Shift of incommensurate antiferromagnetic peaks in $La_{2-x}Sr_xCuO_4$

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(Dated: 20 November, 2002)

Abstract

Neutron scattering experiments on $La_{2-x}Sr_xCuO_4$ (LSCO) have revealed that the incommensurate antiferromagnetic peaks do not lie exactly on the symmetry axes ($q_x = \pm\pi$ or $q_y = \pm\pi$), but are slightly shifted from them. In this paper, a scenario for such a "shift" is presented in terms of the anisotropy of t' (diagonal hopping integral on the square lattice) in the slave-boson scheme of the two-dimensional t-J model. The predictions of the present theory based on fermiology are found to be different from those based on the "spin-charge stripes" hypothesis. This difference will serve to clarify a factor responsible for incommensurate antiferromagnetic correlations in LSCO systems.

PACS numbers: 71.10.Fd, 74.25.Ha, 74.72.Dn

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I. INTRODUCTION

It is well known that $La_{2-x}Sr_xCuO_4$ (LSCO) shows incommensurate (IC) antiferromagnetic correlations, which are observed as four peaks around (π, π) in the neutron scattering experiments[1]. As an origin of such IC correlations, mainly two scenarios have been proposed: (i) "charge stripes" formation or their fluctuations[2], and (ii) fermiology of the quasi-one-dimensional (q-1D) Fermi surface (FS)[3–5]. Although two scenarios provide different concepts for the understanding of LSCO systems, the discrimination between them has not been successful experimentally.

Recently, elastic neutron scattering experiments have revealed the "shift" of IC peaks[6, 7]: the IC peaks do not lie exactly on the symmetry axes, $q_x = \pm\pi$ or $q_y = \pm\pi$, but are slightly shifted from them. The magnitude of the shift is much larger than that expected from the orthorhombic lattice distortion, which indicates that the shift is an intrinsic property of IC peaks[7]. From the "spin-charge stripes" viewpoint, this shift has been argued in terms of the possible realization of the slanted charge stripes[8]. From the fermiology viewpoint, on the other hand, it has been proposed that the anisotropy of t' [the next nearest-neighbor (n.n.) hopping integral on the square lattice], which is expected in the low-temperature orthorhombic (LTO) structure, can be a key factor of the shift[3]. In this scenario, it was predicted that the shift is absent in the low-temperature tetragonal (LTT) structure. Quite recently, this prediction has been confirmed in $La_{1.875}Ba_{0.125-x}Sr_xCuO_4$[9].

In this paper, motivated by such an experimental support, we investigate in detail the shift of IC peaks from the fermiology viewpoint. We calculate the dynamical magnetic susceptibility $\chi(\boldsymbol{q}, \omega)$ numerically in the slave-boson scheme of the two-dimensional (2D) t-J model; the charge density is assumed to be uniform. It is shown that the anisotropy of t' leads to the shift of IC peaks without changing the overall structure of $\mathrm{Im}\chi(\boldsymbol{q}, \omega)$. Although it comes from the slight modification of the FS, the shift is robust against the temperature T, energy ω, and variation of band parameters as long as the IC peaks remain to be well defined. We argue that the observed shift[6, 7, 9] can be understood in the present theory based on fermiology. The predictions of the present theory are different from those based on the spin-charge stripes hypothesis[8]. In the future studies, this difference will serve to clarify a factor responsible for the IC correlations in LSCO systems. In the Appendix, we give an analytic expression of the shift of IC peaks. Part of this work has been published as

conference proceedings[10].

II. MODEL AND FORMALISM

As a model of high-$T_{\rm c}$ cuprates, we take the 2D t-J model on the square lattice:

$$H = -\sum_{i,j,\sigma} t_{ij}\tilde{c}^{\dagger}_{i\sigma}\tilde{c}_{j\sigma} + \sum_{\langle i,j\rangle} J_{ij}\boldsymbol{S}_i\cdot\boldsymbol{S}_j, \tag{1}$$

defined in the Fock space with no doubly occupied sites. Here $\tilde{c}_{i\sigma}$ is an electron operator, and $\boldsymbol{S}_i$ is a spin operator. While the superexchange coupling, $J_{ij} = J_\tau (> 0)$, is assumed only between n.n. spins, the hopping integrals, t_{ij}, are assumed between n.n. sites (t_τ) and next n.n. (t'_τ) sites, where $\boldsymbol{\tau} = \boldsymbol{r}_j - \boldsymbol{r}_i$ denotes the direction. We adopt the slave-boson formalism and introduce the slave particle as $\tilde{c}^{\dagger}_{i\sigma} = f^{\dagger}_{i\sigma}b_i$, where $f_{i\sigma}$ (b_i) is a fermion (boson) operator that carries spin σ (charge e). The spin operator is given by $\boldsymbol{S}_i = \sum_{\alpha\beta}\frac{1}{2}f^{\dagger}_{i\alpha}\boldsymbol{\sigma}_{\alpha\beta}f_{i\beta}$, with Pauli matrix $\boldsymbol{\sigma}$, and the local constraint is described by $\sum_\sigma f^{\dagger}_{i\sigma}f_{i\sigma} + b^{\dagger}_i b_i = 1$ at every site i.

