Van Hove Exciton-Cageons and High-Tc Superconductivity: VIIID
Solitons and Nonlinear Dynamics

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The low-temperature orthorhombic (LTO) phase transition in La$_{2-x}$Sr$_x$CuO$_4$ can be interpreted as a dynamic Jahn-Teller effect, in which the degenerate electronic states are associated with the large densities of states at the two van Hove singularities. The equations describing this phase are strongly nonlinear. This paper illustrates some consequences of the nonlinearity, by presenting a rich variety of exact nonlinear wave solutions for the model.

Of particular interest are soliton lattice solutions: arrays of domain walls separating regions of local low-temperature tetragonal (LTT) symmetry. These arrays have a macroscopic average symmetry higher than LTT. These lattices can display either orthorhombic (‘orthons’) or tetragonal (‘tetrons’) symmetry, and can serve as models for a microscopic description of the dynamic JT LTO and high-temperature tetragonal phases, respectively.

1. Introduction

The two-dimensional van Hove singularity (vHs) was initially introduced as a model[1] to study competition between superconductivity and structural instability. Its possible relevance to high-Tc superconductivity was pointed out by Hirsch and Scalapino[2], who showed that, because of the logarithmically diverging density of states (dos), the form of the BCS equation is modified in a vHs superconductor, leading to much higher values of $T_c$. When the high-Tc superconductors La$_{2-x}$Ba$_x$CuO$_4$ (LBCO) and La$_{2-x}$Sr$_x$CuO$_4$ (LSCO) were first discovered, it was noted that their Fermi surface falls close to a vHs, and it was proposed that the vHs might be responsible for both the high $T_c$ values, as well as the structural transition from the high-temperature tetragonal (HTT) phase to the low-temperature orthorhombic (LTO) phase[3].

However, the LTO phase was found not to split the degeneracy of the two vHs[4], and moreover did not have a large effect on the electronic properties of LSCO, so it was concluded that the LTO transition had nothing to do with the vHs. Now the absence of a structural transition does not rule out a role for the vHs in promoting superconductivity. Indeed, the $T_c$ enhancement depends mainly on the dos peak – i.e., on the $q = 0$ charge susceptibility, and not the inter-vHs $q = 2k_F$ susceptibility[5]. However, Phillips has shown[6] that a simple vHs model cannot explain many details of, e.g., the doping dependence of $T_c$. Most of these problems could be overcome if the vHs also produced short-range structural disorder[7], but, according to Phillips, “there is no experimental evidence which would indicate any relation between the major lattice instabilities” and the vHs[6].

In fact, such evidence is starting to accumulate. First, there is a second structural phase transition in LBCO, this time to a low-temperature tetragonal (LTT) phase[8], which does have a large impact on electronic properties and essentially destroys superconductivity. Moreover, the transition is optimized at a fixed concentration of holes[9], and has the correct symmetry to split the vHs degeneracy[10]. Secondly, a careful reexamination of the LTO-HTT phase boundary has showed that superconductivity is clearly associated with the LTO phase[11]. Finally, it was recently proposed[12-14] that the LTO phase transition is indeed driven by the vHs, but the LTO phase is dynamic, and the average macroscopic symmetry is not representative of the local microscopic state.

This new model describes the structural phase transitions in terms of the interplay between the two electronic saddle points (vHs’s) and the optical phonons associated with tilting modes of the oxygen octahedra, with subsidiary roles played by shear strains and acoustic phonons. The LTT phase involves an essentially static band Jahn-Teller (JT) effect[13], in which the two vHs’s play the role of the degenerate electronic states. As the temperature is raised, there are large fluctuation effects, and the LTO and HTT phases can be described as dynamic and disordered JT phases, respectively[14].
The model Hamiltonian is an extension of the Labbé-Friedel model for the A15 compounds\cite{15,16}. It contains significant nonlinearities; the purpose of the present manuscript is to explicitly display some of these nonlinear features. Analysis of these nonlinear waves should prove useful in understanding the short-range order present in LBCO above the LTT transition, and as fluctuations in other high-\(T_c\) cuprates\cite{17}, and in understanding the role of anharmonicity in enhancing \(T_c\). The present paper introduces a concrete microscopic model which displays the properties postulated for the dynamic JT phase.

Many of the anomalous features are shared by a larger class of materials, the ferroelastics\cite{18}. In addition to the high-\(T_c\) cuprates, this class includes a number of related perovskite compounds and ferroelectrics, including SrTiO\(_3\), and BaTiO\(_3\), and the martensitic phases of the A15’s. Ferroelasticity is in general suggestive of collective dynamic JT effects, with strong electron-phonon coupling. Hence, the present model can be applied to transitions within this larger class of materials. Indeed, the model allows significant electron-phonon coupling even for a filled band, if the Fermi level falls in a gap between two hybridized bands\cite{13}.

The paper is organized as follows. Section 2 shows that corner-sharing of octahedra greatly restricts the possible low-lying states of the lattice, and requires the introduction of defects (solitons) to expand the variety of configurations. A possible model for domain-wall solitons is introduced, and it is shown how this state can provide a microscopic picture for the dynamic JT state of LSCO. In Section 3, the combined electron-phonon equations of motion are introduced, and reduced to a form which is convenient for analyzing the nonlinear wave solutions, both for waves propagating along 100 (\(x\) or \(y\) axes) or 110 (at 45°) directions. Section 4 illustrates the variety of possible wave solutions, both dynamic and static. The low energy waves include both phason-like modes (weak, periodic modulation of the axis of tilt) and soliton-like solutions. These latter can be either isolated domain walls between LTT domains, or arrays of solitons, which display an average macroscopic symmetry which is greater than the true microscopic (LTT) symmetry. The macroscopic symmetry can be either orthorhombic (the corresponding waves are called ‘orthons’) or tetragonal (‘tetrons’). In Section 5, these results are applied to LSCO. The material parameters are estimated, and the energies of the resulting solitons are calculated. Soliton array solutions are predicted to arise for 100-type waves, including static arrays. The energy of individual domain walls is calculated, and compared to microscopic calculations (Appendix II). The relation of the various types of soliton arrays (tetron, orthon, isolated domain walls) and the observed phase transitions (HTT \(\rightarrow\) LTO \(\rightarrow\) LTT) in LSCO/LBCO is discussed. In Section 6, it is suggested that the solitons may be charged, and hence related to domain wall phases postulated earlier in doped LSCO. Finally, Section 7 summarizes the conclusions of this work.

2. Model of Solitons

The essential feature of the dynamic JT effect is that the global symmetry is not indicative of the local symmetry. Such a situation is found in other materials, in particular in the several phase transitions of BaTiO\(_3\)\cite{19}. In the high temperature phases of BaTiO\(_3\), the sample is composed of microscopic domains of the low temperature (distorted) phase, but with different polarization axes in each domain. As the temperature is raised, the axes point successively over two, four, or all eight possible orientations, so that the sample as a whole appears to have higher and higher symmetry. These domains have been directly observed via streaking in electron diffraction patterns\cite{20}, and similar streaking has been observed in high-\(T_c\) compounds\cite{21}.

The tilting in these materials has often been described at the mean-field level in terms of a pseudospin or Potts model, replacing the allowed tilts with equivalent spin states. A closely related mean-field treatment was applied to LSCO in Ref. [14]. A shortcoming of this procedure is that it overlooks the problems associated with corner or edge sharing of octahedra\cite{22}. This corner sharing leads to a long-range interaction between tilts, and requires the introduction of macroscopic defects (solitons as domain walls) to break up the resulting LTT-type order.

Let us illustrate this effect in LSCO. Consider a single octahedron, tilted about the \(x\)-axis (as in the LTT ground state). Since neighboring octahedra are corner-sharing, its nearest neighbors along the \(y\)-axis must be counter-tilted about the \(x\)-axis (again, as in the LTT phase). By induction, the whole row must be similarly tilted, in the absence of some form of excitation – either an anti-tilt along \(x\) or a crossover to a tilt about \(y\). Similarly, if the entire row is tilted about \(x\), the next row along the \(x\)-axis cannot be tilted about the \(y\)-axis, without tipping an oxygen which is shared with the original row. Hence, the second row
would also be tilted about the x-axis. By induction, every row would be tilted about the x-axis. Hence, in
the absence of defects, the ground state would have a quasi-LTT pattern. To lowest order, there is only a
weak interaction between the tilt direction on adjacent rows, so the low energy physics would (in the absence of
defects) be that of rows of x-tilted octahedra, with two possible states for each row (e.g., any particular
cubehedron could have either a + or – tilt about x, which would fix the tilts of all other octahedra on that
row). Hence, this physics would be in the universality class of the one-dimensional Ising model.

