Effects of Orthorhombic Distortion on Magnetic Excitation in t–J Model

Hiroyuki Yamase[1,*] **and Hiroshi Kohno**[2]

1. RIKEN (The Institute of Physical and Chemical Research), Wako, Saitama 351-0198, Japan
2. Graduate School of Engineering Science, Osaka University, Toyonaka, Osaka 560-8531, Japan

Neutron scattering experiments on $La_{2-x}Sr_xCuO_4$ (LSCO) have revealed the incommensurate antiferromagnetic peaks do not lie exactly on the symmetry axes ($q_x = \pm\pi$ and $q_y = \pm\pi$), but are slightly shifted from them. In this paper, a scenario is presented for such 'shift' in terms of the anisotropy of t' (next-nearest-neighbor hopping integral on the square lattice) in the slave-boson scheme of the two-dimensional t–J model. Since the predictions of the present theory are different from those based on the 'spin-charge stripes' hypothesis, further studies of the 'shift' may clarify the factor responsible for the incommensurate antiferromagnetic fluctuations in LSCO systems.

1. INTRODUCTION

It is well known that $La_{2-x}Sr_xCuO_4$ (LSCO) shows the 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).[3,4] 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:[5,6] the IC peaks do not lie exactly on the symmetry axes, $q_x = \pm\pi$ and $q_y = \pm\pi$, but are slightly shifted from them. This 'shift' can be argued in terms of (i) the slanted charge stripes from the 'spin-charge stripes' viewpoint or (ii) the anisotropy of t' (the next-nearest-neighbor hopping integral on the square lattice) from the fermiology viewpoint.[3] It should be noted that the prediction from the latter viewpoint — the 'shift' will be absent in the low-temperature tetragonal (LTT) structure — is confirmed quite recently for $\mathrm{La_{1.875}Ba_{0.125-x}Sr_xCuO_4}$ system.[7]

In this paper, from the fermiology viewpoint we investigate in detail the 'shift' of the IC peaks in the slave-boson scheme of the two-dimensional (2D) t–J model, and discriminate between the present theory and that based on the 'spin-charge stripes' hypothesis. Further studies of the 'shift' of IC peaks may clarify the factor responsible for the IC correlations in LSCO systems.

2. MODEL and FORMALISM

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

$$H = -\sum_{i,\,j,\,\sigma} \left(t_\tau f_{i\,\sigma}^\dagger b_i b_j^\dagger f_{j\,\sigma} + t'_\tau f_{i\,\sigma}^\dagger b_i b_j^\dagger f_{j\,\sigma} \right) + \sum_{\langle i,j\rangle} J_\tau \boldsymbol{S}_i \cdot \boldsymbol{S}_j, \tag{1}$$

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

$f_{i\,\sigma}$ (b_i) is a fermion (boson) operator that carries spin σ (charge e), namely we adopt the slave-boson scheme. $t_\tau (t'_\tau)$ is the hopping integral between the (next) nearest-neighbor sites, and $\boldsymbol{\tau} = \boldsymbol{r}_j - \boldsymbol{r}_i$. $J_\tau (> 0)$ is the superexchange coupling between the nearest-neighbor spins. The constraint (2) excludes double occupations at every site.

Introducing the mean fields, $\chi_\tau \equiv \langle \sum_\sigma f_{i\,\sigma}^\dagger f_{i+\tau\,\sigma} \rangle$, $\langle b_i^\dagger b_{i+\tau} \rangle$ and $\Delta_\tau \equiv \langle f_{i\uparrow} f_{i+\tau\downarrow} - f_{i\downarrow} f_{i+\tau\uparrow} \rangle$, where each is taken to be a real constant independent of lattice coordinates but allowing $\boldsymbol{\tau}$-dependence, and loosing the local constraint (2) to the global one, we obtain the mean-field Hamiltonian. Assuming the boson to be condensed at the bottom of its band, we investigate the fermion part described by

$$H_{\rm MF} = \sum_{\boldsymbol{k},\,\sigma} \xi_{\boldsymbol{k}} f_{\boldsymbol{k}\,\sigma}^\dagger f_{\boldsymbol{k}\,\sigma} + \sum_{\boldsymbol{k}} \Delta_{\boldsymbol{k}} \left(f_{-\boldsymbol{k}\downarrow}^\dagger f_{\boldsymbol{k}\uparrow}^\dagger + f_{\boldsymbol{k}\uparrow} f_{-\boldsymbol{k}\downarrow} \right), \tag{3}$$

where

$$\begin{aligned} \xi_{\boldsymbol{k}} \;&=\; -2\left[\left(t_x\delta + \frac{3}{8} J_x \chi_x \right) \cos k_x + \left(t_y\delta + \frac{3}{8} J_y \chi_y \right) \cos k_y \right. \\ &\qquad \left. + \, t'_\parallel \delta \cos(k_x + k_y) + t'_\perp \delta \cos(k_x - k_y) \right] - \mu \,, \end{aligned} \tag{4}$$

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.