Introducing the mean fields, $\chi_\tau \equiv \langle\sum_\sigma f^{\dagger}_{i\sigma}f_{i+\tau\,\sigma}\rangle$, $\langle b^{\dagger}_i b_{i+\tau}\rangle$ and $\Delta_\tau \equiv \langle f_{i\uparrow}f_{i+\tau\downarrow} - f_{i\downarrow}f_{i+\tau\uparrow}\rangle$, and loosing the local constraint to the global one, we obtain the mean-field Hamiltonian. The mean fields are taken to be real constants independent of lattice coordinate i, but with a possible $\boldsymbol{\tau}$ dependence. Assuming the boson to be condensed at the bottom of its band, we investigate the fermion part described by

$$H_{\rm MF} = \sum_{\boldsymbol{k},\sigma}\xi_{\boldsymbol{k}}f^{\dagger}_{\boldsymbol{k}\,\sigma}f_{\boldsymbol{k}\,\sigma} + \sum_{\boldsymbol{k}}\Delta_{\boldsymbol{k}}\left(f^{\dagger}_{-\boldsymbol{k}\downarrow}f^{\dagger}_{\boldsymbol{k}\uparrow} + f_{\boldsymbol{k}\uparrow}f_{-\boldsymbol{k}\downarrow}\right), \tag{2}$$

where

$$\begin{aligned}\xi_{\boldsymbol{k}} \;=\; & -2\left[\left(t_x\delta + \frac{3}{8}J_x\chi_x\right)\cos k_x + \left(t_y\delta + \frac{3}{8}J_y\chi_y\right)\cos k_y\right. \\ & \left. + t'_{\parallel}\delta\cos(k_x+k_y) + t'_{\perp}\delta\cos(k_x-k_y)\right] - \mu\,,\end{aligned} \tag{3}$$

and $\Delta_{\boldsymbol{k}} = -\frac{3}{4}(J_x\Delta_x\cos k_x + J_y\Delta_y\cos k_y)$. Here δ (μ) is the hole density (chemical potential), and the subscripts $\parallel$ and $\perp$ indicate that $\boldsymbol{\tau}$ is parallel to [110] and [1$\bar{1}$0] (tetragonal notation), respectively.

As shown in Ref. [11], the 2D t-J model has an intrinsic instability to form q-1D FS (breaking the original fourfold symmetry spontaneously) when van Hove points are located near the FS. The same instability was found also by Halboth and Metzner in the Hubbard

model[12], and, following them, we call this instability the Pomeranchuk instability[13]. Although the Pomeranchuk instability is usually masked by the more prominent d-wave pairing instability, we have shown that the presence of small extrinsic anisotropy is sufficient for the q-1D state to manifest in the d-wave state. We have then made a proposal that this symmetry-broken state with q-1D FS is realized in the LSCO systems, which has been reinforced by the subsequent studies on magnetic excitation[4, 5]. To our knowledge, this is the first indication of the Pomeranchuk instability in actual materials.

Since the shift of IC peaks has been observed in LSCO systems, we analyze the shift mainly for the q-1D FS. To reproduce the q-1D FS that is consistent with the data of angle-resolved photoemission spectroscopy in the self-consistent calculation, we introduce the spatial anisotropy as $t_x = t$, $t_y = t(1-\alpha)$, $J_x = J$ and $J_y = J(1-2\alpha)$[11]. The parameter α is determined to fit the FS near $(0, \pi)$ to the observed FS segments[14, 15] as $\alpha = 0.065,\ 0.084,\ 0.065,\ 0.042$ and 0 for $\delta = 0.05,\ 0.10,\ 0.15,\ 0.22$ and 0.30, respectively. We also include the possible coupling to the LTO lattice distortion in LSCO where CuO_6 octahedra tilt around the [110] axis, and introduce the anisotropy as

$$t'_{\parallel} = t', \tag{4}$$

$$t'_{\perp} = \gamma t' \ (\gamma \leq 1). \tag{5}$$

Setting $t/J = 4$ and $t'/t = -1/6$, we determine the mean fields self-consistently for each value of α and γ[16]. At low T, the d-wave singlet pairing [d-wave resonating-valence-bond (d-RVB)] state is stabilized. To obtain the FS, we also determine the mean fields in the so-called uniform RVB (u-RVB) state, where $\Delta_\tau \equiv 0$ is imposed. The FS at $\delta = 0.15$ is shown in Fig. 1. It is seen that the change of the FS due to the anisotropy of t' ($\gamma < 1$) is quite small, but this change leads to the appreciable shift of IC peaks as seen below.

