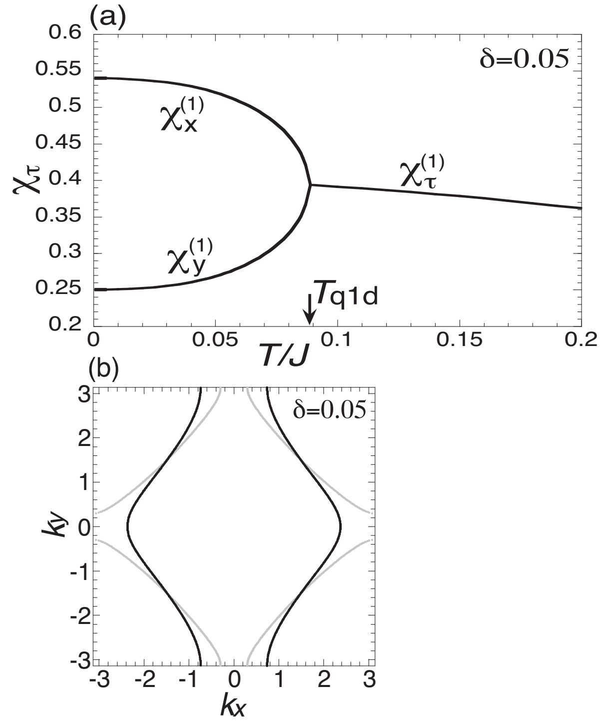

Fig. 1. (a) T-dependence of $\chi_\tau^{(1)}$ under the constraint $\Delta_\tau^{(1)} \equiv 0$. The fourfold symmetry is broken spontaneously below $T_{\rm q1d}$, that is $\chi_x^{(1)} \neq \chi_y^{(1)}$. (b) Fermi surface for $T > T_{\rm q1d}$ (gray line) and that for $T < T_{\rm q1d}$ (solid line).

where $\chi_0(\boldsymbol{q}, \omega)$ is the irreducible dynamical magnetic susceptibility and $J(\boldsymbol{q}) = J(\cos q_x + \cos q_y)$. In eq. (3), we introduce a numerical factor r for convenience. In the RPA, where $r = 1$, $\chi(\boldsymbol{q}, 0)$ diverges at low temperature in a wide doping region $\delta \lesssim 0.17$. This magnetic instability will be an artifact, since such divergence of $\chi(\boldsymbol{q}, 0)$ will be suppressed by higher order corrections to $\chi_0(\boldsymbol{q}, \omega)$. This aspect we take into account phenomenologically by reducing the value of r to 0.35. As a result, the divergence of $\chi(\boldsymbol{q}, 0)$ is limited to the region $\delta \lesssim 0.02$.

3. Result

Focusing our attention on LSCO systems, we take the band parameters as $t^{(1)}/J = 4$, $t^{(2)}/t^{(1)} = -1/6$ and $t^{(3)}/t^{(1)} = 0$.[9] We first impose the constraint $\Delta_\tau^{(1)} \equiv 0$ and determine the mean fields. Figure 1(a) shows $\chi_\tau^{(1)}$ as a function of temperature T. It is found that the fourfold symmetry of $\chi_\tau^{(1)}$ is broken spontaneously below $T = T_{\rm q1d}$ through the second-order phase transition. The resulting FS is q-1d (Fig. 1(b)). We find that this q-1d state is stabilized below $\delta \lesssim \delta_{\rm q1d} \approx 0.13$ at $T = 0$.[10] When we remove the constraint $\Delta_\tau^{(1)} \equiv 0$, the d-wave pairing instability occurs before the q-1d instability and the q-1d state is not stabilized, but the (isotropic) 2d state is.

