Breathers in cuprate-like lattices

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Abstract

All high-T_c superconductors have a layered structure, but the importance of this remains unclear. Some of these layers have chains of atoms with a local symmetry, which facilitates quasi-one-dimensional effects. We describe numerical simulations which suggest that lattice nonlinearities allow the transport of strongly localized and robust packets of vibrational energy (discrete breathers) along these chains. The results support previous studies which correlated these particular structural properties with superconductivity in these cuprates.

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1 Introduction

It has been reported that single layers of cuprate superconducting material, can have a T_c similar to that of the bulk material [6]. This suggests that the underlying pair-bonding mechanism in high-T_c superconductors can be active in a 2D plane of the crystal. In addition, other studies support the idea that the lattice structural and dynamic properties play a critical role in the mechanisms for superconductivity. For example, ref. [7] shows how induced stresses in the lattice at the microscopic level can dramatically change T_c.

Our special interest is in the quasi-one-dimensional anharmonic lattice excitations that can propagate in some atomic planes of theseYBCO-like materials. This was motivated by a previous study [17], where the superconducting properties of cuprates were correlated to the existence of linear chains of atoms, which were conjectured to transport one-dimensional nonlinear waves. Our results provide a realization of these waves in the form of *mobile discrete breathers*, which we have already established in the hexagonal lattice case [13].

The planes of interest here relate to a square lattice that contain linear chains of atoms for which the surrounding lattice has C_2 symmetry, *i.e.* rotations of 180° around the line of the chain leave the lattice unchanged. As a result, a displacement of an atom along the chain direction causes a restoring force

purely in the reverse direction, with no net transverse force. Crystals with a more general C_n symmetry will of course show this same effect. It should be noted that typical doping levels in these superconducting materials does not destroy such C_2 chains [10]. We report here that anharmonic lattice excitations, in the form of highly localized moving breathers, can propagate along the C_2 chains of the flat CuO_2 planes embedded in a 3D structure. Such breathers have been shown to be robust against lateral in-plane spreading. Rough estimates predict that the energies of such breathers can extend from about 0.01 eV to more than 0.5 eV, which is well above the single-phonon energy.

The search for moving breathers in higher dimensional lattices was first motivated by studies on mica minerals. Indirect experimental studies of lattice excitations caused by atomic scattering events in mica suggested that mobile, but very localized, lattice vibrations propagated in C_2 chain directions of this crystal [15]. These conjectured mobile excitations, called "quodons" to reflect their quasi-one-dimensional behavior, appeared to be extremely robust against progressive lateral spreading to adjacent C_2 chains. This lateral stability is the more remarkable because, if the theory is correct, the effect must persist to temperatures of about 600K. This contrasts with the expected rapid degeneration of Toda-like solitons in quasi-2D systems [16]. Some numerical and magneto-mechanical analogue studies of these C_2 chains in terms of 1D moving breathers showed that the concept of a breather was the most promising explanation for the observations [14].

2 Moving breathers

It is well known that some non-linear discrete one-dimensional systems can support localized excitations such as solitons [11] and discrete breathers [1]. A breather is normally contained within a bell-shaped envelope, but unlike a soliton it has internal oscillations. Breathers are generic in lattices, their long lifetime being due to a combined effect of discreteness and nonlinearity [8]. The nonlinearity is responsible for shifting the frequency of such oscillations out of resonance with the phonon bands, while the discreteness ensures the existence of gaps and cut-offs in the frequency range of phonons (which is not the case in continuum-approximation models). The recent experimental observation of breathers in real materials reported in [2] supports these theoretical studies.

Both moving and stationary breathers are possible. Stationary breathers are *exact* solutions of the lattice dynamics, and they are linearly stable in most cases. This is irrespective of the (non-) integrability of the system, just as in the case of lattice solitons [9]. In contrast, moving breathers have a "fast" internal oscillation moving at a phase velocity that exceeds the group velocity of the envelope (the motion of this envelope is slightly slower than the sound velocity). Although the non-integrability of the models suggests that these localized waves are not exact solutions, computer simulations show that they are extremely long-lived. However, up to now they have mainly been studied in 1D systems [12].

We have explored the possibility of creating moving breathers in a fully 2D lattice. Their existence in 2D or 3D lattices posed the problem of preserving the additional localization in the directions transverse to the propagation direction. Radiation to the adjacent chains of atoms is, in principle, to be expected. Nevertheless, we recently found that moving breathers can exist in hexagonal 2D lattices, and showed that they show a remarkable transverse focusing effect [13].

It was natural then to enquire if this behavior was restricted to hexagonal systems. In particular, it was interesting to investigate other 2D structures with a square lattice having both C_2 and non-C_2 crystal chains, in order to test the hypothesis that longitudinal moving breathers need this kind of symmetry. Work done by one of the authors (FMR, [17]) pointed to the high-T_c superconductor layered materials as good candidates for study. It was shown, by molecular mechanical methods, that C_2 chains exist in the flat cuprate layers of $YBa_2Cu_3O_7$, $Y_2Ba_4Cu_6O_{13}$ and La_2CuO_4. In the light of current attempts at understanding the role that the lattice properties play in superconductivity [6, 7, 3], our interest is more than justified.