The irreducible dynamical magnetic susceptibility $\chi_0(\boldsymbol{q}, \omega)$ is calculated as

$$\chi_0(\boldsymbol{q}, \omega) = \frac{1}{4N}\sum_{\boldsymbol{k}}\left[C^{+}_{\boldsymbol{k},\boldsymbol{k}+\boldsymbol{q}}\left(\tanh\frac{E_{\boldsymbol{k}}}{2T} - \tanh\frac{E_{\boldsymbol{k}+\boldsymbol{q}}}{2T}\right)\frac{1}{E_{\boldsymbol{k}} - E_{\boldsymbol{k}+\boldsymbol{q}} + \omega + \mathrm{i}\Gamma}\right.$$
$$\left. + \frac{1}{2}C^{-}_{\boldsymbol{k},\boldsymbol{k}+\boldsymbol{q}}\left(\tanh\frac{E_{\boldsymbol{k}}}{2T} + \tanh\frac{E_{\boldsymbol{k}+\boldsymbol{q}}}{2T}\right)\left(\frac{1}{E_{\boldsymbol{k}} + E_{\boldsymbol{k}+\boldsymbol{q}} + \omega + \mathrm{i}\Gamma} + \frac{1}{E_{\boldsymbol{k}} + E_{\boldsymbol{k}+\boldsymbol{q}} - \omega - \mathrm{i}\Gamma}\right)\right], \tag{6}$$

where $E_{\boldsymbol{k}} = \sqrt{\xi_{\boldsymbol{k}}^2 + \Delta_{\boldsymbol{k}}^2}$, and

$$C^{\pm}_{\boldsymbol{k},\boldsymbol{k}+\boldsymbol{q}} = \frac{1}{2}\left(1 \pm \frac{\xi_{\boldsymbol{k}}\xi_{\boldsymbol{k}+\boldsymbol{q}} + \Delta_{\boldsymbol{k}}\Delta_{\boldsymbol{k}+\boldsymbol{q}}}{E_{\boldsymbol{k}}E_{\boldsymbol{k}+\boldsymbol{q}}}\right) . \tag{7}$$

The value of Γ is a positive infinitesimal, and we adopt $\Gamma = 0.01J$ in the numerical calculation.

The dynamical magnetic susceptibility $\chi(\boldsymbol{q}, \omega)$ is calculated as

$$\chi(\boldsymbol{q}, \omega) = \frac{\chi_0(\boldsymbol{q}, \omega)}{1 + rJ(\boldsymbol{q})\chi_0(\boldsymbol{q}, \omega)} . \tag{8}$$

Here $J(\boldsymbol{q}) = 2J(\cos q_x + \cos q_y)$ and we have introduced a numerical factor r for convenience. In the usual random phase approximation (RPA), we have $r = 1$, which leads to the magnetic instability in a wide doping region. This instability, however, will be an artifact of the present approximation and be suppressed by higher order corrections to the RPA. We include this aspect phenomenologically by taking $r = 0.35$, which limits magnetic instability to $\delta \lesssim 0.02$ in accordance with the phase diagram of LSCO. The choice of r may be arbitrary, but it does not modify the present conclusion including the magnitude of the shift.

III. RESULTS

We first calculate $\mathrm{Im}\chi(\boldsymbol{q}, \omega)$ at low ω $(= 0.01J)$ and low T $(= 0.01J)$ in the d-RVB state. Figures 2(a) and (b) show $\mathrm{Im}\chi(\boldsymbol{q}, \omega)$ around the IC peak for $\gamma = 1$ and 0.8, respectively; the contour lines are drawn on the $\boldsymbol{q}$ plane to show the peak position clearly. For $\gamma = 1$, the IC peak is located on the symmetry axis $q_x = \pi$, namely at $\boldsymbol{q} = (\pi, \pi \mp 2\pi\eta)$. As the anisotropy, measured by $1 - \gamma$, is introduced, the peak shifts away from the symmetry axis to $\boldsymbol{q} = (\pi \pm 2\pi\Delta\eta, \pi \mp 2\pi\eta)$ without changing the overall structure of $\mathrm{Im}\chi(\boldsymbol{q}, \omega)$[17]. (The value of η changes slightly.) This shift is due to the slight modification of the FS (Fig. 1), which changes the scattering wave vector that contributes to the IC peak. In the u-RVB state, similar results are obtained, as shown in Figs. 2(c) and (d). The d-wave gap is not essential to the shift of IC peaks.

