Van Hove Exciton-Cageons and High-T$_c$ Superconductivity: XB: 
Polaronic Coupling in the Doped Material

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A purely ionic interpretation of the tilting mode instabilities in La$_{2-x}$A$_x$CuO$_4$ (A=Sr,Ba) is shown to be not self-consistent: the dominant factor influencing the doping dependence of the interlayer mismatch is the large change in the Cu-O bond length. But such a large dependence of bond length on valence leads to a strong electron-phonon coupling, contradicting the assumption that covalent effects were negligible. This coupling is closely related to the vHs-JT effect. This new insight clarifies the role of the tilt-mode instabilities. The main JT coupling is not to these modes, but to the inter-plane O-O bond stretching modes which split the vHs degeneracy. However, as these modes soften, they couple to the lower-lying tilt modes, so that the ultimate instability has a finite tilt component.

This in turn simplifies the description of the JT instabilities. The tilt modes, while strongly coupled to the electrons, are quadratic in the tilt angle. On the other hand, the bond stretch modes have a large, linear coupling to electrons, with clear polaronic effects. This is connected with the fact that, near a vHs, valence fluctuations are slow and relatively long lived, coupling to local phonon modes. A striking result of this is that there will be a large polaronic band narrowing near the vHs, whether or not the vHs is near the Fermi level. This vHs-localized band narrowing provides a natural explanation for the common occurrence of extended vHs’s.

I. INTRODUCTION

Recent photoemission studies have demonstrated that a van Hove singularity (vHs) falls very close to the Fermi level in optimally doped Bi$_2$Sr$_2$CaCu$_2$O$_8$ (Bi-2212) [1] and YBa$_2$Cu$_3$O$_7$ (YBCO) [2]. This lends strong support to the many proposals that the vHs plays an important role in high-T$_c$ superconductivity [3] in these materials. The vHs’s also couple to many of the phonon modes involved in the various structural phase transitions found in La$_{2-x}$Sr$_x$CuO$_4$ (LSCO) and related compounds [4,5], which leads to a competition between superconductivity and structural transitions in the cuprates.

However, these structural phase transitions are common to most perovskites, many of which are insulating, so the notion that electron-phonon coupling plays an important role has been questioned. The conventional view of these transitions has been that they are purely ionic, driven by the Madelung energy or interlayer strain mismatch, and have little or nothing to do with the electronic system.

This conventional picture has been modified by recent analyses. The perovskites have two classes of distortions, ferroelectric (FE), which generate a dipole moment in the unit cell, and antiferrodistortive (AFD), involving tilting of local octahedra. Cohen [6] has shown that there can be large covalent contributions to the FE instabilities, even when the materials are insulating, if the Fermi level lies in a hybridization gap between two atomic species. (A similar result is discussed in Appendix A4 of Ref. [6]). This has stimulated a great deal of research showing the important role of correlation effects [7] in FE instabilities. Of particular interest is a recent two-band Hubbard model of the FE instability, introduced by Egami, et al. [8], which involves a one-dimensional (1D) version of the three-band Hubbard model regularly applied to the cuprates.

The structural phase transitions in the cuprates are generally AFD, involving tilting of the CuO$_6$ octahedra. Such AFD instabilities are common in other perovskites, and indeed often compete with FE instabilities [4]. However, these AFD instabilities are generally found to be ionic rather than covalent – the tendency towards instability scales linearly with a tolerance factor, $t$, which measures the degree of ionic size mismatch [4], see, e.g., Eq. 1, below). Hence, the present paper provides a reassessment of the role of electron-phonon coupling in the structural instabilities of the cuprates.

