Coexistence of antiferromagnetism and *d*-wave singlet state controlled by long-range hopping integral

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Interplay between antiferromagnetism (AF) and *d*-wave superconductivity (*d*SC) is investigated in the slave-boson scheme of the two-dimensional *t-J* model on the square lattice. So far, it seems that their coexistence is believed to be a general feature. It is, however, reported in this paper that the coexistence is suppressed significantly by t'', the third neighbor hopping. This effect will lead to noticeable material dependence of the possible bulk coexistence of AF and *d*SC.

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I. INTRODUCTION

II. MODEL AND FORMALISM

We analyze the 2D t-J model on the square lattice,

Interplay between antiferromagnetism (AF) and dwave superconductivity (dSC) is one of the most interesting issues in high- T_c cuprates. In particular, it is a fundamental question whether or not the bulk coexistence of AF and dSC is possible. The theoretical studies on the two-dimensional (2D) t-J model[1–4] and extended Hubbard models,[5–8] which are believed minimal for the description of high- T_c cuprates, predict that it is possible. This prediction independent of models might imply a general possibility of bulk coexistence in high- T_c cuprates. However, such a possibility is reported only in La_{2-x}Sr_xCuO₄ (LSCO) systems,[9] and seems to have strong material dependence.

In this paper, we study the material dependence of the coexistence of AF and dSC in the 2D t-J model, specifically, the dependence on the second (t') and third (t'') neighbor hopping integrals. Focus is put on several values around the realistic ones: t'/t = -1/6 and t''/t = 0 for LSCO systems, and t'/t = -1/6 and t''/t = 1/5 for YBa₂Cu₃O_{6+y} (YBCO) systems.[10–12] We find that without t'', the coexistence is realized in a wide doping region, in accordance with the previous work[3]. However, once t'' is introduced, the coexistence is suppressed significantly. This effect of t'' is shown by investigating two routes into the coexistence, namely, the dSC instability in the (metallic) AF state, and the AF instability in the dSC state. We discuss the generality of the present finding, and implications for actual systems.

$H = -\sum_{i,j,\sigma} t^{(l)} \tilde{c}^{\dagger}_{i\,\sigma} \tilde{c}_{j\,\sigma} + J \sum_{\langle i,j \rangle} \boldsymbol{S}_{i} \cdot \boldsymbol{S}_{j}, \qquad (1)$

defined in the Fock space with no doubly occupied sites. Here $\tilde{c}_{i\sigma}(\mathbf{S}_i)$ is an electron (a spin) operator. The $t^{(l)}$ is the *l*th neighbor hopping integral, and we denote $t^{(1)} = t$, $t^{(2)} = t'$ and $t^{(3)} = t''$. The J(>0) is the superexchange coupling between nearest-neighbor sites. We adopt the slave-boson mean-field scheme by writing $\tilde{c}_{i\sigma}^{\dagger} = f_{i\sigma}^{\dagger}b_i$, where $f_{i\sigma}$ (b_i) is a fermion (boson) operator that carries spin σ (charge e), $S_i = \sum_{\alpha\beta} \frac{1}{2} f_{i\alpha}^{\dagger} \sigma_{\alpha\beta} f_{i\beta}$, with Pauli matrix σ , and introducing the following mean fields: for AF, $m \equiv \frac{1}{2} \langle \sum_{\sigma} \sigma f_{i\sigma}^{\dagger} f_{i\sigma} \rangle e^{i \mathbf{Q} \cdot \mathbf{r}_{i}}$, $\mathbf{Q} = (\pi, \pi)$, and for resonating valence bond (RVB), $\chi^{(l)} \equiv \langle \sum_{\sigma} f_{i\sigma}^{\dagger} f_{j\sigma} \rangle$, $\langle b_{i}^{\dagger} b_{j} \rangle$ and $\Delta_{\tau} \equiv \langle f_{i\uparrow} f_{i+\tau\downarrow} - f_{i\downarrow} f_{i+\tau\uparrow} \rangle$, $\tau = x, y$. These mean fields are taken to be real constants independent of sites *i* and *j*. The *d*-wave symmetry $\Delta_0 \equiv \Delta_x = -\Delta_y \neq 0$ is stable at low T and this state is called the d-wave singlet RVB (dRVB). The dSC state is defined as $\Delta_0 \neq 0$ and $\langle b \rangle \neq 0$. In the following, we assume $\langle b \rangle = \sqrt{\delta}$ where δ is the hole density, and focus on the fermion part; the dSCis then associated directly with the dRVB. This assumption is valid at low T and for δ not close to half filling $(\delta \gtrsim 0.02)$.[3] The mean-field Hamiltonian is given by