The γ dependence of $\Delta\eta$ is shown in Fig. 3(a). It is seen that the magnitude of the shift is proportional to the anisotropy of t', namely, $\Delta\eta \propto 1 - \gamma$, in the range we have studied. The suppression of $\Delta\eta$ in the u-RVB is due to the additional scatterings between the FSs near

$(\pi, 0)$ and $(0, \pi)$, which are absent in the d-RVB state where the low-energy scatterings are limited to the region near the Fermi points — d-wave gap nodes on the FS. In the same figure, we also plot $\theta_{\rm Y} = \tan^{-1}(\Delta\eta/\eta)$, a quantity often discussed experimentally. In Fig. 3(b), the δ dependence of $\Delta\eta$ is shown for $\gamma = 0.9$. It is found that the value of $\Delta\eta$ does not change appreciably with δ in the d-RVB state[18]. In the u-RVB state, on the other hand, $\Delta\eta$ decreases at low δ. This is because additional scattering processes, which reduce the shift [Fig. 3(a)], increase at low δ.

Since the shift we have studied comes from the slight modification of the FS (Fig. 1), it is not obvious whether the shift remains appreciable at higher ω and T. We have checked this quantitative aspect up to $\omega = 0.3J$ and $T = 0.1J$. We have found that as long as the IC peak is well defined as a local maximum, the shift survives and its magnitude is comparable to that shown in Fig. 3.

The IC peak also exists at $(\pi \mp 2\pi\eta', \pi)$, which is not equivalent to $(\pi, \pi \mp 2\pi\eta)$ for the present q-1D FS. This IC peak shifts to $(\pi \mp 2\pi\eta', \pi \pm 2\pi\Delta\eta')$ by introducing $1 - \gamma$. (See the lower inset in Fig. 2.) From the calculations in the d-RVB state for $\omega = 0.01J$, we have observed that this value of $\Delta\eta'$ is larger than $\Delta\eta$ by 20-30 % at each δ ($\lesssim$0.20).

We next investigate the shift for different band parameters to show that the shift is a generic feature of the IC peaks in the presence of anisotropy of t' (also see the Appendix): (i) $t/J = 4$, $t'/t = -1/6$ with α fixed to be zero, namely the case of the 2D FS shown in Fig. 4, which was used in the previous studies in LSCO[19, 20], and (ii) $t/J = 4$, $t'/t = -1/6$, $t''/t = 1/5$ with $\alpha \equiv 0$ (t'' being the third neighbor-hopping integral), the case appropriate to YBCO systems[4, 19–21]. For both cases, the shift of IC peaks is seen, although in case (ii) at low ω, the IC peak is well defined as a local maximum only for high δ ($\gtrsim$0.20). The results for case (i) at $\omega = T = 0.01J$ are summarized in Fig. 5. In the d-RVB state, the result is semiquantitatively the same with that in Fig. 3, because only small regions around the Fermi points are effective to the low-energy scattering processes contributing to the IC peaks, and the global shape of FS is not important. In the u-RVB state, the suppression of $\Delta\eta$ is severer than that for q-1D FS. This is due to the difference in weight of additional scattering between the FS near $(\pi, 0)$ and $(0, \pi)$.

IV. DISCUSSION

Having seen our theoretical results on the shift of IC peaks due to the anisotropy of t', we now argue the possibility of the present mechanism to be realized in LSCO systems. The existence of such long-range hopping integral will be reasonable in the actual systems[22–24]. Since the anisotropy of t' is expected from the coupling to the LTO lattice distortion, the shift is expected in the LTO or the *Pccn* structure, and the magnitude of the shift increases with the orthorhombic distortion [Fig. 3(a)]. This is consistent with experiment[9]. The direction of the shift (Fig. 2) is also consistent with experiments[6, 7, 9]. Since such direction is determined uniquely by the tilting axis of the CuO_6 octahedra [Eqs. (4) and (5)], the direction of the shift does not change even for the case that the q-1D band is stacked alternately along the c-axis as proposed in LSCO systems[3, 4]. The shift has been observed around $\delta \approx 0.12$ in the superconducting state and reported as $\Delta\eta \approx 0.002 - 0.006$ (or $\theta_{\rm Y} \approx 1^\circ - 3^\circ$) [7, 9]. Considering the possible realization of q-1D FS in LSCO[3, 4], and taking the results in Fig. 3(a) in the d-RVB[25], we can understand the observed value of $\Delta\eta$ if we assume $1 - \gamma \approx$ 5-15 %. To discuss whether this value of γ is reasonable or not, a microscopic estimation of γ is necessary. A reliable calculation for such estimate, however, is not easy and a quantitative discussion will be beyond the present work. We here try a rough estimation of γ.