The paper is organized around three calculations. First, a mixed ionic-covalent model of the structural transitions is recalled. It is shown that the same model which explained the $T$-dependence of the low temperature orthorhombic (LTO) phase in LSCO [3] can also explain its doping dependence (Section II and Appendix A). [Strictly speaking, the dominant instability is to a phase of short-range order – identified with the pseudogap phase – but the transition temperatures for this phase and the LTO phase are proportional to each other.] While the model must contain a significant ionic contribution, there can also be a significant covalent contribution. Secondly, the purely ionic model for the cuprates is analyzed in more detail, and a number of discrepancies are pointed out. Most importantly, it is found that the dominant factor controlling the doping dependence of the LTO transition is the large compressibility of the CuO$_6$ planes: in ionic terms, there is a large decrease in the Cu-O distance when $O^{2-} \rightarrow O^-$. This analysis is presented in Section III and Appendix B.

This large change of interionic spacing with valence is a signature of large electron-phonon coupling, as found in rare earth compounds [9]. Hence, a purely ionic model
with no electron-phonon coupling is not self-consistent. The contraction of the O-radius couples to a number of phonon modes, but predominantly to in-plane modes, and not to tilting modes. This leads to a reanalysis of earlier results. It is now suggested that the major phonon coupling is indeed with planar modes, which couple quadratically to the much lower frequency octahedral tilt modes. This weak coupling ensures that when the highly coupled bond stretching modes start to soften, the tilt modes go unstable first.

This has important consequences for the vHs-JT effect. The electron-tilt phonon coupling is quadratic in the tilt angle, and hence in the phonon creation operator – a strong violation of Migdal’s theorem. In contrast, the O-O bond stretching mode has a linear JT coupling to the vHs, via the length dependence of the hopping parameter, $t_{CuO}$. The soft mode behavior of, in particular, the O-O stretch modes is discussed in Section IV and Appendix C. Moreover, there is a clear polaronic contribution: as the hole hops around, it carries this lattice distortion with it. These polaronic effects are discussed in Section V and Appendix D. By estimating the magnitude of the polaronic corrections to the bandstructure, it will be possible to make connection with various polaronic or bipolaronic theories of superconductivity.

One striking result is that polaronic effects can explain the existence of extended vHs’s, even when the vHs is away from the Fermi level. Band narrowing effects are localized near a vHs due to the fact that, near a vHs, the material has an ioniccovalent crossover. Electronic motion is slow compared to phonon motion, so valence fluctuations are well defined (Section VI). Section VII summarizes some conclusions, while Appendix E applies some of these results to spin-orbit coupling.

Once it is recognized that strong electron-phonon coupling effects can play an important role in the structural instabilities in the insulating perovskites, it then becomes plausible to assume that they can also drive a competition between structural and superconducting instabilities, when the perovskites are doped. Indeed, undoped SrTiO$_3$ has an antiferrodistortive instability associated with the tilting of the TiO$_6$ octahedra, which is closely analogous to the LTO and low temperature tetragonal (LTT) phases of LSCO, whereas doped SrTiO$_3$ is superconducting – one of the first known members of the family of high-$T_c$ perovskites. A similar competition between tilt-mode instabilities and superconductivity is found in BaK$_{1-x}$Bi$_2$O$_3$ [13]. Interestingly, this is accompanied by softening of the 1D O-O bond stretching modes, which also play an important role in the cuprates, as will be demonstrated below.

**II. STRUCTURAL PHASE TRANSITIONS**

A. Phase Transitions and Pseudogaps

In LSCO/LBCO and related compounds, a number of structural phase transitions are observed. From high temperature to low, the principal phases observed are a high-temperature tetragonal (HTT) phase, where the octahedra appear to be untilted, a low-temperature orthorhombic (LTO) phase, in which the average tilt is about an axis at 45° to the Cu-O bond, and a low-temperature tetragonal (LTT) phase, where the tilt axis is along the Cu-O bond. By substituting Nd for La, it is possible to generate an intermediate (Pccn) phase in which the tilt axis is at an angle between 0 and 45° to the Cu-O bond. The transition temperatures are a strong function of doping, with the LTO transition temperature monotonically decreasing with hole doping, while a full LTT transition is found only in LBCO near a doping $x=0.125$, or in Nd substituted LSCO.