Such one-dimensional chains have very low entropy; for an \( N \times N \) array of atoms there are \( N^2 \) atoms,
but only \( N \) chains, each of which has only two possible orientations, for a total of \( 2^N \) configurations. To
increase the entropy significantly, it is necessary to introduce macroscopic defects into the system. For
instance, it would be preferable to have domains in half of which the tilts lie along the \( y \)-axis, in the other
half along the \( x \)-axis. These domains of LTT-like phase must be separated by domain walls (solitons).
The purpose of the present manuscript is to use the nonlinear equations of the system to develop a model for
these domain walls. If the wells are deep, the domain walls are likely to be narrow – perhaps a single cell
in width. If the wells are shallow (or at high temperatures) the walls can be broad as the octahedral tilt
changes gradually. The average cell size will be given by the balance between surface tension and entropy.

Figure 1 suggests a possible (narrow wall) soliton model of the LTO phase. The circles in Fig. 1
represent the apical oxygens above the \( \text{CuO}_2 \) plane, which would be centered immediately above the Cu
in the undistorted HTT phase. The arrows illustrate the instantaneous local distortion of the apical oxygen’s
position in the tilted state. The figure illustrates two-LTT-like domains, separated by a dynamic domain
wall, with rotating tilt direction, for motion either along a (110) direction (Fig. 1a) or along a (100) direction
(Fig. 1b). In the (110) wave, the domains are composed of diagonal stripes, alternating in tilt along the x-
and \( y \)-axes. The line of atoms along the domain boundary cannot, because of corner sharing, be in a pure
LTT tilt, but will assume a (dynamic) average tilt, as illustrated by the arcs of circles. If the octahedra
within each cell have pure LTT tilts, the structure in the figure would not directly produce any LTO strain,
\( \epsilon_{xy} \). However, there is a pronounced asymmetry to the tilts along directions parallel and perpendicular to the
domain boundaries. Within each row parallel to the boundary, the tilt is uniquely either up or down, so that
the entire domain can readily assume the corrugated pattern characteristic of the LTO phase (i.e., strong
\( \Psi \) coupling to a \( \epsilon_{xy} \) strain. On the other hand, in the perpendicular direction, the up and down tilted rows
are interchanged each time a soliton wall is crossed, making it impossible to generate a global corrugation in
this direction. Moreover, the octahedra comprising the soliton already lead to a net shear strain in the easy
direction.

Thus, the proposed configuration (1) has domains of local LTT symmetry, (2) arranged in such a
pattern as to readily couple to a corrugating shear along a preferred easy axis, to give a \( \text{macroscopic} \) LTO
symmetry. Finally, (3) the domain walls already provide the appropriate shear strain, so that \( \epsilon_{xy} \) should be
approximately proportional to the density of solitons.

It is very often convenient, in dealing with structural phase transitions, to think in terms of pseudospins,
since the magnetic analogs are generally much better developed. Within such a pseudospin model, the solitons
have a very natural interpretation: the two kinds of domain correspond to \( S_z > 0 \) and \( S_z < 0 \), while the
soliton is simply a Néel wall, with \( S_x \neq 0 \) inside the wall.

3. Real-Space Hamiltonian: Intracell and Intercell Coupling

3a. Tilt Equation of Motion

In the present paper, the Hamiltonian will be a simplified form of that introduced in Ref. [14] (Eq.
25 of that paper). The coupling to strains and umklapp electron scattering were found to be relatively
unimportant, and hence will be neglected. Furthermore, it will be assumed that the octahedra are all tilted,
but in random directions, so the pseudorotation operators have the form \( R_1 = R \cos \phi, R_2 = R \sin \phi \), with \( R \)
constant. The Hamiltonian then becomes

\[
H = \sum_i \left( \frac{1}{2} M \dot{\phi}_i^2 + H_{\text{pl}} \right) + \Gamma_0 \sum_{\eta} \left[ \frac{1}{2} M \dot{\phi}_i^2 + \left( \frac{R_2(\tilde{I} - \eta a \hat{y})}{R_2(\tilde{I} + \eta a \hat{y})} \right)^4 + \left( \frac{R_2(\tilde{I} - \eta a \hat{x})}{R_2(\tilde{I} + \eta a \hat{x})} \right)^4 \right] + \frac{\Gamma_0}{2} \left[ R_1(\tilde{I}) + R_2(\tilde{I}) \right] + \frac{\Gamma_0}{2} \left[ R_1^2(\tilde{I}) + R_2^2(\tilde{I}) \right].
\]  

\[ (1a) \]
convenient to explicitly account for this factor, by defining the antiferrodistortive nature of the transition, the tilts of adjacent cells tend to be opposite in phase. It is where
\[ o^3_{b. (110)} \text{ Waves} \]

where the last term is given by Eq. A4 in Appendix I.

\[ H_{epl} = -\tilde{\alpha} e^2 \sum_{n} \frac{R_1(\tilde{l}) - R_1(\tilde{l} + \eta \hat{y})}{2} - \frac{(R_2(\tilde{l}) - R_2(\tilde{l} + \eta \hat{x})}{2} \right) \right| \right|, \]  

(1b)

where \( \eta \) is summed over \( \pm 1 \). It should be noted that \( R_i \) does \textit{not} have the dimensions of a length[13]; rather

\[ R_i^2 = \frac{3}{2} m_O Z^2, \]

where \( m_O \) is the mass of an oxygen atom and \( Z \) is the displacement of the planar oxygen above/below the CuO\(_2\) plane caused by the pseudorotation \( R_i \). This means that the parameter \( M \) is dimensionless,

\[ M = \frac{4}{3} (1 + \eta_{ap}^2) \approx 3.48, \]

where \( \eta_{ap} \approx 1.27 \) is the ratio of the Cu-apical O distance to the Cu-planar O distance.

In Eq. 1b, \( H_{epl} \) is the electron-phonon coupling term in the \( l \)th cell, and the absolute value arises from the JT effect[14]. This absolute value sign leads to unnecessary complications in the analysis, since the model is only approximate to begin with, so a further approximation is introduced. This approximation essentially amounts to Fourier analyzing the electron-phonon term in \( \cos(4n\phi) \), and retaining only the lowest order terms. This procedure is carried out in Appendix I.

The formulation of Eq. 1 is similar to calculations introduced to describe the anomalous polarizability of \( O^{2-} \) in ferroelectrics[23,24], and the resulting nonlinear waves are also similar to those found in ferroelectrics[25]. The equation of motion corresponding to Eq. 1 then becomes:

\[ \frac{M}{R^2} \ddot{\phi}(\tilde{l}) + \frac{\Gamma_0}{8} \sum_{n} \left[ \cos(\phi(\tilde{l})) \sin(\phi(\tilde{l}) - \sin(\phi(\tilde{l} + \eta \hat{x}))^3 - \sin(\phi(\tilde{l})) \cos(\phi(\tilde{l}) - \cos(\phi(\tilde{l} + \eta \hat{y}))^3) \right] \]

\[ + (2\Gamma^a_0 - \Gamma_2) \sin(\phi(\tilde{l})) \cos(\phi(\tilde{l}) \sin^2(\phi(\tilde{l})) - \cos^2(\phi(\tilde{l})) + \frac{2}{R^2} \frac{\partial H_{epl}}{\partial \phi(\tilde{l})} = 0, \]  

(2)

where the last term is given by Eq. A4 in Appendix I.

\subsection*{3b. \( (110) \text{ Waves} \)}

In studying the nonlinear wave solutions of Eq. 2, it is convenient to look for one-dimensional solutions. The simplest such solutions propagate along the \( x \) or \( y \) axes or at \( 45^\circ \). It is assumed that the background state is of HTT symmetry (i.e., \( \sin \phi = \cos \phi = 0 \) except for the modulation produced by the wave), and that the tilt has the same magnitude for all atoms in any plane perpendicular to the propagation direction, but with neighboring cages tilting in the opposite sense. As suggested by Fig. 1, the most interesting solutions are those propagating at \( 45^\circ \), \( (110) \) waves, which include the LTO-like domain walls, and this case will be analyzed in the present section.