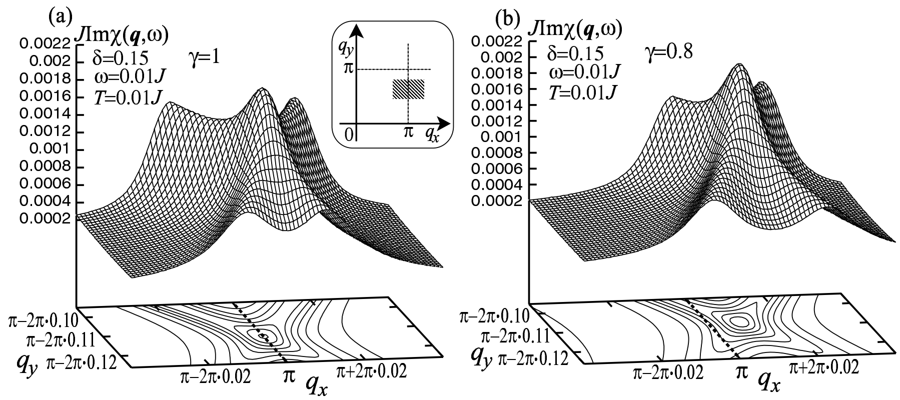

Fig. 1. $\boldsymbol{q}$-dependence of Im$\chi(\boldsymbol{q},\,\omega)$ at ω=T=0.01J for $\gamma = 1$(a) and 0.8(b). On the $\boldsymbol{q}$-plane, the contour lines are drawn to show the peak position clearly; the dashed line is the symmetry axis $q_x = \pi$. In the inset, the scanned $\boldsymbol{q}$-region is shown schematically by the hatch.

As shown in refs.,[3,4] the magnetic excitation in LSCO systems is well understood in terms of the q-1DFS.[8,9] To reproduce the q-1DFS that is consistent with the angle-resolved photoemission spectroscopy,[10] we introduce the spatial anisotropy[8] as $t_x = t$, $t_y = t(1 - 3.78\tan^2\theta)$, $J_x = J$ and $J_y = J(1 - 7.56\tan^2\theta)$. The parameter θ is determined to fit the FS around $(\pi,\,0)$ to the observed FS. We also include the possible coupling to the low-temperature orthorhombic (LTO) lattice distortion where CuO_6 octahedra tilt around the [110] axis, and introduce the anisotropy into t' as $t'_{\parallel} = t'$ and $t'_{\perp} = \gamma t'$ ($\gamma \le 1$). This anisotropy leads to the 'shift' of IC peaks as seen later. Setting $t/J = 4$ and $t'/t = -1/6$, we determine the mean fields self-consistently for each value of θ and γ.[11]

The dynamical magnetic susceptibility $\chi(\boldsymbol{q},\,\omega)$ is calculated in the 'RPA', $\chi(\boldsymbol{q},\,\omega) = \frac{\chi_0(\boldsymbol{q},\,\omega)}{1+rJ(\boldsymbol{q})\chi_0(\boldsymbol{q},\,\omega)}$. Here $\chi_0(\boldsymbol{q},\,\omega)$ is the irreducible part, $J(\boldsymbol{q}) = 2J(\cos q_x + \cos q_y)$ and we introduce a numerical factor r for convenience. While $r = 1$ in the RPA, we use $r = 0.35$ to avoid magnetic instability until $\delta \lesssim 0.02$, in accordance with the phase diagram of LSCO.

3. RESULTS

We calculate Im$\chi(\boldsymbol{q},\,\omega)$ at low $\omega(= 0.01J)$ and low temperature ($T = 0.01J$) where the d-wave singlet order[12] is realized. Figures 1 (a) and (b) show Im$\chi(\boldsymbol{q},\,\omega)$ around the IC peak at $(\pi,\,\pi - 2\pi\eta)$ 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

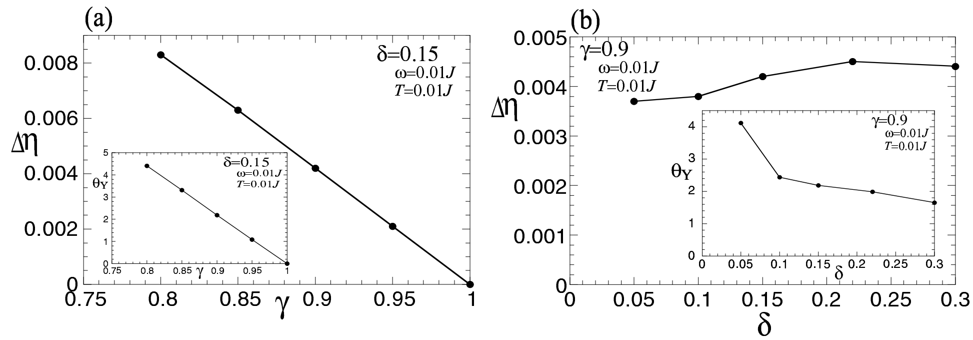

Fig. 2. (a) γ-dependence of $\Delta\eta$ for $\delta = 0.15$. (b) δ-dependence of $\Delta\eta$ for $\gamma = 0.9$. The similar plots for $\theta_{\rm Y}$ (the unit is degree) are shown in the insets.

