



Phonon anomalies and dynamic stripes

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ABSTRACT

Stripe order where electrons self-organize into alternating periodic charge-rich and magnetically-ordered charge-poor parallel lines was proposed as a way of optimizing the kinetic energy of holes in a doped Mott insulator. Static stripes detected as extra peaks in diffraction patterns, appear in a number of oxide perovskites as well as some other systems. The more controversial dynamic stripes, which are not detectable by diffraction, may be universally present in copper oxide superconductors. Thus it is important to learn how to detect dynamic stripes as well as to understand their influence on electronic properties. This review article focuses on lattice vibrations (phonons) that might show signatures of the charge component of dynamic stripes. The first part of the article describes recent progress in learning about how the phonon signatures of different types of electronic charge fluctuations including stripes can be distinguished from purely structural instabilities and from each other. Then I will focus on the evidence for dynamic stripes in the phonon spectra of copper oxide superconductors.

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1. General considerations

Electrons in a doped Mott insulator sometimes form stripe order, consisting of alternating charge-rich lines and charge-poor antiferromagnetic regions. It was predicted theoretically in 1989 [1,2] and discovered in a nickel oxide perovskite in 1994 by neutron diffraction [3]. Static stripe order was subsequently found in some copper oxide perovskites [4]. Diffraction measurements of copper oxide high temperature superconductors do not show magnetic and charge Bragg peaks characteristic of static stripes. However, it was proposed that dynamic stripes, which are much harder to observe than the static ones [5], play an important role in the copper oxide superconductors [6–9].

Periodic charge density modulation, which forms as a result of stripe formation, induces a periodic distortion of the crystal lattice with the same propagation vector. Its magnitude is proportional to the electron-phonon coupling strength. Such distortions can be observed by neutron diffraction as well as scanning tunneling microscopy [5]. Charge density fluctuations associated with dynamic stripes may soften and/or broaden certain phonons signaling an incipient lattice instability. However, structural distortions as well as soft phonons may appear not only because of stripe formation, but also for other reasons. Thus, in order to use phonons as a tool to study dynamic stripes, it is crucial to learn how to distinguish between different origins of soft phonons.

Structural phase transitions can result from purely structural instabilities or from atomic positions reacting to charge density modulation associated with electronic instabilities (such as the tendency to form stripes). In both cases, the phase transition occurs due to a small energy difference between the ground-state structure of low symmetry and a high symmetry structure favored at high temperatures. The high temperature phase is often characterized by a soft phonon mode whose polarization is the same as the “frozen” lattice distortion of the low-T phase. The softening of this mode is most pronounced at the structural transition temperature. In the low temperature phase, the number of phonon branches increases due to the larger unit cell. This phenomenon is called branch folding.

Diffraction is a direct way of detecting structural phase transitions. Static stripes show up in neutron diffraction spectra as extra lattice/magnetic peaks corresponding to charge/spin stripes respectively. Many solids do not undergo structural phase transitions, but exhibit incipient electronic and/or lattice instabilities, which are undetectable by diffraction. In these cases, softening and broadening of phonons (which is often temperature-dependent) provides a unique window on competing phases, which often play an important role in many phenomena including stripe formation.

My goal here is to review recent progress in studies of phonon in correlated electron systems with the focus on phonon anomalies that may be associated with the formation of charge stripes. This article is organized as follows. First I will discuss soft phonons in different systems and demonstrate that, although phonon behavior is very similar near different types of lattice instabilities, it may be possible to distinguish between them. Then, I will focus on the features of soft phonons that may be specific to dynamic stripes.

This article partially overlaps and complements two other recent reviews [10,11].

2. Different types of structural and electronic instabilities

Crystal structure as well as frequencies of atomic vibrations are ultimately determined by interactions between all atomic nu-

clei and all electrons in the crystal, so in this sense all lattice instabilities are driven by electron-phonon coupling. However, one can distinguish between the instabilities caused by electron-phonon coupling directly (which I call structural instabilities), and the instabilities where the electronic state itself undergoes a phase transition, which then pulls the lattice along (which I call electronic instabilities). Stripe formation is an example of the latter.

Phonon measurements can provide insights into mechanisms underlying second order displacive structural transitions that involve soft phonon behavior. In these transitions atomic displacements in a crystal change bond lengths and/or angles, without severing the primary bonds. Such transitions are associated with soft phonons whose eigenvectors are close to the character of the atomic displacements that take place during the transition. The contribution to the Hamiltonian from the soft phonon with the generalized coordinate X , $H(X)$, can always be approximated by adding a double-well potential term to the regular harmonic potential. It is useful to approximate the bottom of the double well potential as:

$$V_{\text{double-well}}(X) = aX^2 + bX^4, \quad \text{where } b > 0.$$

If $a < 0$, the two sides of the well with the minima at $X = \pm\sqrt{-a/2b}$ represent the lattice distortion in one or another symmetry-equivalent direction. At temperatures higher than the barrier between the potential wells, ($k_B T > a^2/4b$), the average structure is undistorted, i.e., $\langle X \rangle = 0$. But the anharmonic potential makes the phonon soft and broad. This broadening and softening becomes enhanced on cooling towards the transition temperature, as the amplitude of the vibration decreases and the phonon feels the anharmonic bottom of the potential more and more. Below T_c , the lattice settles at the minimum of one of the wells with $\langle X \rangle = +\sqrt{-a/2b}$ or $\langle X \rangle = -\sqrt{-a/2b}$, and the phonon hardens and narrows.

If $a > 0$, the phase transition will not occur, but soft phonons induced by anharmonicity and/or electron-phonon coupling may be observed.

Usually (but not always) the phonon spectral function is that of a damped harmonic oscillator. In the limit of weak damping it is close to a Lorentzian centered at the phonon frequency whose linewidth is proportional to the inverse phonon lifetime.

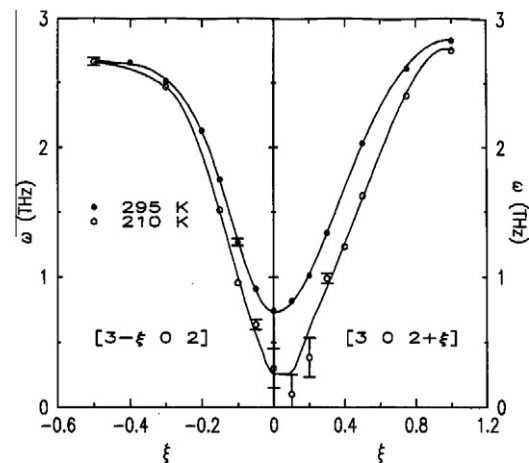


Fig. 1. The dispersion of the soft mode in $\text{La}_{1.67}\text{Sr}_{0.13}\text{CuO}_4$ near the structural phase transition (210 K) and at room temperature (from [12]).

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