The t-J model is an effective Hamiltonian derived from the more microscopic d-p model, which consists of Cu-d and O-p_σ orbitals in the CuO_2 plane. The transfer integrals of the t-J model are estimated as those of the Zhang-Rice singlet formed between the doped p hole and the Cu spin[26]. In the d-p model, the effect of the LTO structure is reflected in the anisotropy of the transfer integral, t_{pp}, between n.n. p orbitals. Microscopically, this comes from two factors, (i) the uniform (alternate) buckling of oxygens along [110] ($[1\bar{1}0]$) due to the tilting of the CuO_6 octahedra around the [110] axis by $\theta_{\rm tilt}$, and (ii) the change of lattice constants $a\,(\,/\!/\,[110]) < b\,(\,/\!/\,[1\bar{1}0])$. To estimate the anisotropy of t_{pp}, we assume a dependence $t_{pp} \propto R^{-\zeta}$ on the distance R between the oxygen sites. In this approximation, we obtain $1 - t_{pp\perp}/t_{pp\parallel} \approx [\zeta + 2)/2] \tan^2\theta_{\rm tilt} + (\zeta - 1.12)(1 - a/b)$ where $t_{pp\parallel}$ ($t_{pp\perp}$) is along [110] ($[1\bar{1}0]$)[27]. We then estimate the anisotropy of t' of the t-J model, following the procedure by Matsukawa and Fukuyama[22]. We have found that the anisotropy of t' depends strongly on the extent of the Zhang-Rice singlet wave function, and have obtained

$1 - t'_\perp/t'_\parallel \gtrsim 1.5(1 - t_{pp\perp}/t_{pp\parallel})$[28]; the factor 1.5 corresponds to the limiting case where the Zhang-Rice singlet is localized at one Cu and its neighboring four O sites. Taking $\theta_{\rm tilt} \approx 2^\circ - 4^\circ$, $a/b \approx 0.99 - 0.995$[29] and $\zeta = 2$[30], we have $1 - \gamma = 1 - t'_\perp/t'_\parallel \gtrsim$ 1-3 %. This value will be encouraging, considering the present level of calculation.

As another scenario, Bosch *et al.*[8] have proposed that the shift of IC peaks comes from the formation of kinks of charge stripes, assuming the lattice commensurability of charge stripes. This scenario provides different predictions from those in the present theory. (i) The shift is expected only in the hole density $\delta \gtrsim 1/8$, and the value of $\Delta\eta$ is proportional to the excess hole density from 1/8, namely $\Delta\eta \propto \delta - 1/8$. In the present theory, on the other hand, $\Delta\eta \propto 1 - \gamma$, and the value of $\Delta\eta$ does not depend on δ appreciably for a fixed γ in the d-RVB state whereas $\Delta\eta$ decreases at low δ in the u-RVB but the noticeable shift remains in $\delta \lesssim 1/8$. (ii) The $\Delta\eta$ can be an order of magnitude larger than in the preset theory. These differences will serve to clarify a factor responsible for the IC peaks in LSCO systems in the future studies.

The "spin-charge stripes" scenario may allow other interpretations for the shift of IC peaks because of its not well-specified nature. In fact, Fujita *et al.*[9] argued that the shift might come from the coupling of charge stripes to the LTO lattice distortion. However, no microscopic analysis have been done so far. Further discussions will be left in the future.

V. SUMMARY

Motivated by the recent neutron scattering experiment, which confirmed our prediction that the shift of IC peaks is absent in the LTT structure, we have investigated in detail the effects of anisotropy of t' on the IC peaks in the slave-boson theory of the t-J model. We have shown that the anisotropy of t' leads to the shift of IC peaks without changing the overall structure of $\mathrm{Im}\chi(\boldsymbol{q}, \omega)$. The magnitude of the shift is proportional to the anisotropy of t', namely, $\Delta\eta \propto 1 - \gamma$. The value of $\Delta\eta$ does not depend appreciably on the hole density in the d-RVB state for fixed γ whereas it decreases at low hole density in the u-RVB state. Although the shift comes from the slight modification of the FS, it is a robust property of the IC peaks in the presence of the anisotropy of t'. We have argued that the observed shift can be understood in the present theory based on fermiology where the charge density is assumed to be uniform. The predictions of the present theory are different from those based

on the spin-charge stripes hypothesis. We hope that this difference will serve to clarify the factor responsible for the IC antiferromagnetic correlations in LSCO systems in the future.

Acknowledgments

We thank M. Fujita and H. Matsukawa for helpful discussions. This work was supported by a Special Postdoctoral Researchers Program from RIKEN and a Grant-in-Aid for COE Research (10CE2004) of Monkasho, Japan

Appendix: Analytic Estimate of the "shift"

We present an analytic formula of the shift of IC peaks at low ω and low T. This formula is valid in the d-RVB state at moderate hole density.