Figure 1 can be used to understand the reduction of the problem to one dimension. For convenience, lines of octahedra parallel to the propagation direction (e.g., A and B in Fig. 1) will be referred to as \textit{columns}, and lines perpendicular to this direction, forming wave fronts, as \textit{rows}. Thus, it can be seen in Fig. 1 that all atoms fall into one of two classes of columns, A or B, and likewise all rows, and that all of the nearest neighbors of an A octahedron are B octahedra. In a one-dimensional, \( 45^\circ \) wave, it will be assumed that all the octahedra within a given row have exactly the same value of \( \phi \), so that the \( \phi(\tilde{l}) \) may be reduced to the one dimensional \( \phi_n \), where \( n \) denotes the successive row in the propagation direction. Because of the antiferrodistortive nature of the transition, the tilts of adjacent cells tend to be opposite in phase. It is convenient to explicitly account for this factor, by defining

\[ \cos(\phi(\tilde{l})) = (-1)^n \cos \phi_n. \]  

(3)

The problem is thus effectively reduced to one-dimensional. For the \( 45^\circ \) waves, Eq. 2a takes the form

\[ \frac{M}{R^2} \phi_n + \frac{\Gamma_0}{8} \sum_{n} \left[ \cos(\phi_n - \sin(\phi_{n+\eta}))^3 - \sin(\phi_n - \cos(\phi_{n+\eta}))^3 \right] - \frac{(2\Gamma^a_0 - \Gamma_2)}{4} \sin 4\phi_n + \frac{2}{R^2} \frac{\partial H_{epl}}{\partial \phi_n} = 0. \]  

(4)
Whereas anharmonic phonons have often been studied as a paradigm for soliton physics, most models assume a diagonal anharmonicity. In contrast, the present model has significant nonlinearity also in the intercell coupling.

Equation 4 has travelling wave solutions of the form:

$$\phi_{n+1}(t + a'/v) = \phi_n(t),$$

(5)

where $a' = a/\sqrt{2}$ is the effective repeat distance, $a$ is the Cu-Cu distance and $v$ is the phase velocity. The continuum limit amounts to expanding

$$\sin\phi_{n\pm 1}(t) = \sin\phi_n(t) \pm \tau \cos\phi_n(t) \dot{\phi}_n(t) + \frac{1}{2} \tau^2 (\cos\phi_n(t) \ddot{\phi}_n(t) - \sin\phi_n(t) \dot{\phi}_n^2(t)),\tag{6}$$

where $\tau = a'/v$, with a similar expansion for $\cos\phi$. Substituting Eq. 6 into Eq. 5 reduces that equation to a single-site form:

$$M \ddot{\phi} - (2\Gamma_0 + 2\Gamma_0 - \Gamma_2) \sin 4\phi + \frac{3\tau^2 \Gamma_0}{8} [\dot{\phi} \sin 4\phi + 2 \ddot{\phi} \sin^2 2\phi] + \Gamma_{ep} [4 \sin 4\phi + \tau^2 (\cos 4\phi - \phi^2 \sin 4\phi)] = 0, \tag{7a}$$

where terms of higher order than $\tau^2$ have been neglected, and the index $n$ has been omitted. The final term of Eq. 7 follows from Eq. A6 of Appendix I, with

$$\Gamma_{ep} = \frac{8 \bar{\alpha} e}{3\pi R^2}.$$ 

(7b)

Equation 7 may be rewritten in dimensionless form by introducing

$$\beta' = \frac{(16\Gamma_{ep} + \Gamma_2 - 2\Gamma_0 - 2\Gamma_0 \bar{R}^2)}{M}, \tag{8a}$$

$$\gamma' = \frac{3\tau^2 \Gamma_0 \bar{R}^2}{32M} = \frac{v_1^2}{4v^2}, \tag{8b}$$

$$\delta' = \frac{\tau^2 \Gamma_{ep} \bar{R}^2}{4M}, \tag{8c}$$

and

$$\alpha = 4\phi, \tag{8d}$$

in which case Eq. 7a becomes

$$\ddot{\alpha} = \frac{(-\beta + \gamma \dot{\alpha}) \sin \alpha}{1 + 4\gamma \cos \alpha}, \tag{9}$$

with $\beta = \beta'/(1 - 4\gamma')$, and $\gamma = (\delta' - \gamma')/(1 - 4\gamma')$. The quantities $\gamma'$ and $\delta'$ are intrinsically positive. In principle, $\beta'$ (Eq. 8a) could be either positive or negative, but will here be taken positive, to stabilize an LTT-like phase (potential minima at $\phi = 0, \pi/2$, etc.). However, $\beta$ in Eq. 9 will be negative when $4\gamma' > 1$ ($v < v_1$), while $\gamma$ may have either sign. When the JT coupling effects dominate over the anharmonicity, then $\delta' > \gamma'$, so $\gamma$ will be positive for fast waves. The velocity $v_1$ is a critical velocity, which separates fast waves ($v > v_1$) from slow waves ($v < v_1$).

3c. (100) Waves

The analysis for (100) waves is very similar to the above analysis for (110) waves. In this Section, a subscript will be added to various symbols to distinguish 100 from 110 waves. Since both waves satisfy the same equation, the symbol will be omitted in subsequent sections, unless it is necessary to distinguish the two types of wave (e.g., in Section 5). Now the wave propagates along the $x$-direction, with rows along $y$. Hence, nearest neighbors along the rows are exactly out of phase,

$$R_1(\vec{l} \pm a\hat{y}) = -R_1(\vec{l}).$$
By a calculation similar to that given above, the \((100)\) wave equation has the same form as Eq. 9, with
the following changes. First, \(\tau_{100} = a/v\), since \(a\) is the distance between rows. Next, since only half of the
neighbors now contribute to the dispersion,

\[ \frac{\gamma'_{100}}{\tau_{100}} = \frac{\gamma'_{110}}{2 \tau_{110}}, \]

with a similar relation for \(\delta'_{100}\). However, since \(a' = a^2/2\), \(\tau_{100}^2 = 2 \tau_{110}^2\), so \(\gamma'_{100} = \gamma'_{110}\) and \(\delta'_{100} = \delta'_{110}\).
Thus, these two corrections compensate. However, there is one last correction, an additional term in \(H_{epn}\),
Eq. A9 in Appendix I. This changes the denominator in the expression for both \(\beta\) and \(\gamma\):

\[ (1 - 4 \gamma') \rightarrow (1 - 4(\gamma' + \delta')). \]

Hence, \((100)\) waves have virtually the same dispersion as \((110)\) waves. Both waves satisfy Eq. 9, with
the only change being the substitution, Eq. 10, for the \((100)\) waves. In Section 5, the significance of this
difference will become apparent. Section 4 analyzes possible solutions of Eq. 9, and hence is applicable to
both types of waves.

4. Nonlinear Wave Solutions

4a. Phase Portraits

A first integral of Eq. 9 can readily be found by setting \(y = \dot{\alpha}\),

\[ \ddot{\alpha} = \ddot{y} = \frac{dy}{d\alpha} \dot{\alpha} = y', \]

so

\[ \int_{y_0}^{y} \frac{ydy}{\gamma y^2 - \beta} = \int_{\alpha_0}^{\alpha} \frac{\sin \alpha d\alpha}{1 + 4 \gamma \cos \alpha}, \]

or

\[ \frac{y^2 - \beta}{y_0^2 - \beta} = \frac{\sqrt{1 + 4 \gamma \cos \alpha_0}}{1 + 4 \gamma \cos \alpha} \equiv F(\alpha), \]

(11)

where \(\alpha_0\) and \(y_0\) are initial values of \(\alpha\) and \(y\) respectively, and \(\beta = \beta/\gamma\). Equation 11 may be reduced to
quadrature:

\[ t = \int_{\alpha_0}^{\alpha} \frac{d\alpha}{\sqrt{F(\alpha)(y_0^2 - \beta) + \beta}}. \]

(12)

This equation must be solved numerically. Equation 11 depends on two parameters \(\hat{\beta}\) and \(\gamma\). In constructing
phase portraits, only \(\gamma > 0\) need be considered, since \(\gamma < 0\) is equivalent to \(\gamma > 0\), but with \(\alpha \rightarrow \alpha + \pi\). The
nature of the phase portraits does change, however, when \(\gamma = \gamma_c = 1/4\). Hence, there are four classes of
phase portrait, corresponding to \(\hat{\beta} >, < 0\), and \(\gamma >, < \gamma_c\). For LSCO, the fast wave solutions are expected
to correspond to \(\beta, \gamma > 0\), and slow waves to \(\beta, \gamma < 0\). The corresponding phase portraits (\(\dot{\alpha}\) vs \(\alpha\)) are
illustrated in Figs. 2 (\(\beta, \gamma > 0\)), 3 (\(\beta < 0, \gamma < 0\)), and 4 (\(\beta < 0, \gamma > 0\)). The lines with filled circles in these
figures are separatrices, dividing regions of qualitatively different kinds of wave behavior. The following
subsections will describe the various kinds of waves which can be generated.