$$H_{\rm MF} = \sum_{\boldsymbol{k}} \Psi_{\boldsymbol{k}}^{\dagger} \left(\begin{array}{ccc} \xi_{\boldsymbol{k}} & -\Delta_{\boldsymbol{k}} & -2Jm & 0\\ -\Delta_{\boldsymbol{k}} & -\xi_{\boldsymbol{k}} & 0 & -2Jm\\ -2Jm & 0 & \xi_{\boldsymbol{k}+\boldsymbol{Q}} & -\Delta_{\boldsymbol{k}+\boldsymbol{Q}}\\ 0 & -2Jm & -\Delta_{\boldsymbol{k}+\boldsymbol{Q}} & -\xi_{\boldsymbol{k}+\boldsymbol{Q}} \end{array} \right) \Psi_{\boldsymbol{k}}, (2)$$

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with a global constraint $\sum_{\sigma} \langle f_{i\sigma}^{\dagger} f_{i\sigma} \rangle = 1 - \delta$. The \boldsymbol{k} sum is over the magnetic Brillouin zone $|k_x| + |k_y| \leq \pi$ and

$$\Psi_{\boldsymbol{k}}^{\dagger} = \left(f_{\boldsymbol{k}\uparrow}^{\dagger} \ f_{-\boldsymbol{k}\downarrow} \ f_{\boldsymbol{k}+\boldsymbol{Q}\uparrow}^{\dagger} \ f_{-\boldsymbol{k}+\boldsymbol{Q}\downarrow} \right) , \qquad (3)$$

$$\xi_{\boldsymbol{k}} = -2 \left[\left(t\delta + \frac{3}{8}J\chi^{(1)} \right) \left(\cos k_x + \cos k_y \right) + 2t'\delta \cos k_x \cos k_y + t''\delta \left(\cos 2k_x + \cos 2k_y \right) \right] - \mu , (4)$$

$$\Delta_{\boldsymbol{k}} = -\frac{3}{4}J\Delta_0 \left(\cos k_x - \cos k_y \right) , \qquad (5)$$

with μ being the chemical potential. The mean fields are determined by solving the following self-consistent equations numerically:

$$m = \frac{1}{N} \sum_{\boldsymbol{k}}^{'} \frac{Jm}{D_{\boldsymbol{k}}} \left(\frac{\eta_{\boldsymbol{k}}^{+}}{\lambda_{\boldsymbol{k}}^{+}} \tanh \frac{\lambda_{\boldsymbol{k}}^{+}}{2T} - \frac{\eta_{\boldsymbol{k}}^{-}}{\lambda_{\boldsymbol{k}}^{-}} \tanh \frac{\lambda_{\boldsymbol{k}}^{-}}{2T} \right), \quad (6)$$
$$\chi^{(1)} = -\frac{1}{2N} \sum_{\boldsymbol{k}}^{'} \frac{\xi_{\boldsymbol{k}}^{-}}{D_{\boldsymbol{k}}} (\cos k_{x} + \cos k_{y})$$
$$\times \left(\frac{\eta_{\boldsymbol{k}}^{+}}{\lambda_{\boldsymbol{k}}^{+}} \tanh \frac{\lambda_{\boldsymbol{k}}^{+}}{2T} - \frac{\eta_{\boldsymbol{k}}^{-}}{\lambda_{\boldsymbol{k}}^{-}} \tanh \frac{\lambda_{\boldsymbol{k}}^{-}}{2T} \right), \quad (7)$$

$$\Delta_{0} = -\frac{1}{2N} \sum_{\boldsymbol{k}} (\cos k_{x} - \cos k_{y}) \\ \times \left(\frac{\Delta_{\boldsymbol{k}}}{\lambda_{\boldsymbol{k}}^{+}} \tanh \frac{\lambda_{\boldsymbol{k}}^{+}}{2T} + \frac{\Delta_{\boldsymbol{k}}}{\lambda_{\boldsymbol{k}}^{-}} \tanh \frac{\lambda_{\boldsymbol{k}}^{-}}{2T} \right), \quad (8)$$
$$\delta = \frac{1}{2N} \sum_{\boldsymbol{k}} \left(\frac{\eta_{\boldsymbol{k}}^{+}}{\lambda_{\boldsymbol{k}}^{+}} \tanh \frac{\lambda_{\boldsymbol{k}}^{+}}{2T} + \frac{\eta_{\boldsymbol{k}}^{-}}{\lambda_{\boldsymbol{k}}^{-}} \tanh \frac{\lambda_{\boldsymbol{k}}^{-}}{2T} \right). \quad (9)$$