I have suggested that these transitions are representative of a dynamic Jahn-Teller (JT) transition. The LTT phase would involve a predominantly static distortion, the LTO a dynamic tunneling between two adjacent LTT tilts, and the HTT tunneling among all four tilts. The Pccn phase could be explained as an intermediate phase, where there is some LTO tunneling, but still a static LTT component. The HTT→LTO transition is a transition between two dynamic JT phases, driven by intercell coupling associated with corner sharing of planar O’s and long range strain forces. If the microscopic average local tilt is unchanged between the LTO and HTO phases, there may be little change in the electronic properties at the transition – this appears to be the case experimentally. However, it is possible that there is an additional transition within the HTT phase, associated with the onset of a tilting instability, which does couple more strongly to electronic degrees of freedom. Such a crossover from the tunneling phase to an undistorted phase is a common feature of many dynamic JT transitions [14].

This dynamic tilting onset can be identified with the ‘pseudogap’ phase recently found by Hwang, et al. [14] in LSCO, at a temperature $T^*$, Fig. 1. Below this temperature, there is evidence for significant changes in the electronic properties of the material: the susceptibility starts to drop below $T^*$, and the anomalous temperature-dependence of the Hall effect first appears. I have suggested that this anomalous temperature dependence follows from the gradual opening of the short-range-ordered dynamic-JT phase structural gap, and signals the gradual crossover from the large Fermi surfaces to the small pockets seen in transport measurements. Hwang, et al., found a striking scaling of the pseudogap properties – the curves at different dopings all scaled to a universal behavior when plotted as functions of $T/T^*$. The LTO phase transition has a similar scaling, with $T_{LTO} \approx T^*/2$ for all dopings.

The dynamic JT model is consistent with frozen
phonon calculations by Cohen, et al., which find that in LBCO the HTT phase is unstable, and the LTO phase metastable with respect to the LTT phase \(^{11}\). A similar pseudogap is found in YBCO, associated with peaks in the susceptibility \(^{17}\) and heat capacity \(^{18}\). This is associated with the onset of a pyramidal tilting instability seen in neutron diffraction \(^{19}\) and related phonon anomalies \(^{20, 22}\). This was originally interpreted as a spin gap \(^{22}\), possibly with spin-phonon coupling \(^{20, 24}\), but the recent evidence is suggestive of a gap in both charge and spin channels.

Hence, I would identify this pseudogap phase with the onset of the JT-tilting instability. Thus, the calculations of this paper should refer to the \(T^*\) transition. Since, however, most of the experiments are on the LTO phase, I will make use of the scaling found by Huang, et al. to compare the calculations for \(T^*\) with experimental data for \(T_{\text{LTO}} \sim T^*/2\).

It should not be overlooked that such a dynamic JT effect is itself a potentially important (and highly anomalous) source of low energy excitations, which could act as additional bosons for causing electrons to pair up. As early as 1941, Teller was speculating that the dynamic JT effect could provide the driving mechanism for (conventional) superconductivity \(^{25}\).

\section*{B. Doping Dependence of LTO Transition}

In the ionic picture for the cuprates, the structural instabilities are driven by interlayer bond-length mismatch \(^{20}\). The unit cell in the CuO\(_2\) layer is larger than that in the LaO layer, with the degree of mismatch measured by the tolerance factor

\[ t = d_{\text{LaO}}/\sqrt{d_{\text{CuO}2}}, \]

where \(d_{\text{LaO}}\) is the effective LaO distance in the LaO plane, with a similar definition for \(d_{\text{CuO}2}\). Commensurability strains will arise in LSCO whenever \(t\) difference from unity. Mismatch problems become more severe at lower temperatures, gradually causing the CuO\(_2\) layers to buckle – either by octahedral tilts in LSCO or by layer dimpling in YBCO (there may also be a pyramidal tilt instability in YBCO). Indeed, the structural instability can be interpreted in a purely ionic model, with the transition temperature proportional to the degree of mismatch.

