

Phonon induced stripe formation and the isotope effect on T^* in high- T_c superconductors

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A theoretical understanding of the mesoscopic striped phase, common to many HTSC, is still incomplete. Specifically it remains unclear, whether and how the stripes are related to superconductivity. At present the formation of the striped phase is mostly thought to arise from antiferromagnetic fluctuations which also act to drive the hole pairing through a d -wave order parameter. The two new independent experimental findings of: (i) a correlation of hole doping with phonon anomalies; and (ii) a huge isotope effect on the stripe formation temperature T^* , question the role of antiferromagnetic fluctuations as driving mechanism, and certainly suggest strongly that electron-phonon interaction induced effects have to be incorporated in any model for HTSC.

In the following it will be shown that the striped phase can be related to charge ordering stemming from strong electron-phonon interactions reminiscent of polaron or Jahn-Teller polaron formation, but extended to account for nonlinear effects. In order to simplify the complex dynamics of the copper oxides we concentrate on the CuO_2 planes only and model them by a two-dimensional nonlinear electron-phonon interaction Hamiltonian. This Hamiltonian can be diagonalized with respect to electronic and phononic degrees of freedom where both subsystems, electrons and phonons, experience strong renormalizations. Even though similar approaches have been used previously, the present model is extended here to account for nonlinear effects (proportional to λ_4 in Eq.(1) below) by using higher order density-density multiphonon interactions and combining them with linear onsite, proportional to λ_1 , and intersite, with strength λ_2 , electron-phonon couplings:

$$\begin{aligned}
 & -\lambda_1 \sum_j u_j^{(1)} n_j - \lambda_2 \sum_j \left(u_{j+1}^{(2)} - u_{j-1}^{(2)} \right) n_j + \\
 & + \lambda_4 \sum_j \left[u_j^{(1)} n_j \left\{ 3u_j^{(1)} n_j - 2 \left(u_j^{(1)} \right)^2 - 4n_{j\uparrow} n_{j\downarrow} \right\} \right] \quad (1)
 \end{aligned}$$

Here $u^{(1)}$, $u^{(2)}$ are the displacement coordinates of the oxygen, copper ion, respectively, in the j 'th unit cell with $j=1 \dots N$. The p electron density at site j is given by $n_j = c_j^\dagger c_j$. In our approach the electron-phonon coupling to the oxygen p -electrons is onsite and included since this is known to be the dominant term in transition metal oxides. A phonon mediated p - d charge transfer is possible through the intersite coupling term proportional to λ_2 . The higher order density-density multiphonon terms stabilize the $2p^6$ configuration of O^{2-} . The exact nonlinear solutions for the lattice frequencies and displacement coordinates have been described previously where a two mode model was used. In order to obtain the electron-phonon and doping induced effects on the electronic structure, we relate the ratio of λ_1 / λ_4 to doping, i.e., the strength of harmonic coupling to the density-density multiphonon terms simulates the effects of doping which increases the local instability of the oxygen ion. The electronic energies are renormalized through the electron-phonon coupling as:

$$E_{k,q}^2 = \varepsilon(k, k-q)^2 + \Delta^2(q),$$

where $\varepsilon(k, k-q)$ is the band energy and

$$\begin{aligned}
 \Delta^2(q) = \pi \varepsilon_F \left[\sqrt{\lambda_2^2 \omega_q u_q^{(2)} + \sqrt{\lambda_1} \omega_q u_q^{(1)}} \cdot \right. \\
 \left. \cdot \left\{ 1 + \sqrt{\frac{\lambda_4}{\lambda_1}} \left[w_q u_q^{(1)} + w_q^2 \left(u_q^{(1)} \right)^2 \right] \right\} \right], \quad (2)
 \end{aligned}$$

where the ω_q , u_q , respectively, are the momentum q -dependent lattice frequencies and displacement coordinates obtained from solving the nonlinear equations of motion of the coupled system. The Fourier transform of Eq.(2) describes the real space charge modulations caused by strong electron-phonon coupling.