$q_x = \pi$. As the anisotropy, measured by $1-\gamma$, is introduced, the peak shifts away from the symmetry axis to $\boldsymbol{q} = (\pi + 2\pi\Delta\eta,\, \pi - 2\pi\eta)$ without changing the overall structure of $\mathrm{Im}\chi(\boldsymbol{q},\, \omega)$. (The value of η changes slightly.) The γ-dependence of $\Delta\eta$ is shown in Fig. 2(a). It is seen that the degree of the 'shift' is proportional to the anisotropy of t', namely $\Delta\eta \propto 1-\gamma$. In Fig. 2(b), the δ-dependence of $\Delta\eta$ is shown for $\gamma = 0.9$. The value of $\Delta\eta$ does not change appreciably with δ. In the insets of Figs. 2(a) and (b), we also plot the quantity, $\theta_{\rm Y} = \tan^{-1}\frac{\Delta\eta}{\eta}$, which is often discussed experimentally. (Note that η has appreciable δ-dependence.[3,4])

4. DISCUSSION AND CONCLUSION

We now compare the present results with the experimental data.[5–7] Since the anisotropy of t' will come from the possible coupling to the LTO lattice distortion, the 'shift' is expected only in the LTO or the *Pccn* structure, and the degree of the 'shift' increases with the orthorhombic distortion (Fig. 2(a)). This is consistent with experiment.[7] The direction of the shift (Fig. 1(b)) is also consistent with experiments.[5–7] The observed values of the 'shift', $\theta_{\rm Y} \approx 1^\circ - 3^\circ$ or $\Delta\eta \approx 0.002 - 0.006$, can be understood semiquantitatively, since we expect[3,13] the anisotropy of t' more than a few percents in the actual systems.

As another scenario, Bosch *et al.*[14] propose that the 'shift' of IC peaks comes from the formation of the kink in the 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 $\delta \gtrsim 1/8$, and the value of $\Delta\eta$ is proportional to the excess hole density from 1/8, namely $\Delta\eta \propto (\delta - 1/8)$. On the other hand, in our theory, $\Delta\eta \propto 1-\gamma$, and the value of $\Delta\eta$ does not depend on δ appreciably for a fixed γ. (ii) The

$\Delta\eta$ can be an order of magnitude larger than in the preset theory.

Because of the unspecified character of charge stripes, it seems to allow other interpretations of the 'shift' of IC peaks. Fujita *et al.*[7] argue that the 'shift' comes from the possible coupling of charge stripes to the LTO lattice distortion. However, no semiquantitative studies have been done so far. We leave further discussions in the future.

Finally, we should note a possible link to the 'spin-charge stripes' *order* in the present theory. Since the present theory describes the *fluctuations* of the IC antiferromagnetism (AF), we can not exclude a possibility that the *ordered state* of IC-AF is accompanied by charge stripes. However, even if it would be the case, our semiquantitative analysis demonstrates that the essence of the 'shift' lies in the anisotropy of t', not the charge-stripes formation.

ACKNOWLEDGMENTS

H.Y. thanks M. Fujita for helpful discussions. This work is supported by a Special Postdoctoral Researchers Program from RIKEN and a Grant-in-Aid for COE Research (10CE2004) of the Ministry of Education, Science, Sports and Culture, Japan.
* Corresponding author. E-mail: yamase@riken.go.jp

REFERENCES

1. K. Yamada *et al.*, *Phys. Rev. B* **57**, 6165 (1998) and references therein.
2. J. M. Tranquada *et al.*, *Nature* **375**, 561 (1995).
3. H. Yamase and H. Kohno, *J. Phys. Soc. Jpn.* **69**, 332 (2000).
4. H. Yamase and H. Kohno, *J. Phys. Soc. Jpn.* **70**, 2733 (2001).
5. Y. S. Lee *et al.*, *Phys. Rev. B* **60**, 3643 (1999).
6. H. Kimura *et al.*, *Phys. Rev. B* **61**, 14366 (2000).
7. M. Fujita *et al.*, cond-mat/0203321.
8. H. Yamase and H. Kohno, *J. Phys. Soc. Jpn.* **69**, 2151 (2000).
9. C. J. Halboth and W. Metzner, *Phys. Rev. Lett.* **85**, 5162 (2000).
10. A. Ino *et al.*, *Phys. Rev. B* **65**, 094504 (2002).
11. In the presence of $\theta(\neq 0)$ and $\gamma(<1)$, the full self-consistent calculations were not done in the previous study.[3]
12. Precisely, a bit of the extended s-wave singlet order mixes in the q-1D state.[8]
13. H. Yamase and H. Kohno, in preparation.
14. M. Bosch *et al.*, *Phys. Rev. B* **63**, 092501 (2001).