In undoped La\(_2\)CuO\(_4\), the LTO transition can equally well be described by either a purely ionic model or a model with considerable electron-phonon coupling \(^{3}\) (due to the strong correlation effects, this would be a spin-Peierls coupling, although the distinction is not obvious at the mean-field level). However, the transition could not be interpreted purely in terms of Fermi surface nesting; the ‘bare’ phonon frequency \(\omega_0\) was always found to be imaginary, stabilized by anharmonic effects. This imaginary frequency could be caused by a combination of covalency effects and interlayer strains,

\[ \omega_0^2 = \omega^2 - \alpha n_h - \Gamma^* T^* \]

(see Eq. 32c of Ref. \(^{3}\)). Here \(n_h = 1 + x\) is the number of holes, \(T^*\) is the interlayer strain, proportional to the lattice mismatch, \(\omega_0\) is the bare frequency, and \(\Gamma^*\) and \(\alpha\) are appropriate coupling constants. The middle term of Eq. 2 is a covalency effect. Note that there is no electron-hole symmetry within the antibonding state: the maximum frequency reduction corresponds to an empty band, \(n_h = 2\). The electron-hole symmetry is restored only when both antibonding and bonding bands are considered. Thus, the maximum covalent effects arise in the insulating state, in a hybridization gap between two atomic levels. The last term would indicate a strong phonon-phonon (anharmonic) contribution to the phase transitions.

In Appendix A, this analysis is extended to include the doping dependence of the LTO transition. Doping reduces the interlayer mismatch in two ways, by substituting the larger Sr\(^{2+}\) for La\(^{3+}\), and by hole doping the CuO\(_2\) planes. Insofar as the holes go predominantly onto O’s, this amounts to replacing O\(^{2-}\) by the much smaller O\(^{1-}\). Thus, in the doped material the layer mismatch is reduced, so the tilting instability is driven to lower temperatures. Detailed calculations based on this picture can provide a semi-quantitative description of the LTO transition, Fig. 2. The data in Fig. 2 come from experiments on pure Sr doping (summarized by Takahashi, et al. \(^{27}\)), and on Nd substitution studies \(^{28}\). Once again, it is found that the transition can be explained equally well by either a purely ionic model, or a mixed ionic, electron-phonon model. The three frames of Fig. 2 correspond to the three models of Fig. 3 of Ref. \(^{3}\), with zero (a), weak (b), or strong (c) electron-phonon coupling. As in that reference, all three models provide comparable fits to the data.

In principle, the Nd substitution studies could help clarify the situation, since Nd is isovalent with La, and Nd substitution should lead to only ionic size effects, with no doping of the CuO\(_2\) layers. However, even this data can be fit by any of the above models.

What is one to make of this? The principle of Occam’s razor would say that since the purely ionic model (Fig. 2a) provides the simplest interpretation of the data, then \textit{in the absence of any other evidence for electron-phonon coupling}, this ionic model is preferred. On the other hand, the cuprates are high-T\(_c\) superconductors, with considerable evidence for phonon anomalies in the vicinity of T\(_c\), and with a strong isotope effect when the materials are doped away from optimum T\(_c\). In this case, Fig. 2c can be taken as evidence that the structural transitions are compatible with a strong electron-phonon coupling. In fact, much more can be said. As the next Section will explain, a careful analysis of the purely ionic model strongly suggests that there should be strong electron-phonon coupling.
III. CU-O COMPRESSIBILITY AND STRONG ELECTRON-PHONON COUPLING

A. Doping Dependence of the Lattice Mismatch

In this Section, the ionic model is analyzed in detail, to better understand the doping dependence of the tolerance factor. We can begin by relating the interlayer strain $T_1$, Eq. 2, to the lattice mismatch. (The middle term of Eq. 2 has a weak doping dependence, since $n_h$ only varies from 1 to 1.2; it can be incorporated into a renormalized $\omega_0$.) If the equilibrium cell size of the CuO$_2$ plane is $a_1$ and of the LaO plane $a_2$, then the two layers will accommodate to one another at an intermediate cell size $a$, with $a_2 < a < a_1$. This will involve a compressional strain $\epsilon_1 \simeq (a - a_1)/a_1$ on the CuO$_2$ plane, and a tension $\epsilon_2 \simeq (a_2 - a)/a_2$ on the LaO plane. The equilibrium lattice size $a$ is found by minimizing the elastic energy