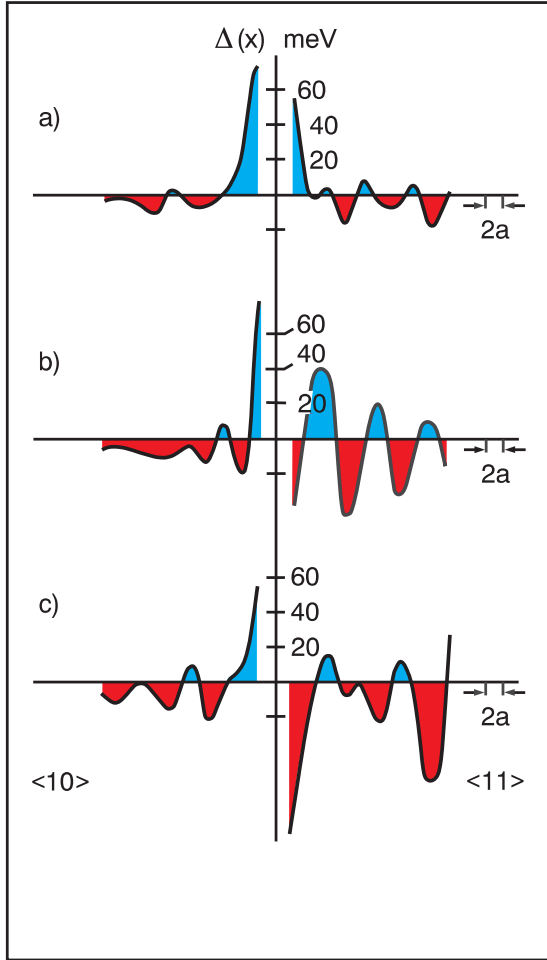


Figure 1: Real space variations of the electron-phonon interaction induced gap with $\lambda_1/\lambda_4 = 0.138$ a), $=0.276$ b), $=0.413$ c) along $\langle 10 \rangle$ and $\langle 11 \rangle$ direction with lattice constant a .

The results are shown in Fig. 1 for various ratios of λ_1/λ_4 . For small values of this ratio (Fig. 1a) modulations in the charge distribution already show up along $\langle 10 \rangle$ and $\langle 11 \rangle$. For larger values of the ratio a striped phase clearly appears along $\langle 11 \rangle$ and changes periodicity with increasing λ_1/λ_4 with additional features growing in the $\langle 10 \rangle$ direction. It is important to note that the dynamical ionic displacements are inserted in Eq.(2) and directly cause the excitation spectrum described above. This strong correlation between ionic and electronic degrees of freedom is clearly reminiscent of polaron formation.

In order to correlate the above features with the experimental data we first replace the ^{16}O oxygen ion mass by its ^{18}O isotope and carry out the same self-consistent iteration scheme to solve for frequencies and displacement coordi-

ates to determine Δ and its real space equivalent. The results are shown in Fig. 2 for the same parameters as those used in Fig. 1. It is evident from Fig. 2 that even for small ratios of λ_1/λ_4 charge ordering is present and persists also at higher values but with a different periodicity. It is especially striking that the amplitude of the charge modulation is much more enhanced as compared to Fig. 1.