The situation corresponding to Fig. 4 does not appear to arise in LSCO. However, it could occur
under special circumstances, and since the resulting waves are strikingly different (particularly for \(\gamma > \gamma_c\)),
solutions for this case will be discussed in Section 4d.

4b. Fast Wave Solutions

For \(\beta > 0\) and \(0 < \gamma < \gamma_c\), the typical phase space profile (\(\dot{\alpha}\) vs \(\alpha\)) is shown in Fig. 2a. This diagram
periodically repeats outside the range illustrated, \(\alpha \rightarrow \alpha + 2n\pi\), \(n\) integer. The overall nature of the phase
portraits can be understood by noting that, for \(\gamma \rightarrow 0\), Eq. 9 reduces to the equation of a pendulum. Hence,
there will be low energy solutions corresponding to oscillations about a single potential minimum, and higher energy solutions in which the octahedron hops between adjacent minima (the ‘pendulum’ undergoes complete $2\pi$ rotations). The finite values for $\gamma$, due to intercell coupling, lead to all the complications discussed below.

In Fig. 2a, there are two separatrices, the nature of which can best be understood by looking at a series of typical orbits, Fig. 5. These orbits all correspond to the parameters $\beta = \gamma = 0.2$, $\alpha_0 = 0$, with different choices of $y_0 = \dot{\alpha}(t = 0)$. This corresponds to moving up the left hand axis of Fig. 2a. Here and below, the waveforms are found by numerical integration of Eq. 12. For the parameters of Fig. 5, the first separatrix occurs at $y_0 = y_1$, with $0.816 < y_1 < 0.817$. For $y_0 < y_1$, Fig. 2a shows that there are $\alpha$ values which are not sampled (the phase space plot passes through $\dot{\alpha} = 0$). The resulting orbit is consequently a bounded periodic orbit. For $y_0 > y_c$, all values of $\alpha$ are sampled, and, since $\dot{\alpha}$ never vanishes, $\alpha$ increases monotonically.

An analytic formula for $y_1$ can readily be found from Eq. 11. From Fig. 2a, the separatrix has initial conditions $\alpha_0 = 0$, $y_0 = y_1$, and passes through the point $\alpha = \pi$, $y = 0$. Then Eq. 11 may be rearranged to

$$y_1^2 = \hat{\beta}(1 - \frac{1 - 4\gamma}{1 + 4\gamma}),$$

which yields $y_1 = 0.8165$ for $\beta = \gamma = 0.2$. The time to travel from $\alpha = 0$ to $\alpha = \pi$ is

$$t = \frac{1}{\sqrt{\hat{\beta}}} \int_0^{\pi} \left(1 - \frac{1 - 4\gamma}{1 + 4\gamma \cos \alpha}\right)^{-1/2} d\alpha.$$ (13b)

When $\alpha = \pi - \alpha'$ with $\alpha' << 1$, the integrand is $\sim 1/\alpha'$. Thus, the integral diverges logarithmically: the separatrix is a ‘single kink’ soliton, varying once from $-\pi$ to $+\pi$ as $t$ varies from $-\infty$ to $+\infty$.

The second separatrix corresponds to $y_0 = y_2 = \sqrt{\hat{\beta}}$. From Eq. 9, it can be seen that $\ddot{\alpha} = 0$ when $y_0 = y_2$. Hence, $\dot{\alpha} = y_2$ remains constant, and $\alpha$ increases linearly with time. For $y_0 > y_2$, $\alpha$ again increases monotonically with time. However, now $\dot{\alpha}$ is larger near $\alpha = (2n + 1)\pi$, than near $0$, $2n\pi$, so $\alpha$ tends to linger near the potential minima (lower slope near $2n\pi$). In contrast, for $y_0 < 1$, the orbit tends to avoid the potential minima. The extreme case is for the separatrix $y_0 = y_1$, where the orbit is a single kink, Eq. 13. These high-$\alpha$ solutions are not of much interest, since they also correspond to high energies; the low energy solutions are those which spend most of their time near the potential minima.

Figure 6 shows a number of different periodic orbits, for $y_0 < y_1$. The low energy waves are the small amplitude, nearly sinusoidal waves which remain close to $\alpha = 0$. These correspond to waves in an LTT-type phase: the octahedra are all tilted in nearly the same x-direction ($\phi = \alpha/4 \simeq 0$, but the tilt axis wanders back and forth as the wave progresses. As the amplitude increases, the waves become increasingly nonsinusoidal, tending to spend more time near the potential maxima $\alpha = \pm \pi$. These are not of importance, being high energy waves, but qualitatively similar slow waves are of great interest, and are discussed further in Section 4c.

4c. Slow Waves: Soliton Lattices in the ‘LTO Phase’

When $v$ becomes less than $v_1$, the signs of both $\beta$ and $\gamma$ change. This sign change is completely compensated for by shifting $\alpha \rightarrow \alpha + \pi$, as can be seen by comparing Figs. 2 and 4. Thus, the periodic orbits of Fig. 6 can be interpreted as fast wave solutions, using the left hand axis, or equivalently as slow wave solutions (with $\beta$, $\gamma$ of same magnitude but opposite sign), using the right hand axis. This simple switch has a profound effect on the nature of the low energy solutions. Now the small amplitude waves are high energy waves, corresponding to small oscillations about the unstable energy maximum $\phi = \pi/4$.

On the other hand, the large amplitude waves are now low energy solutions, because they spend most of their time near potential minima at $\phi = 0$ or $\pi/2$. These are soliton lattice solutions, and a particular solution is displayed in Fig. 7. Corresponding to the periodic solutions for $y_0 < y_1$, there are unbounded solutions for $y_0 > y_1$. The most interesting of these are ones, such as illustrated in Fig. 8, which again form soliton lattices.

Since these are travelling wave solutions, Eq. 5, the spatial dependence can be restored by substituting $t \rightarrow t - x/v$, where in the lattice case, $x = n\alpha'$, with $n$ an integer. Hence, Fig. 7 can be thought of as an illustration of the spatial variation of $\phi$ at a fixed instant of time. Finally, in the limit of a static solution
\( v \to 0 \), Fig. 7 would be the spatial profile of a static domain array, transforming from domains of x-tilted LTT phase (\( \phi = 0 \)) to domains of y-tilted LTT phase (\( \phi = \pi/2 \)), precisely as in Fig. 1.

The bounded orbit solutions (Figure 7) may be called ‘orthons’, in that a static array of orthons would produce a phase of average macroscopic orthorhombic symmetry – the material keeps switching back and forth between an x-tilted domain and a y-tilted domain. The unbounded solutions (Figure 8) are ‘tetrions’ in that they switch periodically between domains of tilt \(+x, +y, −x, −y, +x\), ..., to produce an average tetragonal symmetry.

The distinction between orthons and tetrions can be more clearly understood by analyzing the associated strains. From Ref. [13,14], it is known that the orthorhombic shear strain \( e_{xy} \) is proportional to the product \( R_1 R_2 \), whereas the LTT phase (in a single layer) is associated with \( e_- = e_{11} - e_{22} \propto R_2^2 - R_1^2 \). Figure 7b,c (8b,c) plot the values of \( \cos 2\phi \) and \( \sin 2\phi \), which should be proportional to \( e_- \) and \( e_{12} \), respectively, in the orthon (tetron) wave. Within the individual domains, there is a large value of \( e_- \). However, the sign of \( e_- \) alternates in successive domains, so that the macroscopic average value of \( e_- \) vanishes. In contrast, the octahedral shear strain \( e_{12} \) is non-zero only within the domain walls. However, for an orthon, this strain has the same sign in every domain wall, so that there is a net macroscopic shear \( < e_{12} \), proportional to the domain wall density. For a tetron, the shear strain is equally likely to be positive or negative. Thus, despite the presence of many LTT-type domains, the tetron has on average no macroscopic shear strains, leading to a macroscopic HTT symmetry.

