Study of Phonon Anomalies in Stripe phase of High T_c Cuprates

Eiji Kaneshita [1], Masanori Ichioka, Kazushige Machida

Department of Physics, Okayama University, Okayama 700-8530, Japan

Abstract

We theoretically investigate phonon anomalies in various high T_c cuprates in terms of stripe concept. They could be caused by coupling with charge translational modes of stripes. The phonon self-energy correction is evaluated by taking into account the collective stripe modes. The coupling with stripes causes a phonon dispersion gap when the phonon dispersion has a steep slope around $2\boldsymbol{Q}$. No gap appears when the phonon spectrum has a flat dispersion around $2\boldsymbol{Q}$. Thus it turns out that these are depending on the slope of the phonon dispersions.

Key words: collective modes; phonons ; spin-density waves ; Hubbard model

1. Introduction

Recently, a remarkable series of neutron experiments on various cuprates [1–7] has been done to reveal unequivocally the phonon dispersion anomalies: such as a gap-like structure around the reciprocal point which coincides with the wave number of the charge stripe states. Therefore, the gap seems to be due to the coupling with the dynamical charge stripes.

According to the neutron experiments, the phonon spectra of a breathing mode in $La_{2-x}Sr_xCuO_4$ (LSCO) [1–3] have a dispersion softened over the area from $(0, \frac{\pi}{2})$ to $(0, \pi)$: This origin is discussed in several papers [8–10] without considering stripes. These experiments have shown that the phonon dispersion also has a jump at the slope around $(0, \frac{\pi}{2})$.

In our previous paper [11], we showed the coupling with the collective stripe modes cause a gap on the phonon dispersion, by means of random phase approximation (RPA), on the metallic vertical stripe state. In this paper, we discuss the dispersion jump by varying the stripe periodicity for insulating or metal vertical stripe cases.

[1] E-mail:eiji@mp.okayama-u.ac.jp

2. Model and formulation

We start with the Hubbard model

$$H = \sum_{i,j,\sigma} t_{i,j} c^{\dagger}_{i,\sigma} c_{j,\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}, \quad (1)$$

where σ is a spin index, $t_{i,j} = t$ (t') for the (next) nearest neighbor sites i and j, to describe a stable stripe state. For $\frac{t'}{t} = -0.2$ ($\frac{t'}{t} = 0.0$), we obtain a metallic (insulating) state as a ground state. The mean-field ground state [12,13] and RPA [14] yield a rich structure for individual and collective excitation spectra of spin and charge channels. In this paper, especially, we are interested in the dynamical charge susceptibility $\chi_{nn}(\mathbf{q}, \omega) = \langle\langle n; n \rangle\rangle_{\mathbf{q},\omega}$ because the charge translational mode, which appears in χ_{nn}, is directly coupled to the phonons and most relevant to the phonon renormalization. We calculate $\langle\langle n_\uparrow; n_\uparrow \rangle\rangle$ and $\langle\langle n_\uparrow; n_\downarrow \rangle\rangle$ by means of RPA [14], and obtain $\chi_{nn}(\mathbf{q}+l_1\mathbf{Q}, \mathbf{q}+l_2\mathbf{Q}, \omega)$, which is characterized by l_1, l_2 to represent the Umklapp process resulting from periodicity of stripes.

Once the charge translational mode is yielded, we obtain the renormalized phonon spectrum from an Dyson-like equation [11]: The equation is formed by matrix

$$\sum_{m'}\{\delta_{lm'} - |g|^2 D_0(\mathbf{q}+l\mathbf{Q}, i\omega_n)$$
$$\chi_{nn}(\mathbf{q}+l\mathbf{Q}, \mathbf{q}+m'\mathbf{Q}, i\omega_n)\}$$
$$\times D(\mathbf{q}+m'\mathbf{Q}, \mathbf{q}+m\mathbf{Q}, i\omega_n)$$
$$= D_0(\mathbf{q}+l\mathbf{Q}, i\omega_n)\delta_{lm}, \qquad (2)$$

where $D_0(\mathbf{q}, i\omega_n) = -2\omega_\mathbf{q}/(\omega_n^2 + \omega_\mathbf{q}^2)$ represents the unperturbed phonon Green's function and $\omega_\mathbf{q}$ is the unperturbed phonon dispersion.

Taking the softening into account, we assume the dispersion for the unperturbed phonon as follows:

$$\omega_\mathbf{q} = -\frac{A}{2}(1 - sn(q_x + K))sn(\frac{q_y}{q_x}2K + K)$$
$$+\frac{A}{2}(1 + sn(q_x + K)) + B \qquad (3)$$

for $|q_x| \geq |q_y|$ and $q_x \leftrightarrow q_y$ for $|q_x| < |q_y|$, where $sn(q)$ is the elliptic function and K complete elliptic integral with modulus k.