$$\delta = \frac{1}{N} \sum_{\boldsymbol{k}} \left(\frac{\eta_{\boldsymbol{k}}}{\lambda_{\boldsymbol{k}}^{+}} \tanh \frac{\lambda_{\boldsymbol{k}}}{2T} + \frac{\eta_{\boldsymbol{k}}}{\lambda_{\boldsymbol{k}}^{-}} \tanh \frac{\lambda_{\boldsymbol{k}}}{2T} \right) . \tag{9}$$

Here $\lambda_{\mathbf{k}}^{\pm} = \sqrt{\eta_{\mathbf{k}}^{\pm 2} + \Delta_{\mathbf{k}}^{2}}$ is the quasiparticle energy in the coexistent state, $\eta_{\mathbf{k}}^{\pm} = \xi_{\mathbf{k}}^{\pm} \pm D_{\mathbf{k}}$ is that in the AF state, $D_{\mathbf{k}} = \sqrt{\left(\xi_{\mathbf{k}}^{-}\right)^{2} + (2Jm)^{2}}, \ \xi_{\mathbf{k}}^{\pm} = (\xi_{\mathbf{k}} \pm \xi_{\mathbf{k}+\mathbf{Q}})/2$, and T (N) is temperature (the total number of lattice sites).

III. RESULTS

Figure 1(a) shows the phase diagram on the plane of T versus δ for the band parameter, t/J = 4, t'/t = -1/6, and t''/t = 0, which will be appropriate to LSCO.[13–15] The $T_{\rm N}$ is the onset temperature of AF, whereas $T_{\rm RVB}^{\rm AF}$ ($T_{\rm RVB}$ and $T_{\rm RVB}^{\rm noAF}$) is that of dRVB in the presence (absence) of AF. The (commensurate) AF phase is stabilized in a wide doping region, $\delta \lesssim \delta_{\rm N} = 0.159$, where $\delta_{\rm N}$ is a critical doping rate of AF ordering at T = 0, and suppresses the dRVB instability ($T_{\rm RVB}^{\rm AF} < T_{\rm RVB}^{\rm noAF}$). These features are already seen in the early work.[3] The δ dependence of the order parameters is shown in Fig. 1(b). With decreasing δ , the AF is realized through a second-order transition and it suppresses Δ_0 and $\chi^{(1)}$. Figure 1(c) shows

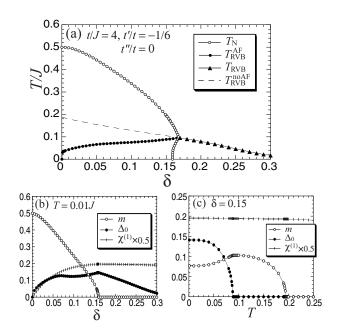


FIG. 1: (a) The phase diagram on the plane of T and δ for t/J = 4, t'/t = -1/6 and t''/t = 0. The $T_{\rm N}$ is the onset temperature of AF, and $T_{\rm RVB}^{\rm AF}$ ($T_{\rm RVB}$ and $T_{\rm RVB}^{\rm noAF}$) is that of dRVB in the presence (absence) of AF. (b) δ dependence and (c) T dependence of the order parameters at T = 0.01J and $\delta = 0.15$, respectively.

the *T* dependence of the order parameters. Both the AF and the *d*RVB are realized through a second-order transition, and the *d*RVB ordering is accompanied by a small suppression of AF. (This suppression is not clear at low δ , because of large *m*.) The change of $\chi^{(1)}$ is negligible below $T_{\rm N}$ and $T_{\rm RVB}^{\rm AF}$, that is, the coherency of fermion's hopping is not disturbed appreciably.

The primary finding of the present study is a significant effect of t''. Figure 2(a) shows the phase diagram with the inclusion of t''/t = 0.2, which will be appropriate to YBCO. The phase diagram is qualitatively different from Fig. 1(a); the dRVB instability in the AF state is strongly suppressed in a range of moderate hole density. The order parameters, especially m and Δ_0 , also behave differently. Figure 2(b) shows that the AF is realized through a first-order-like transition as a function of δ , accompanied by the rapid suppression of dRVB. As a function of T, on the other hand, we see in Fig. 2(c) that while the AF order develops continuously below (higher) $T_{\rm N}$, it suddenly drops once the dRVB sets in through a nearly first-order transition. This is seen in the region close to $\delta_{\rm N}=0.128$. Away from this region, T dependence is similar to Fig. 1(c).