The IC peak is located at $\boldsymbol{q}^{\rm I} = (\pi,\, \pi - 2\pi\eta)$ for $\gamma = 1$, namely, on the symmetry axis, $q_x = \pi$. This means that another equivalent scattering wave vector, $\boldsymbol{q}^{\rm II} = \boldsymbol{q}^{\rm I} - (2\pi,\, 0)$, also contributes to the IC peak (umklapp process). In the d-RVB state, such wave vectors are given approximately by the $2\boldsymbol{k}_{\rm F}$ scattering wave vector, $\boldsymbol{q}^{\rm I} = 2\boldsymbol{k}_{\rm F}^{\rm I}$ and $\boldsymbol{q}^{\rm II} = 2\boldsymbol{k}_{\rm F}^{\rm II}$, that is,

$$\xi_{\frac{1}{2}\boldsymbol{q}^{\rm I}} = \xi_{\frac{1}{2}\boldsymbol{q}^{\rm II}} = 0\,, \tag{A.1}$$

because these wave vectors correspond to the scattering between the regions near the Fermi points for the realistic parameters. We extend this analysis to the case of $\gamma \neq 1$ by setting $\boldsymbol{q}^{\rm I} = (\pi + 2\pi\Delta\eta,\, \pi - 2\pi\eta)$. From Eq. (A.1) we obtain

$$\eta = \frac{1}{\pi}\sin^{-1}(\mu/F_y)\,, \tag{A.2a}$$

$$\Delta\eta = \frac{1}{\pi}\tan^{-1}\left[-\frac{(1-\gamma)F'\cos\pi\eta}{F_x + (1+\gamma)F'\sin\pi\eta}\right]\,, \tag{A.2b}$$

where $F_\tau = -2(t_\tau\delta + \frac{3}{8}J_\tau\chi_\tau)$ with $\tau = x$, y, and $F' = -2t'\delta$. We see $\Delta\eta = 0$ for $\gamma = 1$ as expected. We argue the validity of this estimation through the comparison with the direct numerical calculation of ${\rm Im}\chi(\boldsymbol{q},\, \omega)$ for both q-1D and 2D FSs.

The values of η from Eq. (A.2a) (open symbols) are plotted in Fig. 6 as a function of δ, compared with those from numerical calculation of ${\rm Im}\chi(\boldsymbol{q},\, \omega)$ (solid symbols). We see that η is reproduced quite well at high δ, but the numerical errors get larger at low δ. This is because (i) effects of the d-wave gap, the amplitude of which becomes larger at low δ, is not

included sufficiently in the present estimation, and (ii) the RPA enhancement factor is not considered, which becomes prominent near the magnetic instability point. A more precise analytic expression is given in ref. [4] as Eq. (B·2), but such analysis can not be applied to the present case of $\gamma \neq 1$.

In Fig. 7, we compare the $\Delta\eta$ from Eq. (A.2b) (open symbols) with those from the numerical calculation of $\mathrm{Im}\chi(\boldsymbol{q}, \omega)$ (solid symbols) for several choices of δ and γ. The error in the analytic formula of $\Delta\eta$ at low δ is due to the same reasons as η. At moderate hole density, we see a good agreement. At $\delta \approx 0.30$, however, the numerical error becomes large in contrast to Fig. 6. This is probably due to the smallness of the d-wave gap, and the contribution from other scattering wave vector is not negligible on the scale of $\Delta\eta$.

We have seen that Eq. (A.2) is valid for moderate hole density. This equation describes the essential features of the shift of IC peaks. First, it clearly shows the relation, $\Delta\eta \propto 1-\gamma$, and the higher-order corrections come from the γ dependence of χ_τ and μ. Second, it shows that the δ dependence of $\Delta\eta$ is small, as seen from the saturation behavior of $\Delta\eta$ in Fig. 7. This saturation comes from the δ dependences, $F_\tau \propto \delta$ at high δ and $F' \propto \delta$, which cancel in Eq. (A.2b).

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[25] It seems reasonable to take the d-RVB state for discussing magnetic excitation spectrum in the superconducting state. But we can not deny possibility that the u-RVB state may be better for such a discussion, because calculations in the d-RVB predict the magnetic gap at the IC peak, which is, however, not observed around $\delta \approx 0.12$ experimentally. (See the discussion in Ref. [4].) Although this problem is not relevant to the present discussion on the quantitative aspect of $\Delta\eta$ around $\delta \approx 0.12$, it should be resolved in the future since the δ dependence of $\Delta\eta$ depends on which state is taken [Figs. 3(b) and 5(b)].

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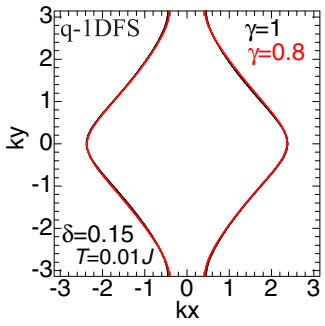

FIG. 1: (Color) The q-1D FS determined self-consistently for $\gamma = 0.8$ (red line) and $\gamma = 1$ (solid line) at $\delta = 0.15$. The band parameters are chosen as $t/J = 4$ and $t'/t = -1/6$ with $\alpha = 0.065$, and $\Delta_\tau \equiv 0$ is imposed. For $\gamma < 1$, the FS near $(\pi/2, \pi/2)$ and that near $(-\pi/2, \pi/2)$ move in opposite ways; the difference in magnitude is due to the shift of μ.