$$E_e = \frac{1}{2} C_1 \epsilon_1^2 + \frac{1}{2} 2 C_2 \epsilon_2^2; \quad (3a)$$

or

$$a = \frac{C_1 a_1 + 2 C_2 a_2}{C_1 + 2 C_2}; \quad (3b)$$

(The 2 in front of $C_2$ comes from the fact that there are two LaO layers.) This ensures that the stresses in the various layers are balanced,

$$T_1 = -2T_2,$$

where $T_i = C_i \epsilon_i$. Because of the stress-balance equation, the only free parameter is $T_2$, or equivalently $a_2 - a$. Hence, $T_{LTO}$ is a function only of $a_2 - a$. This is convenient, because $a$ is the measured radius, and the doping dependence of $a_2$ can be estimated from tables of ionic radii. In contrast, evaluation of $a_1$ requires knowledge of how hole doping modifies the Cu and O radii. In Appendix B, the parameter $a - a_2$ is estimated as a function of doping, and this result is used to derive the theoretical curves in Fig. 2 (see Eq. A2). As a result of the calculation, the largest contribution to the doping dependence of the transition is found to be the large ionic size change associated with $O^{2-} \rightarrow O^-$, with estimates for the $O^-$ radius that are about 14-21% smaller than that of $O^{2-}$.

The same calculation can also explain the Nd substitution results. The Nd ion is smaller than the La (1.163 Å for Nd$^{3+}$ vs. 1.216 Å for La$^{3+}$), so Nd substitution will worsen the mismatch, and hence should enhance the structural transition temperature. This is indeed observed: there is a strong variation of $T_{LTO}$ with Nd content (Fig. 2), which is quantitatively well described by the present model. However, the in-plane area of the orthorhombic cell, $ab$, is virtually unchanged by Nd substitution. This suggests that the cell size is fixed by the CuO$_2$ planes, while changing the La-Nd size leads predominantly to changes in incommensurability strains.

Correspondingly, it is found that increases in Sr doping lead to large decreases in $ab$.

This can be understood from Eq. 3b. If $C_1 \gg C_2$, then $a \approx a_1$, so the cell area will be independent of the Nd substitutions in the LaO layer, as observed. This is consistent with the expectation that the LaO layer should be more compressible than the CuO$_2$ layer [24]. Moreover, the CuO$_2$ layer is already compressed via the distortion of the CuO$_6$ octahedra, with the four planar O’s moving closer to the Cu, the two apical O’s moving away. (This is a molecular JT effect, which splits the degeneracy of the $d_{x^2-y^2}$ and $d_{z^2}$ orbitals on the Cu.) Hence, it will be hard to produce any additional CuO$_2$ compression (in the absence of hole doping).

In order to explain the pressure dependence of the LTO transition temperature, $dT_{LTO}/dp < 0$, Zhou, et al. [25] suggested that the Cu-O bond length is more compressible than the La-O bond length. This result is surprising, and is not consistent with the above finding, $C_1 \gg C_2$. Schilling and Klotz [26] have suggested that the anomalous $T_{LTO}(p)$ may be due to pressure induced charge transfer. While the sign of the charge transfer is the same as that found in other cuprates, direct Hall effect measurements have not found evidence for a pressure dependence of the hole concentration in LSCO.

B. Large Electron-phonon Coupling to In-Plane Phonons

The above calculations reveal that the purely ionic model is not self-consistent. The dominant factor in explaining the Sr doping dependence of the LTO transition is the large dependence of the O radius on valence. However, it is well known in rare earth compounds, that such large ionic contractions lead to large electron-phonon coupling, accompanied by lattice softening and elastic anomalies [12].