4d. \( \gamma > \gamma_c \)

When \( \gamma > \gamma_c \), Figs. 2b, 3b, 4b, the slope \( \alpha \) passes through a critical value at special angles \( \alpha_c \) such that \( \cos \alpha_c = 1/\sqrt[4]{\gamma} \) (Eq. 11). For \( \beta > 0 \), \( \alpha \) diverges when \( y_0 > \beta \) (case A) and \( \alpha \to 0 \) when \( y_0 < \beta \) (case B), leading to strikingly different behavior. In case A, the resulting soliton lattices are qualitatively similar to those found for \( \gamma < \gamma_c \), except that \( \alpha \) jumps discontinuously from \( \alpha_c \) to \( 2\pi - \alpha_c \). Similar behavior arises when \( \beta < 0 \) (case C), as a tetron lattice. (For case C, orthon arrays with \( \alpha \) discontinuities are also possible.) This discontinuous jump means that the interface is abrupt, and its properties must be calculated on a microscopic model, and not in the continuum limit.

For case B, the solutions are again periodic oscillations, similar to those in Fig. 6. However, the lines \( \alpha = \alpha_c, 2\pi - \alpha_c \) divide these oscillations into those centered on \( 2n\pi \) and those centered on \( (2n + 1)\pi \).

Soliton arrays with jump discontinuities are an intriguing possibility, but are found only in case C. While such a situation does not appear to arise in LSCO for 100 or 110 waves, it might still occur in other directions or in materials with different parameters. Thus, if anharmonic effects were stronger, it would be possible to have \( \beta' > 0 \), but \( \delta' < \gamma' \), so \( \beta < 0 \).

4e. Static Solutions

Some care must be exercised in examining the static limit of Eq. 9. The static solutions of Eq. 9 correspond to \( v \to 0 \), or equivalently \( \tau \to \infty \); however, the time derivatives are really derivatives with respect to \( t - x/v \). Hence, changing to spatial derivatives requires multiplying \( \ddot{\alpha} \) or \( \ddot{\alpha}' \) by \( v^2 \) before taking the limit. Hence, the static limit of Eq. 9 still has the form of Eq. 9, but with the superscript dots now signifying spatial derivatives, with \( \beta \to -\beta'/4\gamma'v^2 \) and \( \gamma \to -(\delta' - \gamma')/4\gamma' \). That is, both \( \beta \) and \( \gamma \) are expected to be negative in this limit. In this case, the phase profiles are identical to the slow waves, discussed in Section 4c.

4f. Energy of a Soliton

While the above analysis shows what kinds of nonlinear waves are possible, no account was taken as to the energy of the wave, to see which waves are probable. The low energy waves will be those which are close in energy to the ground state of the system – i.e., to the LTT phase with \( \phi \) a multiple of \( \pi/2 \). These low-energy waves can be of two forms. First, there are ordinary phasons – nearly sinusoidal excitations of small amplitude away from the LTT phase, as in Fig. 6.

More interesting, however, are the soliton lattice solutions, Figs. 7-9. These will be low energy states when the steps are flat topped and lie close to an LTT value, \( \phi = n\pi/2 \), for integral \( n \). Orthons of this form can be generated from Eq. 11 by choosing \( y_0 = 0 \) and \( \alpha_0 \) small. As \( \alpha_0 \) gets progressively smaller, the steps become flatter and the periodicity increases. In the limit \( \alpha_0 \to 0 \), the solution approaches the
separatrix, which is an isolated soliton. In the opposite limit, choosing \( \alpha_0 = 0 \) and \( y_0 \) small generates low energy tetron arrays.

The energy per unit cell associated with the wave can be found from Eq. 1. Applying the same transformations as to the equation of motion, the energy is found to be

\[
E = \frac{M \tilde{R}^2}{2} \dot{\phi}^2 - (\beta_e - \gamma_e \dot{\phi}^2) \cos 4\phi + \delta_e \ddot{\phi} \sin 4\phi,
\]

with

\[
\beta_e = \left( \frac{8 \Gamma_{ep} + \Gamma_2 - 2 \Gamma_0 - 2 \Gamma_0}{16} \right) \tilde{R}^4,
\]

\[
\gamma_e = \left( \frac{4 \Gamma_{ep} - 5 \Gamma_0} {16} \right) \tilde{R}^4 \tau^2,
\]

\[
\delta_e = \left( \frac{\Gamma_{ep} - \Gamma_0} {8} \right) \tilde{R}^4 \tau^2,
\]

\[
\tilde{M} = M - \frac{3 \Gamma_0 R^2 \tau^2}{8}.
\]

The static limit of Eq. 14 follows from the substitution

\[
\tau \frac{d}{dt} \rightarrow - \frac{d}{d\xi},
\]

with \( \xi = x/a' \) (for (110) waves). Denoting the spatial derivative on the right side of Eq. 16 by a prime, Eq. 14 becomes

\[
E = E_0 \left( - \frac{3}{8} \dot{\phi}^2 - (\beta_e - \gamma_e \dot{\phi}^2) \cos 4\phi + \delta_e \ddot{\phi} \sin 4\phi \right),
\]

with

\[
E_0 = \Gamma_0 \tilde{R}^4,
\]

\[
\beta_e = \frac{8 \eta_{ep} + \eta_2 - 2}{16},
\]

\[
\gamma_e = \frac{4 \eta_{ep} - 5}{16},
\]

\[
\delta_e = \frac{\eta_{ep} - 1}{8},
\]

and \( \eta_{ep} = \Gamma_{ep}/\Gamma_0, \eta_2 = (\Gamma_2 - 2 \Gamma_0)/\Gamma_0 \). The static limit of the parameters of Eq. 9 can also be expressed in terms of the \( \eta \) parameters. However, these differ for 110 and 100 waves:

\[
\beta_{110} = - \frac{8}{3} (16 \eta_{ep} + \eta_2 - 2),
\]

\[
\gamma_{110} = - \frac{1}{12} (8 \eta_{ep} - 3).
\]

\[
\beta_{100} = -8 \left( \frac{16 \eta_{ep} + \eta_2 - 2}{8 \eta_{ep} + 3} \right),
\]

\[
\gamma_{100} = - \frac{1}{4} \left( \frac{8 \eta_{ep} - 3}{8 \eta_{ep} + 3} \right).
\]

Note that \( \hat{\beta} \) remains the same for both kinds of waves.

Figure 10 illustrates the energy per unit cell, Eq. 17, for the oscillatory sloutions of Fig. 6, assuming \( \eta_{ep} = 2, \eta_2 = 0 \). [N.B.: This is only done for illustrative purposes. Strictly speaking, the assumed \( \eta \) values are not consistent with the parameters of Fig. 6; this will be corrected in Section 5, after the parameters relevant to LSCO have been estimated.] For simplicity, the energy associated with only one half-cycle of
oscillation (i.e., a single soliton) is explicitly displayed. In this case, the soliton has a simple lineshape, the energy being dominated by the term \( \hat{\beta}_e \) (Eq. 18b). The linewidth is \( \sim 5a/\sqrt{\hat{\beta}} \), and the profile quickly becomes independent of soliton spacing – i.e., there is very little soliton-soliton interaction in the present model.

5. Applications to LSCO

Numerical estimates for the above parameters follow from the calculations of Ref. [13]. These calculations may underestimate the parameters, since it was assumed that the HTT→LTO transition represents the onset of tilting, \( \hat{R} \neq 0 \), whereas it is more probable that \( \hat{R} \) is finite in the HTT phase, but with \( < \cos \phi > = 0 \). Furthermore, the value of \( \hat{R} \) is taken from the measured tilt, whereas this macroscopic average value may only be about half as large as the instantaneous microscopic value[14]. With these caveats, the best estimates are from parameter sets 10 and 11 of Table II of Ref. [13]. The resulting parameter values are summarized in Table I. The Table also includes values for the crossover velocity, \( v_1 \), where

\[
\frac{v_1^2}{16M\hat{R}^2} = \frac{3E_0a^2}{16M\hat{R}^2}.
\]

Note the striking difference of \( \gamma \) values for the two types of waves. For 110 waves, \( \gamma \) is large and negative, dominated by the electron-phonon coupling. However, for 100 waves, \( |\gamma| \) is always restricted to be less than \( \gamma_c = 1/4 \). Hence, the slow wave and static solutions for 100 waves are described by the phase profiles of Fig. 3a, and include orthons, tetrons, and isolated kinks. By contrast, the 110 waves correspond to Fig. 3b, so the low energy solutions are phasons: weak periodic modulations of the tilt axis about some LTT state.