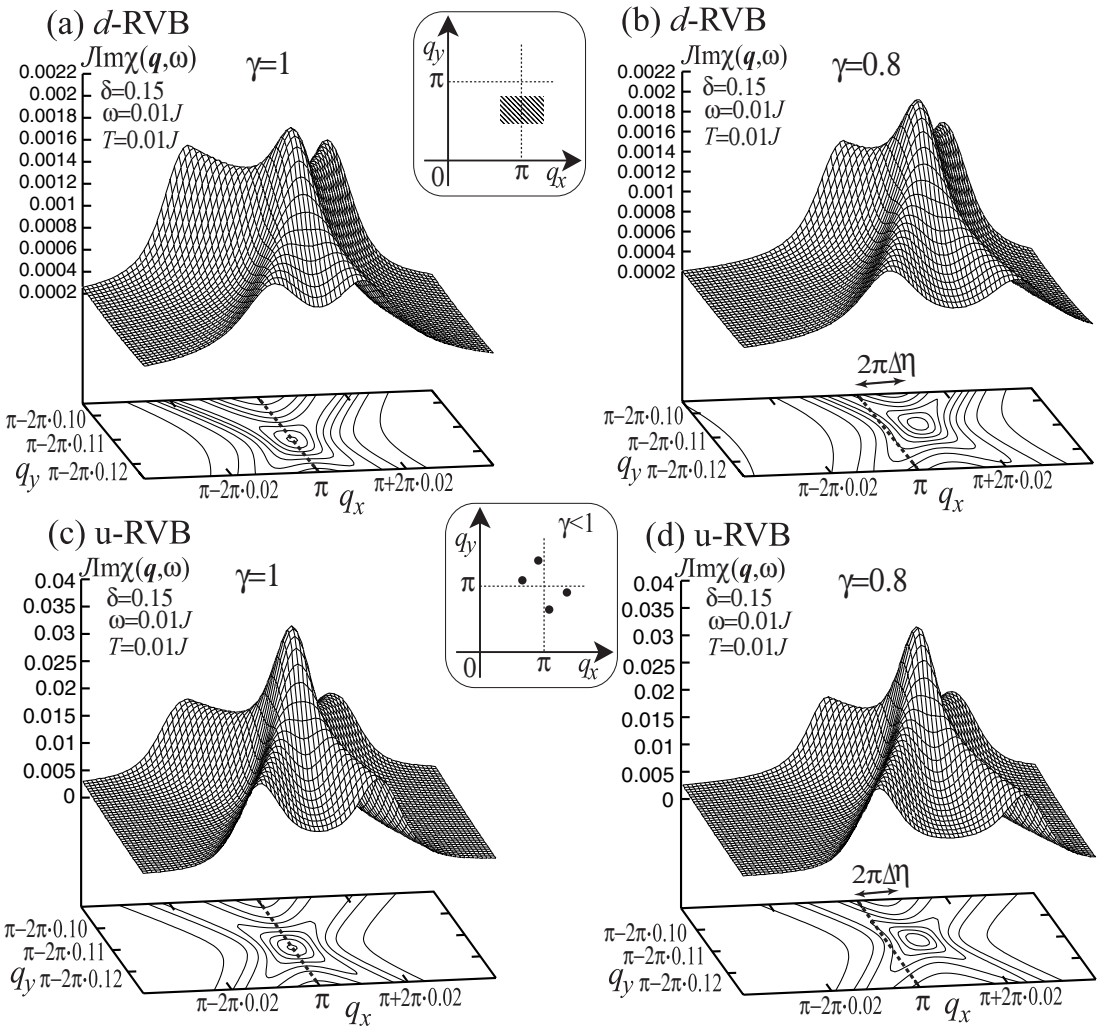

FIG. 2: $\boldsymbol{q}$ dependence of Im$\chi(\boldsymbol{q}, \omega)$ at ω=T=0.01J for $\gamma = 1$ and 0.8 in the d-RVB [(a) and (b)] and u-RVB [(c) and (d)] states. On the $\boldsymbol{q}$ plane, the contour lines are drawn to show the peak position clearly; the dashed line is the symmetry axis $q_x = \pi$. In the upper inset, the scanned $\boldsymbol{q}$ region is shown schematically by the hatch, and the lower inset sketches the IC peak positions (solid circles) for $\gamma < 1$.