3 The model for cuprates

Figure 1 shows the 2D copper-oxide layer of a typical YBCO compound that we used for our simulations. As before, we chose to model the system by means of *lattice dynamics* (LD). We use pair potentials between the atoms of the plane, and simulate the 3D environment of the crystal via a layer of fixed atoms sitting above (and below) the plane. The Hamiltonian of the system can be written as

$$H = \sum_{ij,l} \left[\frac{1}{2} m_l \dot{\vec{x}}^2_{ij,l} + V_l(\vec{x}_{ij,l}) + \frac{1}{2} \sum_{<i'j',l'>} W_{ll'}(\vec{x}_{ij,l}, \vec{x}_{i'j',l'}) \right], \qquad (1)$$

where $\vec{x}_{ij,l}$ is the 2D vector for the displacement of the atom l in unit cell (i, j), $W_{ll'}$ represents the various inter-atomic pair potentials, and V_l is the on-site potential generated by the fixed atoms above and below. In our particular case this on-site potential, which has to mimic the presence of the structure in which the CuO_2 plane is embedded, was constructed using the actual positions of atoms in the neighbouring layers of the YBCO structure.

We have made a major simplification by ignoring the motion of atoms in the adjacent planes. If the other planes were rigid, this would already be a good approximation, since the forces due to atoms in adjacent planes would be modeled by the on-site potentials. However, we know that the atoms in the other planes are not fixed, so it may be that in a full 3D model the energy of the breather is radiated in the third dimension. A counter-argument is that in many cases, in a full 2D model, the breather shows a strong self-focussing effect in one dimension, with the atoms in the adjacent chains exhibiting an oscillatory motion with no nett perpendicular transport of energy. Our hypothesis is that this effect extends to 3D in some lattices. There is supporting experimental evidence for this. It is reported that, in silicon, breathers (quodons) can propagate

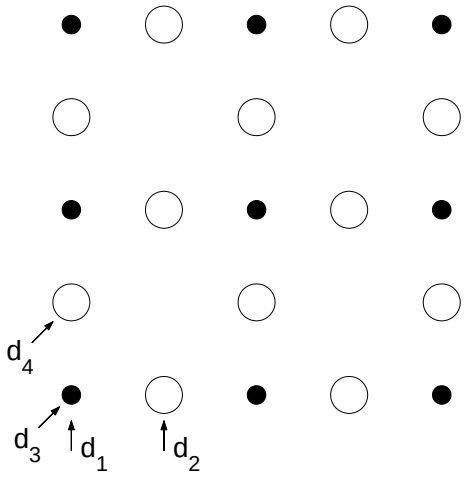

Figure 1: Schematic figure of the CuO_2 plane of atoms in some high-T_c materials. This was the structure used in the simulations, with corresponding fcc layers of fixed atoms sitting symmetrically above and below.

in certain C_2 directions with flat paths of order 1μ [23]. We plan to make some full 3D simulations of cuprate materials in the near future.

We experimented with both Lennard-Jones ($(a/r)^{12} - 2(a/r)^6$) or Morse ($\frac{1}{2}\left(1 - e^{-(r-a)}\right)^2$) potentials, both for the inter-atomic and the on-site interactions. They provide a good approximation to realistic potentials once we neglect long-range Coulombic interactions. We included interactions to nearest and next-nearest neighbours.

We have assumed that the forces between the atoms can be approximated by radial forces, thus neglecting angular (i.e. "three-body") forces. One reason for this is of course to avoid the necessity of engaging in a full MD time-dependent simulation. Once the results with the simpler lattice model are more fully understood, a more accurate calculation will be appropriate. However the effects we observe suggest that the key point is the C_2 symmetry discussed above, and the fact that for small deviations from movement *along* the crystalographic directions, the transverse forces are small. Molecular-mechanics studies of the potential energy surfaces on the relaxed structures of HTSC structures [17] suggest that a full model will also have these key features.

We should stress however, that we do not require the initial disturbance to be in line with a crystalographic direction. Simulations show that breathers travelling along the crystalographic direction can be excited by perturbations at quite a large angle ($\approx 15^\circ$) to the eventual line.

