Phonon anomalies due to stripe collective modes in high $T_c$ cuprates

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Phonon anomalies observed in various high $T_c$ cuprates by neutron experiments are analyzed theoretically in terms of the stripe concept. The phonon self-energy correction is evaluated by taking into account the charge collective modes of stripes, giving rise to dispersion gap, or kink and shadow phonon modes at twice the wave number of spin stripe. These features coincide precisely with observations. The gapped branches of the phonon are found to be in-phase and out-of-phase oscillations relative to the charge collective mode.

The pairing mechanism of high $T_c$ superconductors has been still highly debated since its discovery over a decade ago. The debates are mainly centered on how to describe the normal state above its superconducting transition $T_c$. Recently, a remarkable series of neutron experiments on various cuprates has been done to reveal unequivocally the phonon dispersion anomalies at the particular reciprocal point. The phonon anomalies differ slightly in their appearance, ranging from a sharp dispersion jump to the dispersion kink. This depends on the materials; La$_2$CuO$_4$ (LSCO) [1, 2, 3] or YBa$_2$Cu$_3$O$_{6-x}$-y (YBCO) [4, 5, 6, 7, 8] or the focused phonon modes such as breathing mode, or bond-stretching mode, etc. This ubiquitous phenomenon for which proper explanation has not been given so far is interesting because not only it gives a clue to pairing mechanism in high $T_c$ cuprates, but more importantly it gives a key to better understanding the normal state properties with full of mysteries.

It is known now that in underdoping La$_{2-x}$Sr$_x$CuO$_4$ the incommensurate static magnetic peaks at $Q$ are observed around $(\pi, \pi)$ point in two dimensional CuO$_2$ plane (here the lattice constant $a$ is unity) by neutron experiments [9]. As doping proceeds with $x$, the ordering vector $Q$ rotates precisely at the insulator-metal transition ($x = 0.05$) by 45° around $(\pi, \pi)$ point, corresponding to spin modulation change from the diagonal stripe $Q = (2\pi(\frac{1}{2} \pm \delta), 2\pi(\frac{3}{2} \pm \delta))$ to the vertical stripe $Q = (2\pi(\frac{1}{4} \pm \delta), 0)$ or $(0, 2\pi(\frac{3}{4} \pm \delta))$ where $\delta \sim x$. In higher doping region the incommensurability $\delta$ almost saturates at a particular value $\delta \sim \frac{1}{8}$. The same 45° rotation of the magnetic superspots is also observed in (La, Nd)$_{2-x}$Sr$_x$CuO$_4$, corresponding to the metal-insulator transition, further lending this superspot rotation to the universal mechanism to drive a metal-insulator transition upon doping. In this material [10] and La$_{2-x}$(Sr,Ba)$_x$CuO$_4$ [11] the concomitant static charge superspots at $2Q$ are found by neutron scatterings.

These characteristics coincide nicely with the incommensurate spin density wave or stripe picture [12, 13] in which a solitonic midgap state occupies excess holes completely (partially) in an insulating (metallic) state, giving rise to a microscopic charge and spin segregation characteristic to topological doping. The partially occupied midgap state is observed directly by recent angle-resolved photoemission experiment [14] near $(\pi, 0)$ point as a parallel Fermi surface sheet which is responsible to metallicity of doped CuO$_2$ plane [15].

As for YBCO, although experimental verification of true static magnetic order comes only from $\mu$SR [16] which reports a similar phase diagram to LSCO in doping vs. static magnetic ordering, there are several common characteristics mentioned above [17], including neutron scatterings [18]. Thus it is expected that the stripe picture may be applicable to YBCO [19]. Numerous other experiments such as write-out effect for charge order by NMR [20], detailed transport measurements [21], etc. and theories [22], collectively point to support the idea that the stripe concept may be applicable to doped CuO$_2$ plane in general.

Here we are going to demonstrate that the phonon anomalies observed in various cuprates are a direct manifestation of existence of the low-lying collective charge excitations associated with stripes. Physically, the $\pi$-phase shifting domain walls accommodate excess holes and the remaining antiferromagnetic regions are intact. The domain wall motion, or the charge collective oscillation, is strongly coupled with the particular phonon mode, such as breathing or bond-stretching modes. Both electron and phonon systems are mutually influenced by the others to lower the total energy. The spin and charge inhomogeneity is a universal phenomenon in doped CuO$_2$ plane, out of which high $T_c$ superconductivity is created. This process is still beyond our understanding at the moment, but this identification, we believe, is important towards this step. This is particular true for YBCO where there is no defining experiment to uncover the charge collective modes which has been elusive so far. Since the stripe concept, although originally derived from mean field approximation [12, 13], may be valid for describing a doped Mott insulator, or at least, the stripe is a convenient “vehicle” to accommodate excess holes, it is worthwhile to pursue this identification.