Figure 11 illustrates the energy of a soliton wall, using Eqs. 18 and 19 to estimate all parameters, and using typical values \( \eta_{ep} = 8 \), \( \eta_2 = 0 \), and \( E_0 = 5.5meV \). Shown are both the total energy (solid line) and the various components (corresponding to Eqs. 18a-d). The shape is more complicated than found in Fig. 10, because the term in \( \hat{\gamma}_e \) (Eq. 18c) becomes comparable to that in \( \hat{\beta}_e \) when \( |\hat{\beta}| \) is large.

By integrating the energy profile, the total interface energy \( E_w \) (plotted as energy per column width) can be found, and is plotted in Fig. 12 as a function of the spacing between successive domain walls, \( d_w \). In the present theory, the tilt-tilt interaction is short ranged, and this is reflected in Fig. 12 by the fact that there is virtually no soliton-soliton interaction until the solitons are less than two cells apart. Below this separation, the tetrons have lower energy than the orthons. However, it is unlikely that a continuum theory should be trusted at such small length scales – note that the width of the domain wall is less than a single cell across. The limiting energy of a single soliton at large separation is found to be nearly linear in \( \eta_{ep} \):

\[
E_w \simeq \frac{E_0}{2}(\eta_{ep} - 1.3),
\]

There are a number of additional factors which will give rise to longer range soliton interaction. For instance, the strains associated with the tilting give rise to direct coupling of more distant cells[14]. Moreover, the electronic energy lowering is produced by the splitting of the vHs degeneracy within the LTT-like domains. If the domain walls approach one another too closely, the domains will cease to have a well-defined LTT-like character, and the vHs splitting will decrease. This is equivalent to a repulsive interaction between domain walls.

Using the present equations, it is possible to calculate the energy associated with a static domain wall exactly, for a given microscopic configuration, Fig. 13. Such calculations are presented in Appendix II. These calculations are still approximate, in that the simple distortions assumed do not display the correct corner sharing behavior. The resulting energy is very similar to the calculations of this section. The wall energy is found to satisfy an equation of the form of Eq. 20, but with different numerical coefficients, which depend explicitly on the assumed wall thickness. The minimum wall energy corresponds to an abrupt wall, as in Fig. 13a.

It is tempting to relate the various nonlinear waves to the various phases found in LSCO and related compounds – the isolated solitons separating large grains of LTT phase, the orthons associated with the LTO phase, and the tetrons with the HTT phase. If this correspondence is valid, then what distinguishes the various phases, and in particular, what constitutes a phase transition? Presumably, this is accomplished
by coupling to macroscopic strains: e.g., in the LTO phase, the macroscopic average shear strain, $\epsilon_{xy}$. As shown in Ref. [14], inclusion of strain coupling makes the effective tilt-tilt interaction longer ranged, and hence could stabilize an orthorhombic or tetragonal phase. [This same model could be applied to BaTiO$_3$, in which case, the long-range coupling would be via the ferroelectric polarization.]

6. Charged Solitons?

In the above sections, it has been shown that the LTO phase of LSCO can be interpreted as a dynamic JT phase, or equivalently as a soliton lattice with domains of LTT phase separated by domain walls of a different phase, closer to the usual LTO phase. This nanoscale phase heterogeneity is very reminiscent of another grain boundary phase postulated[7,26] to exist in this system – a phase separation of holes associated with doping LSCO away from the optimal hole concentration at which the vHs coincides with the Fermi level.

In this earlier model, the phase separation arises because the electron-phonon coupling is strongest exactly at the vHs, leading to a minimum in the free energy at precisely that concentration. (There is a close relation to Hume-Rothery phases in alloys.) The size of the domains is restricted, because the hole concentration is different in the two phases – i.e., the domains are charged, and the domain size is limited by Coulomb effects. The lowest energy phase turns out to be a grain boundary phase, with the LTT domains forming one phase, and the domain walls constituting a second, microscopic LTO-like phase. Near the vHs, it is possible to have a pure LTT phase. As the material is doped away from the vHs toward half-filling, the LTO phase becomes more stable, and the size of the LTT domains decreases. If, as found above (Fig. 7), the orthorhombic shear strain is taken as proportional to the domain wall density, this is exactly what is found experimentally in LSCO – that $\epsilon_{12}$ increases as the material is doped away from the vHs ($x$ decreased below $\sim 0.15$).

There are a number of similarities between the doping-induced grain boundary phase and the soliton lattice. Indeed, it is possible that the solitons are charged. This could arise if the strains in the domain wall, associated with corner sharing, lead to a modification of the shape of the octahedron – i.e., a change of the Cu to apical O bond length. A reduction of this bond length would reduce the splitting between the Cu $d_{3z^2-r^2}$ and $d_{x^2-y^2}$ levels, which can lead to a different degree of charge transfer into the Cu-O$_2$ planes, as well as to a direct change in the shape of the Fermi surface. These changes will have similar effects to the charge bunching postulated in the earlier work[26], in that the density of planar Cu holes will be different in the domains and in the walls. It is of interest to note that a number of experiments have detected structural anomalies in the cuprates, often at temperatures very close to $T_c[17]$, which are related to tilting of the octahedra, and generally include a change of the Cu to apical O bond length.

7. Conclusions and Discussion

The present paper is the fourth in a series of closely related works which have introduced the idea that the LTO phase of LSCO is a dynamic JT phase. It is perhaps appropriate to briefly summarize what has been accomplished to date, and what remains to be done. The formal model was introduced in B[13], and static JT solutions were displayed, emphasizing the first appearance of a macroscopic tilt, $\hat{R} \neq 0$. The dynamics of the model, wherein the tilt axis could bob about, assuming one of four preferred orientations, is discussed in C[14] at the mean-field level, and in D, the present manuscript, in terms of a microscopic picture of nonlinear wave solutions. The first paper, A[12], introduced the concept of the dynamic vHs-JT phase, and provided a simplified model calculation which reproduced the general doping dependence of the phase diagram. In particular, it answered the vexing question of why, if superconductivity can only be found in the LTO phase[11], the highest superconducting transition temperatures occur in the doping range in which the LTO phase is least stable.

Prior to these papers, the vHs model seemed to provide an interesting framework for interpreting many of the phenomena associated with high-$T_c$ superconductivity[7,27], but also predicted a strong competition with structural instabilities (charge density wave phenomena) of a form which could not be clearly identified with the major phase transitions of the high-$T_c$ cuprates. While the discovery of the LTT phase provided a first link between structural instability and the vHs, the present model clearly demonstrates for the first time a close relation between the vHs and the LTO phase, the dominant phase in which high-$T_c$ superconductivity arises. Moreover, the model paints this LTO phase as a highly unusual, dynamic and nonlinear phase, of just
the form wherein one might expect to observe the anomalous normal-state and superconducting properties actually found in the cuprates. The close similarity between the present model and the earlier picture of short-range structural disorder\[7,26\] should be noted.

While the present equations display a rich variety of nonlinear wave solutions, it should be kept in mind that these equations are already approximations, and that the more exact equations\[13\] should have even stronger nonlinearities. In particular, it was assumed that the tilting of the individual octahedral cages sets in at considerably higher temperatures, so that the average tilt $\bar{R}$ can be considered constant. Moreover, while the term $H_{ep}$ in Eq. 1 accounts for the role of the electronic excitations in modifying the structural transition, the back-reaction of this structural change on the electronic properties has not been discussed. In particular, what is the effect of the domain walls on the splitting of the vHs? Indeed, in a dynamic JT phase, it is unclear what the ‘band structure’ means, when the Brillouin zone itself may be a local function of time and space (c.f. the spatial variation of the orthorhombic splitting in Figs. 7 and 8).

It should be noted that these complications are ‘interesting’ in that they are likely to lead to a rich variety of anomalous behavior, both in the superconducting and normal states, comparable to that observed experimentally in the cuprates.