Why does t'' have such significant effects and lead to the sharp contrast between Fig. 1 and Fig. 2? To under-

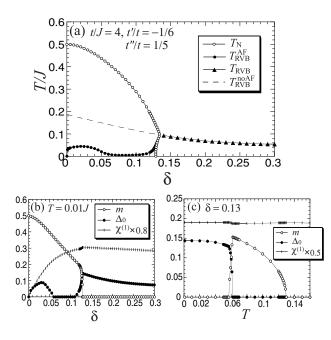


FIG. 2: (a) T- δ phase diagram for t/J = 4, t'/t = -1/6, and t''/t = 1/5. (b) δ dependence and (c) T dependence of the order parameters at T = 0.01J and $\delta = 0.13$, respectively.

stand this, we analyze the onset equation of dRVB,

$$T_{\rm c} = \frac{3}{16N} \sum_{\boldsymbol{k}} (\cos k_x - \cos k_y)^2 \\ \times \left(\frac{2T_{\rm c}}{\eta_{\boldsymbol{k}}^+} \tanh \frac{\eta_{\boldsymbol{k}}^+}{2T_{\rm c}} + \frac{2T_{\rm c}}{\eta_{\boldsymbol{k}}^-} \tanh \frac{\eta_{\boldsymbol{k}}^-}{2T_{\rm c}}\right).$$
(10)

Here $T_{\rm c}$ is $T_{\rm RVB}^{\rm AF}$ for $m \neq 0$ and $T_{\rm RVB}^{\rm noAF}$ for $m \equiv 0$. The bands in the AF state $\eta_{\mathbf{k}}^{\pm}$ are shown in Fig. 3(a) together with those for $m \equiv 0$. Since the $\eta_{\mathbf{k}}^{+}$ is pushed up to high energy and only $\eta_{\mathbf{k}}^{-}$ extends to low energy, the term with $\eta_{\mathbf{k}}^{-}$ is relevant in Eq. (10). For $m \equiv 0$, on the other hand, both terms with $\eta_{\mathbf{k}}^{\pm}$ contribute. Thus, $T_{\rm RVB}^{\rm AF}$ is generally lowered from $T_{\rm RVB}^{\rm noAF}$. The degree of this suppression is controlled mainly by $\eta^{-}(\pi, 0)$ because of the *d*-wave form factor in Eq. (10). To measure $\eta^{-}(\pi, 0)$, we consider the following quantity:

$$W(t',t'') \equiv [\eta^{-}(\pi/2,\pi/2) - \eta^{-}(\pi,0)]/4\delta \quad (11)$$

= $2t'' - t'$. (12)

For the present parameter, t' < 0 and $t'' \ge 0$, W(t', t'')is positive. This means that the Fermi surface (FS) or the hole pocket is formed around $(\pi/2, \pi/2)$ [Fig. 3(b)] independent of the values of t' and t''.[16] Since the area of the hole pocket is determined uniquely by δ , the band parameter dependence of $\eta^{-}(\pi/2, \pi/2)$ is weaker than that of $\eta^{-}(\pi, 0)$ for a fixed δ . Hence, the relative value of $\eta^{-}(\pi, 0)$ among different band parameters will be measured by W(t', t''). That is, the larger value of 3

W(t', t'') means the larger magnitude of $\eta^{-}(\pi, 0)$, which suppresses $T_{\text{RVB}}^{\text{AF}}$ more significantly [see Eq. (10)]. To demonstrate this explicitly, we first take t'' = 0 and plot $T_{\text{RVB}}^{\text{AF}}$ as a function of $\delta/\delta_{\text{N}}(\leq 1)$ for several choices of t' in Fig. 4(a). As expected, $T_{\text{RVB}}^{\text{AF}}$ is suppressed with increasing |t'| or W(t', t''). The degree of the suppression depends on $\delta/\delta_{\rm N}$ and is most enhanced in a moderate doping region. This is because the AF order is not so strong near $\delta/\delta_{\rm N} \approx 1$ [see Fig. 1(b)], on one hand, and the hopping terms renormalization by δ [see Eq. (4)] makes their effects ineffective at low δ , on the other hand. The point is that compared with this t' effect, t'' will have a much more significant effect, since t'' has a prefactor 2 in Eq. (12) and the finite value of t'' will generally imply a finite t', which contributes to W(t', t'') additively. This is demonstrated in Fig. 4(b) by choosing several t''. We see a significant suppression even at small t''/t. (The recovery of $T_{\rm RVB}^{\rm AF}$ in $\bar{\delta}/\delta_{\rm N} \lesssim 0.4$ comes from the reduction of t' and t'' effects at low δ [see Eq. (4)].) It is to be noted that the present effect is a special feature of the band parameter, t' < 0 and $t'' \ge 0$, where W(t', t'') is most enhanced.[16]