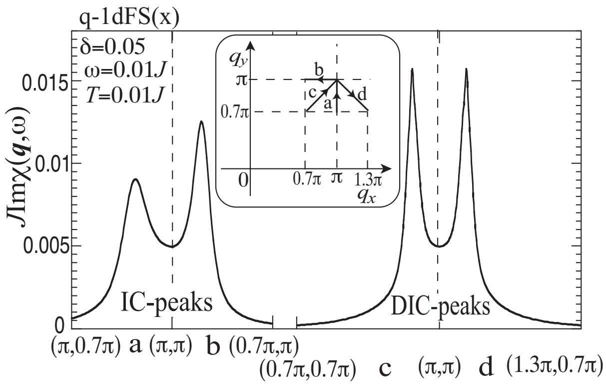

Fig. 2. $\boldsymbol{q}$-dependence of Im$\chi(\boldsymbol{q}, \omega)$ for the q-1dFS(x) ($\chi_x^{(1)} > \chi_y^{(1)}$) in the d-wave pairing state. The inset shows the $\boldsymbol{q}$-scan directions.

To investigate the origin of the q-1d instability, we expand the free energy in terms of $\delta\chi \equiv (\chi_x^{(1)} - \chi_y^{(1)})/2$ up to the second order under the constraint $\Delta_\tau^{(1)} \equiv 0$:

$$F - F_0 \sim \frac{3J}{4}(1-a)(\delta\chi)^2 \,, \tag{4}$$

where F_0 is the free energy in the (isotropic) 2d state. The right-hand side in eq. (4) originates from the J-term in eq. (1), and

$$a = \frac{3J}{4}\frac{1}{N}\sum_{\boldsymbol{k}}\left(-\frac{\partial n_F}{\partial \xi_{\boldsymbol{k}}}\right)(\cos k_x - \cos k_y)^2 > 0 \,, \tag{5}$$

with n_F being the Fermi-Dirac distribution function. We see that the coefficient, $1-a$, in eq. (4) becomes negative below $T = T_{\mathrm{q1d}}$, signalling an instability toward the q-1d state. Since the factor $-\frac{\partial n_F}{\partial \xi_{\boldsymbol{k}}}$ in eq. (5) limits $\boldsymbol{k}$ to a region close to the FS, and the factor $(\cos k_x - \cos k_y)^2$ takes a maximum at $(\pi, 0)$ and $(0, \pi)$, the q-1d instability is driven mainly by the fermions on the FS near $(\pi, 0)$ and $(0, \pi)$. On the other hand, such fermions are also responsible to the d-wave pairing instability, which thus competes with the q-1d instability. We find that the condensation energy for the d-wave pairing state is larger than that for the q-1d state.[10] Therefore, the q-1d state is not stabilized when the constraint $\Delta_\tau^{(1)} \equiv 0$ is removed.

Nonetheless, when we introduce a small spatial anisotropy, $t_x^{(1)} \neq t_y^{(1)}$ and $J_x \neq J_y$, as a weak perturbation coming from the coupling to the low-temperature tetragonal (LTT) lattice distortion[11,12] or its fluctuations[13] in LSCO systems, it is found[10] that the anisotropy is largely enhanced with decreasing T and the q-1d state is realized even in the d-wave pairing state, although the anisotropy is somewhat suppressed by the onset the d-wave pairing order.

We next investigate the magnetic excitation spectrum Im$\chi(\boldsymbol{q}, \omega)$ for the q-1dFS(x), where $\chi_x^{(1)} > \chi_y^{(1)}$, in the d-wave pairing state. In Fig. 2, we show the $\boldsymbol{q}$-scan through the IC-peak