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### Appendix I: Approximate Electron-Phonon Coupling Term

In this Appendix, an approximate form for the electron-phonon coupling term, Eq. 1b, will be derived. Following the discussion of Section 3, this term can be written

$$H_{epn} = -\frac{\tilde{\alpha}^c R^2}{4} \left| \sum_n [(\cos\phi_n - \cos\phi_{n+1})^2 - (\sin\phi_n - \sin\phi_{n+1})^2]\right|. \quad (A1)$$

Expanding $\sin\phi_{n+1}$, $\cos\phi_{n+1}$ as in Eq. 6, this becomes

$$H_{epn} = -\frac{\tilde{\alpha}^c R^2}{2} |4\cos2\phi - \tau^2(2\dot{\phi}\sin2\phi + 3\dot{\phi}^2\cos2\phi)|, \quad (A2a)$$

$$H_{epn} = -\frac{\tilde{\alpha}^c R^2}{2} (4 - 3\tau^2\dot{\phi}^2) \sqrt{1 + \mu^2} |\cos(2\phi + \nu)|, \quad (A2b)$$

where the index $n$ on $\phi$ is omitted, $\mu = 2\tau^2\dot{\phi}/(4 - 3\tau^2\dot{\phi}^2)$, and $\sin\nu = \mu/\sqrt{1 + \mu^2}$. Figure 14a illustrates $H_{epn}$ in the case of perfect intercell coupling, $\cos\phi_{n+1} = -\cos\phi_n$ ($\phi = \dot{\phi} = 0$). Deviations from this coupling reduce the amplitude of $H_{epn}$ and shift the phase of $\cos2\phi$.

The absolute value signs in Eq. A2 lead to the cusps in Fig. 14a, and can complicate the analysis. Since $H_{epn}$ is an effective potential for the tilt phonons, rounding the cusps at the potential maxima should have negligible effect on the problem. Hence, the Fourier expansion may be utilized:

$$|\cos2\phi| = \frac{2}{\pi} \left( 1 + \sum_{n=1}^{\infty} \frac{2(-1)^n}{4n^2 - 1} \cos4n\phi \right). \quad (A3)$$

Keeping only the constant and $n = 1$ terms provides a reasonable first approximation (dashed line in Fig. 14a).

What enters into the equations of motion is not $H_{epn}$ but its derivative with respect to $\phi_n$, which may be written

$$\frac{\partial H_{epn}}{\partial \phi_n} = (\pm) \frac{\tilde{\alpha}^c R^2}{2} [4\sin2\phi + \tau^2(\dot{\phi}\cos2\phi - \dot{\phi}^2\sin2\phi)], \quad (A4a)$$

$$= (\pm) \frac{\tilde{\alpha}^c R^2}{2} (4 - \tau^2\dot{\phi}^2) \sqrt{1 + \mu^2} \sin(2\phi + \nu'), \quad (A4b)$$

where, to order $\tau^2$, $\mu' = \mu$ and $\nu' = \nu$, and the term $(\pm)$ comes from the absolute value signs in Eq. A1: the minus sign applies whenever the quantity within ||'s in Eq. A1 is negative. The resulting quantity, plotted
in Fig. 14b, has discontinuous jumps whenever the $\cos2\phi$-term changes sign, Fig. 14a. Because of these discontinuities, the Fourier series requires more terms for an adequate representation:

$$\pm \sin 2\phi = \frac{8}{\pi} \sum_{n=1}^{\infty} \frac{n(-1)^{n+1}}{4n^2 - 1} \sin 4n\phi.$$  \hspace{1cm} (A5)

Figure 14b shows the Fourier series for one term (dashed line) and for two (dotted line). The one term series is nonetheless qualitatively correct, particularly in the region of the potential minima, so this approximation is adopted for the main text. In the present case, this amounts to replacing

$$\pm \sin (2\phi + \nu) \rightarrow \frac{8}{3\pi} \sin (4n\phi + \nu),$$  \hspace{1cm} (A6)

so

$$\frac{\partial H_{epn}}{\partial \phi_n} = \frac{4\bar{\alpha} \epsilon \bar{R}^2}{3\pi} [4\sin 4\phi + \frac{\tau^2}{2} (\dot{\phi}\cos 4\phi - \dot{\phi}^2 \sin 4\phi)].$$  \hspace{1cm} (A7)

There is one last complication. The terms $H_{ep,n \pm 1}$ also depend on $\phi_n$, so their derivatives must be added to Eq. A7 to give the total potential contribution. By reasoning similar to the above, it can be shown that

$$\frac{\partial H_{ep,n+1}}{\partial \phi_n} + \frac{\partial H_{ep,n-1}}{\partial \phi_n} = \frac{\partial H_{epn}}{\partial \phi_n},$$  \hspace{1cm} (A8)

except possibly when $\cos 2\phi_n$ is changing sign. In this case, it is possible that, e.g., $\partial H_{ep,n+1}/\partial \phi_n$ will change sign before $\partial H_{epn}/\partial \phi_n$ (Fig. 14b). In this case, its contribution would tend to cancel rather than add. This effect will tend to smooth out the discontinuity in Fig. 14b. Furthermore, the correction will be small in the smoothed form of the restoring force (dashed line in Fig. 14b). Hence, this complication is neglected, and Eq. A8 is assumed to hold throughout. This amounts to doubling the contribution of $H_{epn}$, accounting for a factor of 2 in Eq. 2 and subsequent equations.

Finally, the above analysis can be repeated for (100) waves, as in Section 3c. In this case, Eq. A7 becomes

$$\frac{\partial H_{epn}}{\partial \phi_n} = \frac{4\bar{\alpha} \epsilon \bar{R}^2}{3\pi} [4\sin 4\phi + \frac{\tau^2}{2} (\dot{\phi}\cos 4\phi + 1 - \dot{\phi}^2 \sin 4\phi)].$$  \hspace{1cm} (A9)

Note that this differs from Eq. A7, in that the $\tau^2$ terms are half as large, and there is an extra term multiplying $\dot{\phi}$.

**Appendix II: Microscopic Domain Wall Energy Calculations**

For narrow domain walls (only a few unit cells thick), it is possible to directly calculate the domain wall energy from Eq. 1, for any assumed pattern of tilt angles. In this Appendix, the calculation is presented for the three configurations illustrated in Fig. 13. In this figure, the dashed lines enclose the regions of canted cells – everything outside the dashed lines is assumed to be in perfect LTT order. (For the abrupt wall of Fig. 13a, there are no cells ‘within’ the wall.) The domain wall energy is defined as the excess energy over the ground state energy within a single domain. For an LTT-type domain, e.g., $\cos \phi = 0$ everywhere, this minimum energy is, for a single cell,

$$E_{min} = \left( \frac{\Gamma_0 + \Gamma_2^a}{2} \right) \bar{R} + 2\bar{\alpha} \epsilon \bar{R}^2.$$  \hspace{1cm} (B1)

(Recall that the terms involving $\Gamma_0^a$ and $\Gamma_2$ are on-site terms, while the terms in $\Gamma_0$ and $\bar{\alpha} \epsilon$ involve sums over nearest neighbors.)

For the abrupt wall of Fig. 13a, all atoms remain tilted about the x or y axes, so there is no wall energy contribution from the terms involving $\Gamma_2$ or $\Gamma_0^a$. Here, y is defined as parallel to the domain wall and x perpendicular to it, with the positive x direction pointing to the right of the figure. The terms in $\Gamma_0$ and $\bar{\alpha} \epsilon$.
are affected by the wall, since the cells nearest the walls have neighbors in a less than optimal configuration. For instance, for the top left atom in the figure, the excess energy due to $\Gamma_0$ is

$$\Delta E_\Gamma = \frac{\Gamma_0 R^4}{4} (2 \times 1 + 0 + \left(\frac{1}{2}\right)^4 - 2).$$

Here the first term in parentheses is due to the term involving nearest neighbors along $y$, the next to the neighbor along $-x$, the third along $+x$ (i.e., across the domain wall); the final term is the subtraction of the energy for the undistorted state (absence of the domain wall). For the top right atom, the analogous term is

$$\Delta E_\Gamma = \frac{\Gamma_0 R^4}{4} (2 \times 0 + 1 + \left(\frac{1}{2}\right)^4 - 2).$$

For the electron-phonon term, taken from Eq. A1, the net wall energy due to both atoms is

$$\Delta E_\alpha = -\tilde{\alpha}_e R^2 (|2 \times 1 - \left(\frac{1}{2}\right)^2| + |1 + \left(\frac{1}{2}\right)^2 - 0| - 4).$$