We start with the Hubbard model $H = \sum_{i,j,\sigma} t_{i,j} c_{i,\sigma}^\dagger c_{j,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow}$ to describe a stable stripe and its excitations. The mean-field ground state [13, 15] and random phase approximation (RPA) [13] yield a rich structure for individual and collective excitation spec-
The phonon dispersion is directly coupled to the phonons and the dynamical charge susceptibility \(\chi_{nn}(q, \omega) = \langle \langle S_{zz}^{(1)}(0) ; S_{zz}^{(2)}(q) \rangle \rangle_{q, \omega} \), and the dynamical charge susceptibility \(\chi_{nn}(q, \omega) = \langle \langle n; n \rangle \rangle_{q, \omega} \). The RPA equation for \(\chi_{S_{zz}S_{zz}} = \langle \langle S_{zz}^{(1)} ; S_{zz}^{(2)} \rangle \rangle \) is written as \(\chi_{S_{zz}S_{zz}}(r_1, r_3, \omega) = \chi_0^{zz}(r_1, r_3, \omega) + U \sum_{r_2} \chi_0^{zz}(r_1, r_2, \omega) \chi_{S_{zz}S_{zz}}(r_2, r_3, \omega) \) with non-interacting susceptibility \(\chi_0^{zz} \). After Fourier transformation to \(k\)-space, this is reduced to a matrix equation of \(\chi_0^{zz} \) and \(\chi_{S_{zz}S_{zz}} \). By solving it, we obtain \(\chi_{zz}(q + l_1 Q, q + l_2 Q, \omega) \). There, \(q + l_1 Q \) and \(q + l_2 Q \) are, respectively, outgoing and incoming wave vectors. They can change by \((l_1 - l_2) Q \) through the Umklapp process, since the underlying electronic state is spatially modulated with the periodicity \(Q \). In a similar manner, we calculate \((n\uparrow; n\uparrow)\) and \((n\uparrow; n\downarrow)\), and obtain \(\chi_{zz}(q + l_1 Q, q + l_2 Q, \omega) \) and \(\chi_{nn}(q + l_1 Q, q + l_2 Q, \omega) \).

The spin modes \(\chi_{zz}(q, \omega) \equiv \chi_{zz}(q, q, \omega) \) give rise to collective excitation at the ordering vector \(Q \) and its odd-harmonic points as a Goldstone mode. The charge mode \(\chi_{nn}(q, \omega) \equiv \chi_{nn}(q, q, \omega) \) exhibits the collective excitations at \(q = 2Q, 4Q \ldots \). There, \(\chi_{zz} \) gives spin wave, when we assume that the magnetization points to the \(z \) axis. The translational phason modes appear in \(\chi_{nn}(z, z) \), which correspond to the motion of the charge (spin) stripe \(\parallel \). Among various individual and collective motions associated with stripes, the phason mode in the charge oscillation is directly coupled to the phonons and most relevant to the phonon renormalization. In Fig.1, \(\text{Im}\chi_{nn}(q, \omega) \) is shown around \(q = 2Q = (0, \pi/2) \) along the \(q_x \) and the \(q_y \) directions. This particular charge mode with the anisotropic velocities is situated at \(2Q \). The motion parallel (perpendicular) to \(2Q \) vector corresponds to the compression (meandering) motion of stripes with high (low) velocity. In the following we illustrate typical results for the metallic vertical stripe \(\parallel \) which is stable with \(Q = (\pi, \pi/2) \) for the electron filling per site \(n = 0.82 \) and the parameters are fixed as \(t_L = 4.0 \) and \(t_F = -0.2 \). (\(t(\tau) \) is the (next) nearest neighbor hopping integral). The main features of the results do not much depend on the choice of these values. We note that \(t \) is an order of 0.5eV and the phonon energy \(\omega \sim 80\text{meV} \) for the breathing mode or bond-stretching mode which is coupled strongly to the electronic state. We focus on an energy range of typically \(\frac{\pi}{a} \sim 0.1 \) in the following. All the energy is scaled by \(t \).