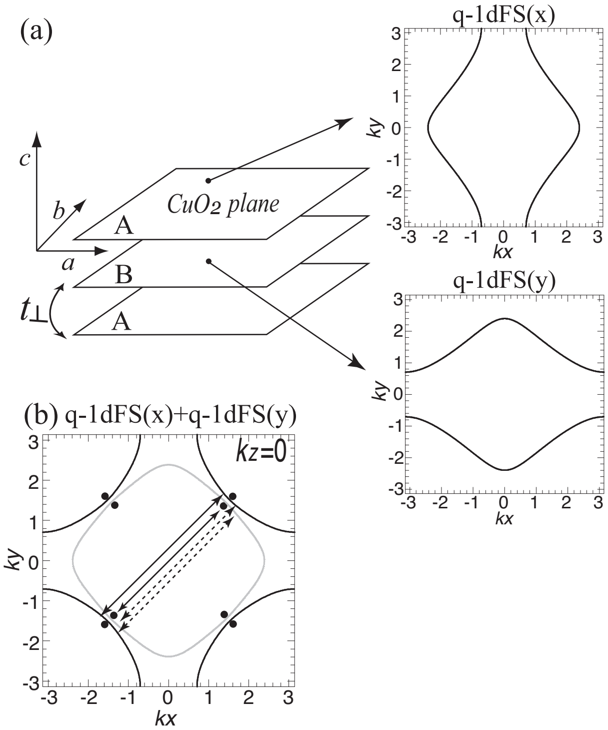

Fig. 3. (a) The alternate stacking of the q-1dFS(x) and the q-1dFS(y) along the c-axis. (b) The resulting FSs, q-1dFS(x)+q-1dFS(y), in the presence of the interlayer hopping $t_\perp$. They consist of the inner FS (gray line) and the outer FS (solid line). The scattering processes between the d-wave gap nodes (solid circles) on the FSs, which may cause the DIC-peak at $\boldsymbol{q} = (\pi \mp 2\pi\eta_c,\, \pi \mp 2\pi\eta_c,\, 0)$, are shown by the solid lines with arrows for the intraband scattering process and by the dashed lines with arrows for the interband scattering process. (Each process is a little shifted away for clarity.)

positions at $(\pi,\, \pi - 2\pi\eta_a)$ and $(\pi - 2\pi\eta_b,\, \pi)$, and the DIC-peak positions at $(\pi - 2\pi\eta_c,\, \pi - 2\pi\eta_c)$ and $(\pi + 2\pi\eta_d,\, \pi - 2\pi\eta_d)$. The IC-peaks lack the fourfold symmetry as expected, but the overall line shapes are 2d rather than 1d even for the q-1dFS. In the DIC-peaks, on the other hand, the fourfold symmetry is retained, since $\mathrm{Im}\chi(\boldsymbol{q},\, \omega)$ is symmetric under $q_x \to 2\pi - q_x$.

We find that with the inclusion of a small interlayer hopping $t_\perp$, the fourfold symmetry in the DIC-peaks can be broken drastically. We take a model that the q-1dFS is stacked alternately along the c-axis (Fig. 3(a)). This alternate stacking may be reasonable if we consider the coupling to the LTT lattice distortion[11,12] or its fluctuations,[13] which will induce the spatial anisotropy alternating along the c-axis. As a c-axis dispersion $\epsilon_{\boldsymbol{k}}$, we take $\epsilon_{\boldsymbol{k}} \propto t_\perp \cos\frac{k_x}{2} \cos\frac{k_y}{2} \cos\frac{k_z}{2}$, which is consistent with the symmetry of the crystal structure in LSCO systems where the adjacent CuO_2 plane is relatively shifted by $[\frac{1}{2},\, \frac{1}{2},\, \frac{1}{2}]$ (tetragonal notation). The resulting FS, shown in Fig. 3(b), recovers the fourfold symmetry.

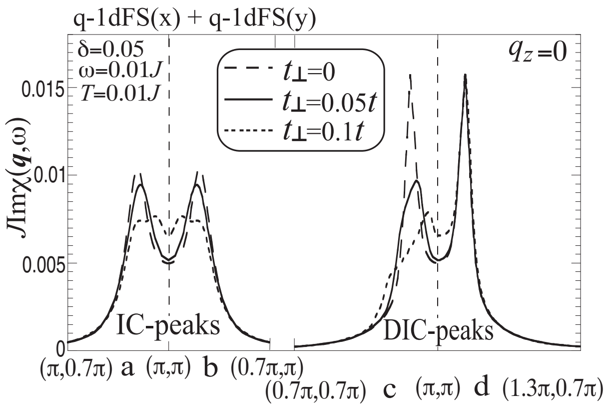

Fig. 4. $\boldsymbol{q}$-dependence of $\mathrm{Im}\chi(\boldsymbol{q},\,\omega)$ for several choices of $t_\perp$ in the d-wave pairing state for the q-1dFS(x)+q-1dFS(y) shown in Fig. 3(b).