3. Results and conclusion

We show the renormalized phonon spectral functions $-\frac{1}{\pi}\mathrm{Im}D(\mathbf{q}, \mathbf{q}, i\omega_n \to \omega + i\eta)$ in Fig. 1, where the spectrum for the metallic state (a) is also showed to compare with those for the insulating states (b) and (c): (a) $\boldsymbol{Q} = (\pi, \frac{3\pi}{4})$, $n = 0.82$, (b) $\boldsymbol{Q} = (\pi, \frac{7\pi}{8})$, $n = 0.875$, (c) $\boldsymbol{Q} = (\pi, \frac{3\pi}{4})$, $n = 0.75$. The spectrum for metallic state has a gap at $2\boldsymbol{Q}$. This gap comes from the charge collective mode of stripes and the band folding of phonon dispersion due to the periodic structure of stripes[11].

In the insulating state with $\frac{t'}{t} = 0.0$, on the other hand, $2\boldsymbol{Q}$ is shifted to $(\frac{\pi}{4}, 0)$ because the filling changes to one hope per stripe. Around $2\boldsymbol{Q}$, the phonon dispersion is flat. While a weak anomaly appears there, it has no gap-like structure. Instead, another type of anomaly appears around $2\boldsymbol{Q}$ although it has a weak intensity. It also gives rise to the band folding of phonon dispersion due to the periodic structure of stripes.

We can also consider the case $2\boldsymbol{Q} = (0, \frac{\pi}{2})$ as in the metallic case by decreasing n. It is shown in Fig. 1(c), where a gap structure appears at $2\boldsymbol{Q}$ in the phonon spectrum. Therefore, the difference between Fig. 1(a) and Fig. 1(b) cases is not due to the system properties whether metal or insulator but on the slope of the phonon dispersion rather. It is because the dispersion is flat around $2\boldsymbol{Q}$ in the insulating case that no gap appears there.

Hence we get the following conclusion: the coupling with the collective stripe mode and the phonon mode doesn't necessarily cause a gap on the phonon spectrum, depending on the slope of the phonon dispersion around $2\boldsymbol{Q}$, even though another anomaly probably appears there.

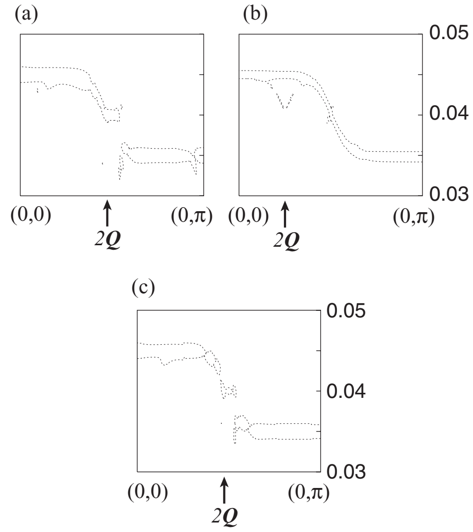

Fig. 1. Renormalized phonon spectral functions for a metallic state (a) and insulating states (b) and (c). We set the parameters as follows: $|g|^2 = 0.001$, $A = 0.005$, $B = 0.04$, $k = 0.9999$ and $\frac{U}{t} = 4.0$, $\frac{t'}{t} = -0.2$ (a) and 0.0 (b, c).

References

[1] R. J. McQueeney, *et al.*, Phys. Rev. Lett. **82** (1999) 628.

[2] R. J. McQueeney, *et al.*, Phys. Rev. Lett. **87** (2001) 077001.

[3] L. Pintschovius, M. Braden, Phys. Rev. B**60** (1999) R15039.

[4] H. A. Mook, F. Doğan, Nature **401** (1999) 145.

[5] Y. Petrov, *et al.*, cond-mat/0003414.

[6] H. A. Mook, F. Doğan, cond-mat/0103037.

[7] R.J. McQueeney, *et al.*, cond-mat/0105593.

[8] C. Falter, M. Klenner, G. A. Hoffmann, Phys. Rev. B **55** (1997) 3308. C. Falter, G. A. Hoffmann, Phys. Rev. B **61** (2000) 14537.

[9] M. Braden, W. Reichardt, S. Shiryaev, S.N. Barilo, cond-mat/0107498.

[10] K. Park, S. Sachdev, Phys. Rev. B **64** (2001) 184510.

[11] E. Kaneshita, M. Ichioka, K. Machida, Phys. Rev. Lett. **88** (2002) 115501.

[12] K. Machida, Physica C **158** (1989) 192. M. Kato, K. Machida, H. Nakanishi, M. Fujita, J. Phys. Soc. Jpn. **59** (1990) 1047.

[13] K. Machida, M. Ichioka, J. Phys. Soc. Jpn. **68** (1999) 2168. M. Ichioka, K. Machida, J. Phys. Soc. Jpn. **68** (1999) 4020.

[14] E. Kaneshita, M. Ichioka, K. Machida, J. Phys. Soc. Jpn. **70** (2001) 866. Also see, M. Ichioka, E. Kaneshita, K. Machida, J. Phys. Soc. Jpn. **70** (2001) 818.