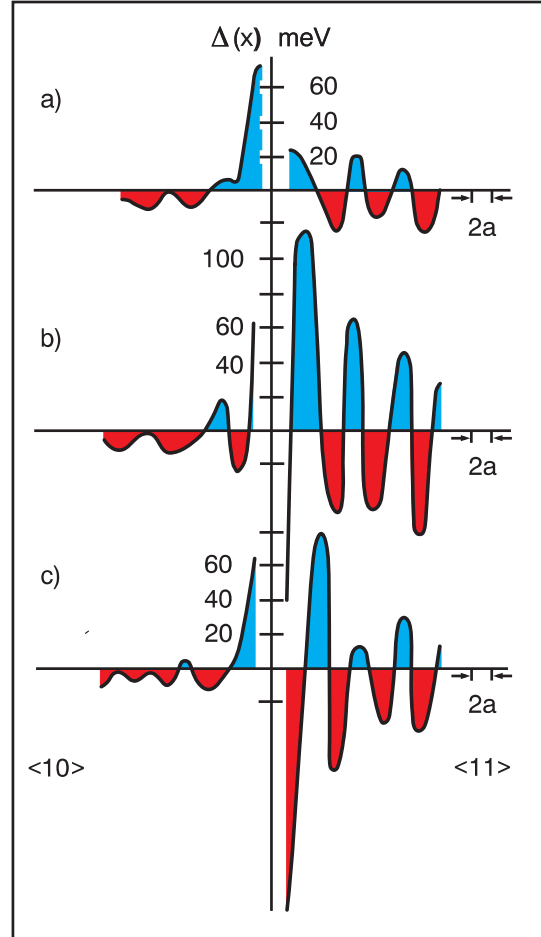


Figure 2: Real space variations of the electron-phonon interaction induced gap with $\lambda_1/\lambda_4 = 0.138$ a), $=0.276$ b), $=0.413$ c) along $\langle 10 \rangle$ and $\langle 11 \rangle$ direction with lattice constant a . The oxygen ion mass is enhanced by a factor $18/16$ as compared to Fig. 1.

The stripe formation temperature T^* can be related to the electron-phonon interaction induced gap:

$$k_B T^* = 2.28 \epsilon_F \exp(-2b)$$

$$\text{with } 2b = \int_0^{\epsilon_F} dx \tanh \frac{1/2\beta F}{F} + \ln 2 + O\left(\frac{\Delta^2}{\epsilon_F^2}\right)$$

$$\text{and } F = \sqrt{x^2 + \Delta^2}$$

The gap varies strongly in real space, but we provide an estimate for the effect on T^* by comparing the average gap value Δ for the same parameters calculated for ^{16}O with those found in ^{18}O . T^* and $2b$ can then be evaluated self-consistently for fixed ϵ_F and representative results are given in Tab. 1.

From e.g., Figs. 1 b), 2 b) an enhancement in Δ by at least a factor of 3 is observed which leads to an enhancement factor of T^* of 1.41. Even though this is less than observed experimentally our result provides the correct trend. It is important to note here that the experimental observation of the isotope effect is limited by three factors which have to be present simultaneously. (i) The time scale of the experiment has to be faster than 10^{-14} s in order to capture the additional ionic dynamics; (ii) the length scale must be local, i. e., of the order of a few lattice constants in order to reproduce the local spatial variations in the charge distribution and the ionic displacements; (iii) the spatial experimental resolution must be better than 10^{-9} cm, since this is the scale of the ionic displacements contributing to the stripe formation. Correspondingly the experimental detection of an isotope effect on T^* will be limited to very few methods.

Table 1. *Dependence of T^* and $2b$ on the electron-phonon interaction induced average gap Δ .*

Δ [meV]	$2b$	T^* [K]
20	0.588	110.2
40	0.36	138.4
60	0.247	155.03
80	0.186	164.7

To summarize, it has been shown that stripe formation with charge ordering follows from strong nonlinear electron-phonon effects which lead to strong modulations in the phonon induced gap in the electronic degrees of freedom. The isotope effect on T^* is a natural consequence of these effects. Yet it should be kept in mind that the time and length scales of these effects are restricted and consequently limit their experimental detectability.

Q-dependent anomalies in the phonons are expected at an incommensurate wave vector, and a variation of these anomalies with doping is expected. Even though our model oversimplifies the dynamics of HTSC, it yields qualitative agreement with striking new experimental data.