Using this FS, we calculate $\mathrm{Im}\chi(\boldsymbol{q},\,\omega)$ for several choices of $t_\perp$; q_z is fixed to 0. Figure 4 shows that the IC-peaks get broader with $t_\perp$ and retain the fourfold symmetry around $(\pi,\,\pi)$ because of the symmetry of $\mathrm{Im}\chi(\boldsymbol{q},\,\omega)$ under the transformation $(q_x,\,q_y) \to (q_y,\,q_x)$. However, we find a drastic breaking of fourfold symmetry in the DIC-peaks with the small $t_\perp$, that is, the DIC-peak at $\boldsymbol{q}_c^{\mathrm{DIC}} = (\pi \mp 2\pi\eta_c,\,\pi \mp 2\pi\eta_c,\,0)$ is largely suppressed while the DIC-peak at $\boldsymbol{q}_d^{\mathrm{DIC}} = (\pi \pm 2\pi\eta_d,\,\pi \mp 2\pi\eta_d,\,0)$ is not. This symmetry breaking itself is not surprising since $\chi(\boldsymbol{q},\,\omega)$ is not symmetric under the transformation $q_x \to 2\pi - q_x$ for the present c-axis dispersion. But why is such symmetry breaking drastic with the small $t_\perp$?

In the presence of the interlayer hopping, particle-hole scattering consists of two processes, the intraband scattering and the interband scattering: $\chi_0(\boldsymbol{q},\,\omega) = \chi_0^{\mathrm{intra}}(\boldsymbol{q},\,\omega) + \chi_0^{\mathrm{inter}}(\boldsymbol{q},\,\omega)$. It can be shown[14] that $\chi_0^{\mathrm{intra}}(\boldsymbol{q},\,\omega)$ is reduced to $\chi_0^{\mathrm{intra}}(\boldsymbol{q},\,\omega) \propto \sum_{\boldsymbol{k}}(1+\mathrm{sign}(\epsilon_{\boldsymbol{k}}\epsilon_{\boldsymbol{k}+\boldsymbol{q}}))\times\cdots$, and similarly $\chi_0^{\mathrm{inter}}(\boldsymbol{q},\,\omega) \propto \sum_{\boldsymbol{k}}(1-\mathrm{sign}(\epsilon_{\boldsymbol{k}}\epsilon_{\boldsymbol{k}+\boldsymbol{q}}))\times\cdots$: the former (latter) consists of the scattering process with $\epsilon_{\boldsymbol{k}}\epsilon_{\boldsymbol{k}+\boldsymbol{q}} > 0(<0)$. In Fig. 3(b), the possible main low-energy scattering processes of the DIC-peak at $\boldsymbol{q} = \boldsymbol{q}_c^{\mathrm{DIC}}$ are shown. For these processes, the sign of $\epsilon_{\boldsymbol{k}}\epsilon_{\boldsymbol{k}+\boldsymbol{q}}$ is positive. By transforming $q_x \to 2\pi - q_x$ and $k_x \to -k_x$, the possible main scattering processes for the DIC-peak at $\boldsymbol{q} = \boldsymbol{q}_d^{\mathrm{DIC}}$ are obtained; the sign of $\epsilon_{\boldsymbol{k}}\epsilon_{\boldsymbol{k}+\boldsymbol{q}}$ is then negative. Therefore, the DIC-peak at $\boldsymbol{q}_c^{\mathrm{DIC}}$ comes mainly from the intraband scattering process whereas the DIC-peak at $\boldsymbol{q}_d^{\mathrm{DIC}}$ comes mainly from the interband process. That is, the DIC-peaks at $\boldsymbol{q}_c^{\mathrm{DIC}}$ and $\boldsymbol{q}_d^{\mathrm{DIC}}$ are essentially different entities, which leads to the drastic breaking of fourfold symmetry in the DIC-peaks.