In order to study the effects of the stripes on the phonon Green’s function \(D(q + l_1 Q, q + l_2 Q, \omega) \) within RPA, we consider the following standard electron-phonon Hamiltonian: \(H’ = \sum_{k, \sigma_{c}} g \langle \hat{b}_{k+q} \hat{b}^\dagger_{-q} \rangle \langle \hat{c}_{k+q} \rangle \) with \(g \) being the coupling constant. Since the electron bubble in the phonon self-energy correction is nothing but the dynamical charge susceptibility mentioned, we immediately obtain an equation in a matrix form for the thermal Green’s functions \(\sum_{m'} \{ \delta_{mn} - \langle |g|^2 D_0(q + /Q, \omega) \rangle \chi_{nn}(q + l_1 Q, q + l_2 Q, \omega) \} D(q + m'Q, \omega) = D_0(q + l_1 Q, \omega) \delta_{nm} \), where the unperturbed Green’s function \(D_0(q, \omega) = -2\omega_q/(\omega_q + \omega_q^2) \), and \(\omega_q \) is the unperturbed phonon dispersion. Diagonalization of this matrix equation yields the renormalized phonon Green’s function.

We show the renormalized phonon spectral function \(-\frac{1}{2} \text{Im} D(q, q, \omega) \) in Fig.2, where we assume a simple sinusoidal form \(\omega_q \) for \(\omega_q \) as a typical phonon. It is seen from Fig.2 that the dispersion exhibits several characteristic modifications: (A) The discontinuities of the dispersion occur at various points, notably near \(2Q \) where the dispersion cone of the collective charge mode

**FIG. 1:** Dispersion curves of the charge collective mode around \(2Q \). We plot \(\text{Im}\chi_{nn}(q, \omega) \) for two paths along \(2Q \) (a) and perpendicular to \(2Q \) (b).

**FIG. 2:** Renormalized phonon spectral functions for \(|g|^2 = 0.001 \). (a) is logarithmic plot to emphasize the small intensity of the shadow bands. (b) is contour plot shown for high intensity. The simple sinusoidal form is assumed for the unperturbed phonon \((A = -0.01, B = 0.08, k = 0) \).
shown in Fig.1 and the phonon mode intersect. (B) The appearance of the downward hybridized new phonon dispersions. (C) The flat dispersion appears above the gap at $2Q$. (D) The shadow band which is a replica of the original mode is seen.

These features come from the two physical reasons schematically illustrated in Fig.3: The hybridization of the charge collective mode centered at $2Q$ denoted as 1 with the original phonon 2 in Fig.3 and the band-folding due to the periodic structure with the charge ordering vector $2Q$, which amounts to shifting the original dispersion 2, resulting in phonon dispersions; curve 3 ~ 5 in Fig.3. The hybridization of these dispersions gives rise to the reconnected phonon modes in Fig.2.

These main four features (A-D) of the dispersion modification become more evident when the electron-phonon coupling $|g|^2$ increases, or the unperturbed dispersion is situated at lower energy side. The gap size at the discontinuity increases as the original phonon band is widen. It is noteworthy that the discontinuity of the dispersion, or a kink feature and associated new lower mode branching-out from the disconnected lower phonon are reminiscent of the observation on O$_6$ in YBCO by Mook and Doğan[4] (see their Figs.1(d) and (e)). Note also that since the discontinuity point occurs at the intersection of the charge collective mode at $2Q$ and phonons, the observed dispersion anomaly should change with doping: As doping increases the $2Q$ vector increases. This is indeed observed by neutron experiment[6] and also consistent with the doping dependence of the fundamental vector $Q$ of the magnetic peaks[8]. These constitute an internal consistent picture for the stripe origin.

The physical implication of the phonon gap formation is understood by analyzing the phonon oscillation patterns of the upper and lower phonon branches. According to linear response theory, the oscillation patterns are given by $\phi(r, t) = \Sigma_i \frac{1}{\hbar} D(q_i) e^{iQ \cdot r} e^{i\omega t}$ where $\phi(r, t)$ is the lattice displacement and $h_i$ is the external field with the wave number $q$ and the frequency $\omega$. At the wave number $2Q = (0, \frac{\pi}{2})$, the oscillations corresponding to the upper ($\omega = 0.08$) and lower ($\omega = 0.075$) branches shown in Fig.2 are schematically displayed in Fig.4. The four site period oscillations are either in phase or out of phase with the charge oscillation in the electron system which is the phason motion of the stripes.