Adding up the excess energies of these two cells, the wall energy is found to be

$$E_w^\alpha = \tilde{\alpha}_e R^2 - \left(\frac{7}{32}\right) \Gamma_0 R^4$$

$$= \left(\frac{3\pi}{8} \eta_{ep} - \frac{7}{32}\right) E_0 = 1.18 E_0 (\eta_{ep} - 0.186). \quad (B2)$$

This procedure can be repeated for the thicker walls of Figs. 13b, 13c. In each case, the sum involves one additional cell, and there is now an internal degree of freedom, the tilt angle $\theta$ of the cells within the wall. For the one-cell wall, Fig. 13b,

$$E_w^b = \frac{E_0}{4} \left(2 \cos^4 \theta - 3 + \frac{\sin^4 \theta + (1 + \sin \theta)^4}{8} + \frac{\sin^2 2 \theta}{2} \eta_2 + \left(\frac{3\pi \eta_{ep}}{8}\right) [11 - 2\sin \theta - 10\cos^2 \theta - 3 - 2\sin \theta] \right)$$

$$= 2.65 E_0 (\eta_{ep} + 0.047 \eta_2 - 0.133), \quad (B3)$$

where the final numerical form is for the symmetric wall position, $\theta = 45^\circ$. Actually, the term in $\eta_{ep}$ is minimized at $\theta = 0$, and so dominates the wall energy that the total $E_w^b$ also has a minimum at $\theta = 0$ as long as $\eta_{ep} \geq 1$. In fact, this limiting case of $\theta = 0$ corresponds exactly to the abrupt wall situation, Fig. 13a. It is a check of the calculation that Eq. B3 agrees with Eq. B2 in this limit.

The same calculation may be repeated for Fig. 13c. The wall energy is

$$E_w^c = \frac{E_0}{4} \left(-3 - \sin^2 2 \theta + \frac{\sin^4 \theta + (\sin \theta + \cos \theta)^4 + (1 + \cos \theta)^4}{8} + \sin^2 2 \theta \eta_2 + \frac{3\pi \eta_{ep}}{4} [9 - 2\cos \theta - 5\cos^2 \theta] \right)$$

$$= 2.80 E_0 (\eta_{ep} + 0.067 \eta_2 - 0.160), \quad (B4)$$

with the last line holding for $\theta = 30^\circ$. No absolute value signs appear in Eq. B4, since it only makes sense for $\theta \leq 45^\circ$ (otherwise the wall tilt is no longer monotonic). Again, the wall energy actually minimizes at $\theta = 0$, in which case it agrees with Eq. B2. Thus, the minimum wall energy corresponds to the abrupt wall, Fig. 13a. The energy, Eq. B2, should be compared to the continuum theory, Eq. 20. It is seen that the continuum theory underestimates the absolute energy by a factor of about two, but correctly predicts that the wall thickness is of the order of a single unit cell. It should be noted that the calculations of this Appendix employ the full, discontinuous form of the electron-tilt coupling (solid line in Fig. 14a) rather than the smooth approximation (dashed line).

Note that the present model does not fully account for the complications of corner-sharing octahedra. The distortion of, e.g., Fig. 13a is not consistent with a tilting of rigid octahedra. For instance, in Fig. 13a, the top atom to the left of the domain wall is tilting parallel to the wall (the upper apical oxygen is tipped in the positive y direction), so the in-plane oxygen in the right corner of the cell (positive x direction) would be
untitled, for a rigid octahedron. On the other hand, the apical oxygen of the top cell to the right of the wall is tipped in the negative x direction, which would require the same in-plane oxygen to tip below the plane. In the actual corner-shared configuration, neither tilt can be a pure x or y directed tilt. This distortion in turn will cause cells further from the domain wall to be tilted, and may lead to distortions of the shape of the octahedra.

However, a more realistic model, allowing for these distortions, would be considerably more involved. For instance, it would include variations in the Cu-apical O distance, with the ensuing relative change of the Cu $d_{3z^2-r^2} - d_{x^2-y^2}$ level splitting. While these effects may play an important role in the detailed characterization of the domain wall and its excitations, it is hoped that the present simplified model captures the essential nature of the structural nonlinearities of the model.

### Table I: Parameter Values (from Ref. [13])

| fit | $E_0$ (meV) | $\eta_{ep}$ | $\eta_2$ | $\beta$ | $\gamma_{110}$ | $\gamma_{100}$ | $\nu_1$ (m/s) |
|-----|-------------|-------------|----------|--------|----------------|----------------|-------------|
| 10  | 6.4         | 5.6         | 0.7      | 68     | -3.5           | -0.22          | 470         |
| 11  | 4.7         | 9.6         | -2.0     | 65     | -6.2           | -0.23          | 400         |

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Figure Captions

Fig. 1 Proposed domain wall between two LTT domains, for (a) (110) wall or (b) (100) wall. Circles represent apical oxygens in layer above CuO$_2$ plane. Arrow indicates direction of displacement of apical oxygen due to tilting of corresponding octahedron. Dashed lines indicate limits of domain wall, within which tilt direction is variable. Dotted lines indicate two columns of inequivalent atoms, A and B.

Fig. 2 Phase portrait of Eq. 9 for fast waves ($v > v_1$), with $\beta > 0$, $\gamma > 0$. Lines with filled circles indicate separatrices.

Fig. 3 Phase portrait of Eq. 9 for $\beta < 0$, $\gamma < 0$.

Fig. 4 Phase portrait of Eq. 9 for $\beta < 0$, $\gamma > 0$.

Fig. 5 Temporal (or spatial) evolution of fast waves (corresponding to Fig. 2), assuming $\beta = \gamma = 0.2$, $\alpha_0 = 0$, and $y_0 = 2, 1, 0.82, 0.8$, in order of decreasing slope; dashed line is $y_0 = 2$ curve, with expanded horizontal scale (upper axis).

Fig. 6 Oscillatory wave solutions, which can equally correspond to either fast waves (using left-hand axis) or slow waves (right-hand axis). Parameters (for slow waves) are $\beta = \gamma = -0.1$, $y_0 = 0$, and $\alpha_0/\pi = 0.8, 0.4, 0.2, 0.02, 0.002$, in order of increasing amplitude. For clarity, only the first two cycles of each mode are illustrated.

Fig. 7 Orthon solution, assuming $\beta = \gamma = -0.1$. (a) Phase of tilt; (b) $\cos 2\phi$, proportional to the ‘LTT strain’, $e_- = e_{11} - e_{22}$; (c) $\sin 2\phi$, proportional to the orthorhombic shear strain $e_{12}$.

Fig. 8 Tetron solution, with same parameters as Fig. 7.

Fig. 9 Family of tetron solutions, illustrating discontinuous jump in $\alpha$ for $\gamma > \gamma_c = 0.25$. For all curves, $\beta = -1$. Values of $\gamma$ are, from right to left, 0.05, 0.1, 0.2, 0.251, 0.26, 0.3, 0.4, 0.8, 2, and 10 ($\gamma = 100$ is nearly indistinguishable from $\gamma = 10$.) Filled circles show limits of jump in $\alpha$.

Fig. 10 Local energy per unit cell of waves of Fig. 6, assuming $\eta_{ep} = 2$, $\eta_2 = 0$. For simplicity, only one half cycle of period (corresponding to a single kink) is illustrated.

Fig. 11 Local energy per unit cell of single (100) soliton, using parameters appropriate to LSCO: $\eta_{ep} = 8$, $\eta_2 = 0$, $E_0 = 5.5meV$. Solid line = total energy, Eq. 17; dotted line = contribution of $\dot{\beta}_c$; long dashed line = contribution of $\dot{\gamma}_c$; short dashed line = contribution of $\dot{\delta}_c$; dotted line = contribution of $-3\phi'^2/8$.

Fig. 12 Integrated domain wall energy $E_w$ per column, as a function of wall spacing, $d_w$, both for orthon (solid lines) and tetron configurations (dashed lines), for $\eta_{ep} = 8$ or 2.
Fig. 13 Microscopic domain wall configurations, for the calculations of Appendix II, for three different wall thicknesses.

Fig. 14 (a) JT energy, $H_{epn}$. Solid line = Eq. A2b, $\nu = 0$; dashed line = Fourier approximation, retaining only the $n = 0,1$ terms. (b) $\partial H_{epn}/\partial \phi_n$. Solid line = Eq. A4b, $\nu = 0$; dashed line = Fourier approximation, $n = 1$ term only; dotted line = two term ($n = 1,2$) Fourier representation.