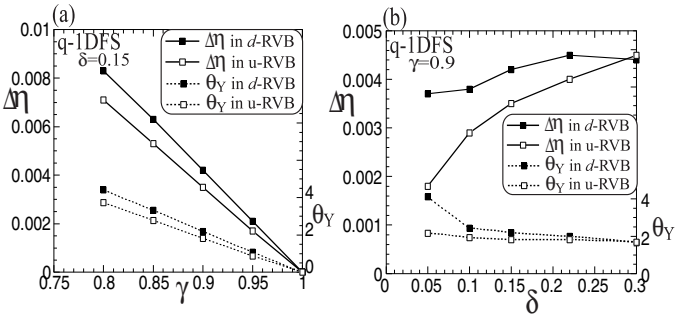

FIG. 3: The shift of IC peaks for the q-1D FS. (a) γ dependence of $\Delta\eta$ for $\delta = 0.15$. (b) δ dependence of $\Delta\eta$ for $\gamma = 0.9$. The calculations are done at $\omega = T = 0.01J$. Similar plots for $\theta_{\rm Y} = \tan^{-1}(\Delta\eta/\eta)$ (the unit is degree) are also shown; note that η has appreciable δ dependence (see Fig. 6).

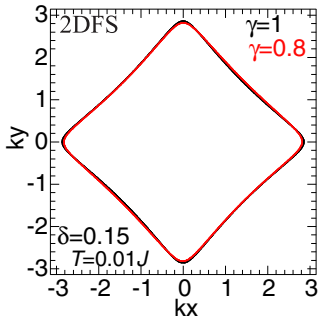

FIG. 4: (Color) The 2D FS determined self-consistently for $\gamma = 0.8$ (red line) and $\gamma = 1$ (solid line) at $\delta = 0.15$. The band parameters are chosen as $t/J = 4$ and $t'/t = -1/6$ with $\alpha \equiv 0$, and $\Delta_\tau \equiv 0$ is imposed.

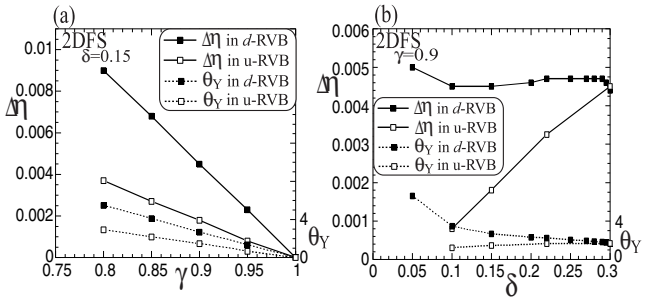

FIG. 5: The shift of IC peaks for the 2D FS; the band parameters are chosen as $t/J = 4$ and $t'/t = -1/6$ with $\alpha \equiv 0$. (a) γ dependence of $\Delta\eta$ for $\delta = 0.15$. (b) δ dependence of $\Delta\eta$ for $\gamma = 0.9$. Similar plots for $\theta_{\rm Y} = \tan^{-1}(\Delta\eta/\eta)$ (the unit is degree) are also shown.

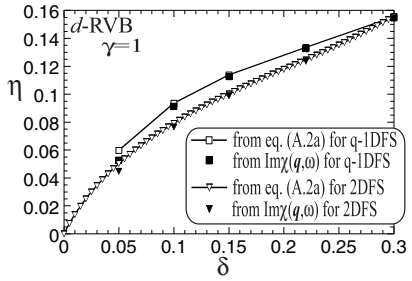

FIG. 6: Comparison of η between the analytic (open symbols) and numerical (solid symbols) estimations for q-1D and 2D FSs with $\gamma = 1$. The analytic one is from Eq. (A.2a) and the numerical one is from $\mathrm{Im}\chi(\boldsymbol{q}, \omega)$ at $\omega = T = 0.01J$ in the d-RVB state.

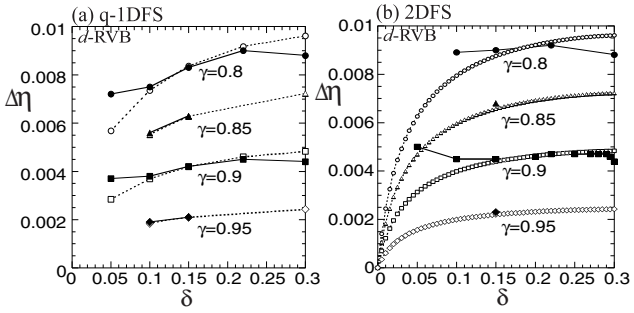

FIG. 7: Comparison of $\Delta\eta$ between the analytic (open symbols) and numerical (solid symbols) estimations for several choices of γ for q-1D FS (a) and 2D FS (b). The analytic one is from Eq. (A.2b) and the numerical one is from $\mathrm{Im}\chi(\boldsymbol{q}, \omega)$ at $\omega = T = 0.01J$ in the d-RVB state.