We show the renormalized dispersions parallel to $2Q$ in Figs.5(a) and (c) and perpendicular to $2Q$ centered at $2Q$ in Figs.5(b) and (d). Here we assume the unperturbed phonon with a steep slope at $(0, \frac{\pi}{2})$, simulating the breathing mode in LSCO with the energy $\sim$80meV. Noticeable features of the modification are: (A) Rather large dispersion discontinuity observed at $2Q$ is seen in Figs.5(a) and (c). (B) It is noted that the shadow mode which is a replica of the original band can be seen in Figs.5(a) and (b). (C) The anomaly continues to extend to the perpendicular direction seen from Figs.5(b) and (d). These features (A-C) coincide with the neutron experiment[1] on LSCO with $x = 0.15$ where at $(\frac{\pi}{2}, 0)$ in the $(q_x, 0)$ scan they observe a sharp drop of the bond-stretching mode (see their Fig.2) and this anomalous behavior continues to the perpendicular direction (see their Fig.4). As they emphasize, the phonon anomaly occurs not because of the simple band-folding effect due to new charge periodicity with 4 lattice period which would result in a gap at the new Brillouin zone boundary at $(\frac{\pi}{2}, 0)$, but the observed gap is at $(\frac{\pi}{2}, 0)$.

The anomalous reciprocal regions for the two perpendicular directions have different widths as seen from Fig.5 because the underlying charge cone is anisotropic as mentioned, yielding different widths (compare the openings of the cones at the center in Figs.1(a) and (b) corresponding to the cones in Figs.5(a) and (b)). Thus it is possible to use it as a kind of spectroscopy, namely, to investigate this anisotropy of the charge collective mode through the
analysis of the phonon anomaly. In fact according to the above experiment [1], the width of the anomalous region in the perpendicular direction is wider than that in the parallel direction. This accords with our result in Fig.5. We can attribute it as arising from the lower velocity of the meandering mode than the compression mode [2].

McQueeney, et al. [3] report that there is no phonon anomaly below $x \leq 0.05$ in LSCO where the static diagonal stripe is stabilized. There are two possibilities: (1) Since the velocity of the collective charge excitation is rather low for the insulating diagonal stripe [2], the phonon mode investigated by them may not be coupled with this excitation, failing to drive the anomaly. (2) As the second possibility, the collective charge excitation could be gapped [2]. There is no low-lying excitation coupled to phonons. In this connection, we point out that in Cr, where the diagonal stripe in the present terminology is realized, neutron experiment to see the phonon anomaly at $2Q$ corresponding to the so-called strain wave or charge order is desirable.

Considering the electron-phonon coupling, we study the phonon anomalies in the stripe state. The phonon anomalies observed mainly by neutron scattering experiments on LSCO and YBCO with various doping levels are accounted for as arising from two physical effects: Hybridization with the charge collective mode at $2Q$ and band-folding of a phonon band. These give rise to reconnection and gap formation in bands. The underlying physics behind the phonon anomalies at the particular reciprocal point, namely $2Q$, is the existence of the collective charge excitations associated with stripes; the translational phason and meandering gapless modes with different velocities situated at every even-multiples of the fundamental vector $Q$ which varies systematically with hole-doping. Thus this also leads to systematic changes of the $2Q$ vector, a fact that the experiments have found (see Fig.4 in Ref.[1]). In order to confirm our identification, further neutron experiments are desirable, in particular to find the yet-uncovered lower modes branching-out downwardly from the phonon discontinuity at $2Q$. Since in principle the phonon anomalies occur for all phonon modes and the observability depends on the electron-phonon coupling constant, lower phonon modes are more favorable for this purpose.

It might be interesting to point out that similar phonon mode anomalies are also found in $(\text{La,Sr})_2\text{NiO}_4$ [25] where the diagonal stripes are stabilized because as mentioned this system is an insulator up to higher dopings, thus $45^\circ$ rotation of the superspots occurs. In yet another non-cuprate superconductor $\text{Ba}_{0.8}\text{K}_{0.2}\text{BiO}_3$, which is related to charge density waves instead of spin density wave here the phonon anomaly of the bond-stretching mode appears at a certain reciprocal point $2Q$. We believe that these anomalies could be analyzed in the same way as in here, which belongs to future problem.

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