To ensure that the 2D scheme is internally consistent, we made some simplifications. The pair potentials used between atoms have to match the bond-lengths that we have chosen as the reference lattice. This means that both the

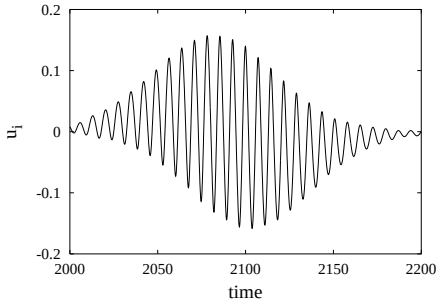

Figure 2: Atomic displacement along the $\mathbf{d_3}$ direction. Units are in fractions of the unit cell length. The asymmetry of the envelope, an oscillation of the "dc" component of the vibrations, is due to the usual bond-stretching phenomenon of soft nonlinear potentials.

inter-atomic and the on-site potentials will have their bond lengths adapted, so that when the atoms are at their reference positions, each bond is in their own relaxed state. Their relative strengths can still be varied, via a prefactor in the potential, without changing the bond length. This is not a big simplification, since one can think of these modified pair potentials as "effective" interactions, where the rest of the contributions to the potential landscape have been integrated. Our lattice dynamics schema provides a good approximation to the problem at hand. Moreover, it has been shown that discrete breathers are a very generic phenomenon, insensitive to the details of the potentials involved [8].

Our simulations confirmed that moving breathers can exist in this system, propagating in some chain directions and being robust against lateral spreading for a wide range of initial starting conditions. Such breathers are somewhat insensitive to the relative strengths of the inter-particle to on-site terms in the system Hamiltonian. As expected from the pair-wise, radial nature of the potentials used, these are *longitudinal* breathers, where the atoms oscillate along the line of propagation, in a nearly out-of-phase motion. They travel over long distances in the lattice, with very weak coupling (radiation) to the phonons. Figure 2 shows the displacement of a typical atom in the C_2 chain as a function of time as the breather passes through. One common feature of all these breathers is that the internal, "fast" vibration has a frequency which is outside the phonon bands of the system (also true for higher harmonics), while the translational velocity is below that of linear sound waves by 20%–60%.

In our model we created moving breathers by giving initial momenta to three consecutive atoms along a chain, for example, in ratios $(-1, 2, -1)$. Over a wide energy range, initial impulses of this type yielded stable moving breathers, after the initial transient (where some percentage of the initial energy is quickly radiated throughout the lattice). We found that breathers could be propagated along directions $\mathbf{d_1}$,$\mathbf{d_2}$, and $\mathbf{d_3}$ (see figure), all of which have C_2 symmetry.

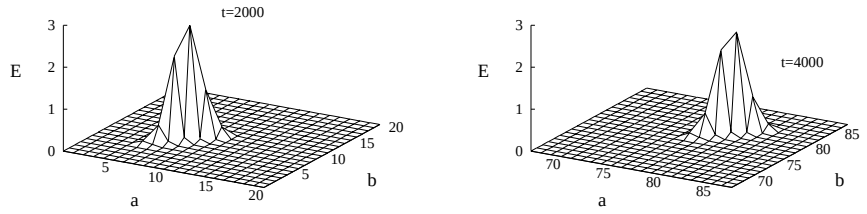

Figure 3: A breather travelling along the $\mathbf{d_3}$ direction (see Fig. 1).

However, direction $\mathbf{d_4}$ does not have this symmetry, and our simulations with the same initial conditions in this direction revealed no sign of breathers.

In fig. 3 we show a typical simulation of a breather envelope, in this case along direction $\mathbf{d_3}$. In this figure, E is the energy of the breather in arbitrary units, and only a (different) part of the lattice has been shown in each case. In between the two snapshots, the excitation has travelled about 100 lattice cells, losing only some 10% of the energy, but remaining as an exponentially localised excitation. Moving breathers in general *are not* expected to be infinitely lived, due to the non-integrability of these lattice models. We find that 2D moving breathers, like their 1D counterparts, exhibit remarkably long lifetimes.

The real energy of such breathers can be estimated by comparing (a) the displacements of atoms from the equilibrium positions during the passage of the breather in a simulation with (b) the unrelaxed lattice defect-energies resulting from displacement of a given atom in an initially energy minimised lattice. The calculation for (b) comes from independent molecular mechanics studies. For La_2CuO_4 an approximate lower limit of 0.01 eV was found for the energy of robust moving breathers, extending upwards to about 0.5 eV.

4 Discussion

Our aim is to explore and better understand the properies of the peculiar layered structure of YBCO-like superconductors. This includes the possibility of interactions of free charges with moving breathers. The present study was motivated by the correlation found in these materials between the high-T_c superconducting property and the existence of C_2 chains [17]. These do not need to be necessarily the C_2 chains of the CuO_2 plane that we studied. Certainly, many materials in the YBCO family contain different chains with C_2 symmetry in other parts of the crystal, such as in layers containing Y or Ca [17]. We have focused on the cuprate layer because this is where the superconductivity is thought to take place.

Some other layered superconducting materials do not have CuO_2 layers. If

breathers are still involved in mediating charge transport in such materials, then the existence of C_n chains elsewhere in the crystal should be a prerequisite for high T_c superconductivity. Such a correlation has been reported for the structurally related family of compounds containing Ni and B [17].

There is some evidence that breathers might interact with free charges on or near the C_2 chains [3]. We are currently studying the interaction between breathers and free charges as a possible coupling mechanism in superconductivity [20, 21, 22].

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