We have seen that t'' is a crucial factor of the *d*RVB instability in the AF state. We next turn to the other side of the phase boundary, the AF instability in the *d*RVB state. This instability is determined by the condition $\chi^{-1}(\mathbf{q}) = \chi_0^{-1}(\mathbf{q}) + 2J(\cos q_x + \cos q_y) = 0$, where

$$\chi_{0}(\boldsymbol{q}) = \frac{1}{4N} \sum_{\boldsymbol{k}} \left[C_{\boldsymbol{k},\boldsymbol{k}+\boldsymbol{q}}^{+} \frac{\tanh \frac{E_{\boldsymbol{k}}}{2T} - \tanh \frac{E_{\boldsymbol{k}+\boldsymbol{q}}}{2T}}{E_{\boldsymbol{k}} - E_{\boldsymbol{k}+\boldsymbol{q}}} + C_{\boldsymbol{k},\boldsymbol{k}+\boldsymbol{q}}^{-} \frac{\tanh \frac{E_{\boldsymbol{k}}}{2T} + \tanh \frac{E_{\boldsymbol{k}+\boldsymbol{q}}}{2T}}{E_{\boldsymbol{k}} + E_{\boldsymbol{k}+\boldsymbol{q}}} \right], (13)$$
$$C_{\boldsymbol{k},\boldsymbol{k}+\boldsymbol{q}}^{\pm} = \frac{1}{2} \left(1 \pm \frac{\xi_{\boldsymbol{k}}\xi_{\boldsymbol{k}+\boldsymbol{q}} + \Delta_{\boldsymbol{k}}\Delta_{\boldsymbol{k}+\boldsymbol{q}}}{E_{\boldsymbol{k}}E_{\boldsymbol{k}+\boldsymbol{q}}} \right), \quad (14)$$

and $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}$. With mean fields determined under the constraint $m \equiv 0$, we calculate $\chi_0(\mathbf{q})$ around (π, π) for several choices of t' and t''. To see the degree of suppression, we have scaled $\chi_0(\mathbf{q})$ in Figs. 5(a) and 5(b) so that the peak height for t' = 0 and for t'' = 0is unity, respectively. While $\chi_0(\mathbf{q})$ is suppressed with increasing |t'| [Fig. 5(a)], we see much more significant suppression with t'' [Fig. 5(b)]. This means that t'' is crucial to suppress the AF instability in the dSC state. [We have checked that this qualitative feature does not depend on T and $\delta(> 0)$.]

Here we note effects of the underlying "FS" in the dRVB, which may be defined as $E_{\mathbf{k}} = 0$ with $\Delta_{\mathbf{k}} \equiv 0$. For $|t'/t| \lesssim 0.2$ at t''/t = 0, the "FS" is electronlike centered at the Γ point. The two clear incommensurate (IC) peaks of $\chi_0(\mathbf{q})$ in Fig. 5(a) come from the nesting of the "FS." For larger |t'/t| or with $t''/t(\gtrsim 0.1)$, the electronlike "FS" changes to a holelike "FS" centered at (π, π) , and loses the nesting property. Figure 5(b) shows that with

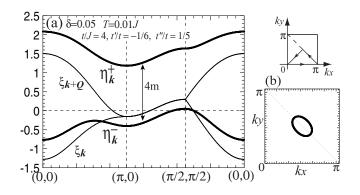


FIG. 3: (a) Energy band in the AF state (thick lines) and in the paramagnetic state with $m \equiv 0$ (thin lines); the energy unit is J. The scanned path is shown in the upper right figure. (b) The Fermi surface in the AF state (thick line).