It should be noted that although we have taken the q-1dFS here, the use of the q-1dFS is not essential to the symmetry breaking in the DIC-peaks, but the form of the c-axis dispersion is. In fact, we find such symmetry breaking also for the 2dFS with the present c-axis dispersion.[14)]

4. Conclusion and Discussion

Focusing our attention on the LSCO systems, we have analyzed the 2d t–J model within the slave-boson mean-filed scheme. We have shown that the J-term has an intrinsic instability toward the formation of the q-1dFS. This instability is driven mainly by the fermions on the FS near $(\pi,\, 0)$ and $(0,\, \pi)$.[15)] The q-1d instability, however, is usually masked by the more prominent d-wave instability. Nonetheless, the presence of the small spatial anisotropy is sufficient for the q-1d state to appear in the d-wave pairing state. By taking the c-axis dispersion $\epsilon_{\boldsymbol{k}} \propto t_{\perp} \cos\frac{k_x}{2} \cos\frac{k_y}{2} \cos\frac{k_z}{2}$, we have also shown that the inclusion of the small $t_{\perp}$ leads to the drastic breaking of fourfold symmetry in the DIC-peaks. This is because the DIC-peak at $\boldsymbol{q}_c^{\rm DIC}$ comes mainly from the intraband scattering process while the DIC-peak at $\boldsymbol{q}_d^{\rm DIC}$ comes mainly from the interband process.

On the basis of the mechanism due to the J-term, we propose a q-1d picture of the FS for LSCO systems as shown in Fig. 3(a).[16)] With this picture, both the angle-resolved photoemission spectroscopy data[17)] and the inelastic neutron scattering data[18)] can be understood consistently.[16,19)] The mechanism due to the $t_{\perp}$-term (Fig. 4) may give a scenario to understand the '1d-like' DIC-peak observed in LSCO with $0.02 \lesssim x \lesssim 0.05$.[3,4)] The following aspects, however, should be noted, which will be crucial to further discussions. (i) The form of the c-axis dispersion, which has not been clarified yet experimentally. (ii) The use of the d-wave pairing state in Fig. 4. This is reasonable from the view of the resonating-valence-bond (RVB) picture,[20)] but would not from the experimental viewpoint since the existence of the spin gap has not been clarified yet in $0.02 \lesssim x \lesssim 0.05$ where the ground state is the spin-glass phase.

In YBCO systems, the band parameters may be taken as $t^{(1)}/J = 4$, $t^{(2)}/t^{(1)} = -1/6$ and $t^{(3)}/t^{(1)} = 1/5$,[9)] for which we have found that the FS is almost 2d at least in $0.05 \lesssim \delta \lesssim 0.30$ even if the small spatial anisotropy is introduced in $t^{(1)}$ and J.[10)] This is because the location of the (original) FS is away from $(\pi,\, 0)$ and $(0,\, \pi)$ more than that for the band parameters appropriate to LSCO systems. Therefore, the mechanism due to the J-term is less effective. The c-axis dispersion in YBCO is proposed to be $\epsilon_{\boldsymbol{k}} \propto t_{\perp}(\cos k_x - \cos k_y)^2$ in the band calculation.[21)] For this c-axis dispersion, $\chi(\boldsymbol{q},\, \omega)$ is equivalent between $\boldsymbol{q} = \boldsymbol{q}_c^{\rm DIC}$ and $\boldsymbol{q}_d^{\rm DIC}$. The present mechanism due to the $t_{\perp}$-term does not work.

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