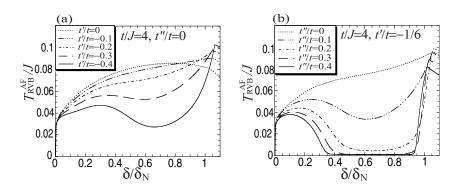


FIG. 4: The doping dependence of $T_{\text{RVB}}^{\text{AF}}$ for several choices of t' (a) and t'' (b). The δ is scaled by δ_{N} ; $\delta_{\text{N}} = 0.151, 0.155, 0.161, 0.161, \text{ and } 0.147 \ (0.159, 0.156, 0.128, 0.109, \text{ and } 0.095)$ for $t'/t = 0, -0.1, -0.2, -0.3, \text{ and } -0.4 \ (t''/t = 0, 0.1, 0.2, 0.3, \text{ and } 0.4)$ in (a)[(b)], respectively.

this "FS" being kept, $\chi_0(q)$ is suppressed significantly by t''. That is, the topology of the "FS" is not relevant to the present finding.

IV. DISCUSSION AND CONCLUSION

We have shown that both the dRVB instability in the AF state (Figs. 1, 2, and 4) and the AF instability in the dRVB state (Fig. 5) are significantly suppressed by t''. Although this effect is found in the slave-boson mean-field scheme with the commensurate AF order, our finding will be rather general in the following senses.

(i) In the analysis of Eq. (11), the *d*RVB instability in the AF state is governed by the quasiparticle energy at $\mathbf{k} = (\pi, 0)$.

(ii) For the AF instability in the *d*RVB state, the suppression of $\chi_0(\boldsymbol{q})$ by t'' (Fig. 5) will be reflected in the full $\chi(\boldsymbol{q})$ beyond the random phase approximation.

(iii) For the band parameter used in Fig. 1, the IC AF order will be more favorable at finite δ and low T. [Note that $\chi_0(\mathbf{q})$ shows the IC peaks in Fig. 5(b) for t'' = 0.] However, essential features may be captured by Fig. 1, since the calculation in the IC AF state[17] shows that the (segments of) FS is located near $(\pi, 0)$ and $(0, \pi)$, which

will not severely block the scattering processes leading to the dRVB instability.

(iv) It is pointed out theoretically [7, 8, 18] that the coexistence of AF and dSC generates the π -triplet order, which should therefore be considered on an equal footing with AF and dSC. Our preliminary calculations, however, show that its effects are not strong enough to modify the present conclusions.

Now we discuss implications for experiments, assuming t'/t = -1/6 and t''/t = 0 for LSCO, and t'/t = -1/6 and t''/t = 1/5 for YBCO.[10–12] Compared with the actual phase diagrams, the AF order is overstabilized in Figs. 1(a) and 2(a). The obtained value of δ_N , therefore, may be regarded as a rough measure of hole density below which there is a possibility that the AF order is stabilized and coexists with dSC especially for LSCO. In this sense, the "1/8 anomalies" are interesting.

The 1/8 anomalies are various anomalies observed around hole density 1/8 in the typical high- T_c cuprates.[19–23] One of anomalies is the possible bulk coexistence of AF and dSC. This possibility, however, is reported only in LSCO[9], not in YBCO and Bi2212. In fact, μ SR data show no precession of the muon spin in YBCO[21] and Bi2212[22] even if Zn impurity is introduced. This material dependence will be understood

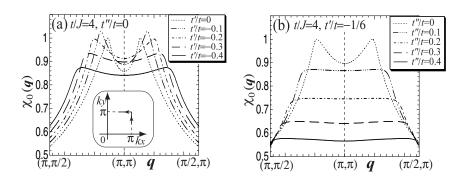


FIG. 5: $\chi_0(q)$ in the *d*RVB state for several choices of t' (a) and t'' (b) at $\delta = 0.15$ and T = 0.01J. The scanned path is shown in the inset of (a). $\chi_0(q)$ is scaled so that the peak height for t' = 0 (a) and t'' = 0 (b) is unity.

by the present effect of t'', since a moderate value of $t''/t(\sim 0.2 - 0.3)$ is expected in both YBCO and Bi2212, and not in LSCO.[10–12]

The search for actual systems, which show a similar phase diagram to Fig. 2(a), is challenging. Such cadidates may include Hg- and Tl-based cuprates.

In conclusion, we have studied the possible bulk coexistence of AF and dSC in the slave-boson scheme of the 2D t-J model. We have found that t'' has a significant effect on the suppression of the coexistence. This effect will be rather general and appear as noticeable material depen-

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Acknowledgments

dence of the possible bulk coexistence of AF and dSC.

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the quasi-1D band proposed by us for LSCO.[12, 14, 15].

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