When electron-phonon coupling arises through the dependence of ionic size on valency, a large number of phonon modes can couple to the distortion. This occurs in other mixed-valence systems as well (see, e.g., Mook, et al. [27]). In the present case, Figure 3 illustrates some of the CuO$_2$ plane phonon modes which should have a strong coupling to the valence fluctuation. Thus, if the O$^-$ is localized on a single site, the local contraction will involve a Cu-Cu bond stretching mode, Fig. 3a. If it can hop between adjacent O’s across an intervening Cu, it will couple to the O-O bond stretching mode, Fig. 3b. These modes are expected to be longitudinal within a single Cu-O-Cu row on a given plane, but in successive rows, the stretch distortions can be either in-phase, as in Fig. 3a,b, or out of phase, as in Fig. 3c,d. It turns out that, due to vHs coupling, the gaps are larger for the out of phase modes, Fig. 3c,d. For completeness, certain other modes are illustrated in Fig. 3e,f. Figure 3e shows a related, ferroelectric
mode, a 2D version of the mode introduced by Egami, et al. [10]. In addition to the optical modes, there can also be coupling to elastic strains (to account for the average, homogeneous effects of volume reductions) and acoustic phonons (for the local, inhomogeneous effects), Fig. 3f. These shear strains function as secondary order parameters for the LTO transition.

Since these are all in-plane modes, it is not clear why the actual observed soft mode involves out-of-plane tilting. A possible explanation is developed in Fig. 3g. The extra hole is assumed to be partially delocalized in the $x$-direction, giving rise to a local shear, shrinking the lattice $x$-axis and increasing the $y$-axis. Since the layer is already under compression, the octahedra rotate about the $x$-axis, to tip the long-bond out of the $a - b$ plane. This would explain the highly anomalous feature of the LTT phase, that the Cu-Cu distance is shorter along the untitled bond than along the tilted one. An analogous effect occurs in the LTO phase.

Recently, Zhou, et al. [31] have also come to the conclusion that in-plane phonon modes play a large role in the dynamic JT effect in LSCO.

Thus, in analyzing the soft-mode instabilities, the following hypothesis will be adopted. The primary electron-phonon interaction involves a planar distortion, but as this softens, it interacts with the lower lying LTT-type tilt mode, leading to an actual soft mode of mixed symmetry. For a first analysis, this additional complication of phonon mode-mode coupling will be ignored, and only the planar mode will be included in the analysis of electron-phonon coupling.

C. Other Problems with the Ionic Model

There are a number of other features of this structural transition which are difficult to understand in a simple ionic picture. First, if the driving force for the transition is a layer mismatch, with the LaO lattice constant being too small, it is somewhat surprising that the LaO plane is buckled rather than flat. Billenge and Egami [32] also questioned the ionic model, noting that the CuO$_2$ planes in Nd$_{2-x}$Ce$_x$CuO$_4$ showed local buckling, even though in the ionic model, they are supposed to be under tension.

More importantly, Fig. 4 shows the doping dependence of the Cu-O bond length found by Radaelli, et al [33]. The detailed form of this dependence is inconsistent with a purely ionic model. There are actually a number of problems. One problem lies in the temperature dependence at fixed $x$. If the tolerance factor were the driving force for the transition, it would be expected that the Cu-O bond length would act like an order parameter, having a strong temperature dependence in the LTO phase. Instead, this bond length has a strong $x$ dependence, but is nearly independent of $T$ in the LTO phase, whereas it has a strong $T$ dependence and weak $x$ dependence in the HTT phase. The LTO-HTT transition occurs when these two bond lengths are equal.

This leads to a second problem: on each side of the phase transition, the stable phase is the one with the longer Cu-O bond length! This is opposite to the prediction of the ionic model, which says that the driving force for the transition is to reduce the Cu-O bond length.

There is also another potential problem. The dot-dashed line in Fig. 4 shows the doping dependence of the equilibrium Cu-O bond length, which agrees with the measured value in the LTO phase, but changes much more rapidly with doping than the experimental value in the HTT phase. The break in slope cannot be explained by the tolerance factor passing through the value unity. Theoretically, this is not expected to happen until $x \approx 0.42$. More importantly, the break in slope occurs at different $x$ values at different temperatures. However, the HTT data all come from the overdoped regime, $x > 0.15$. It is known [33] that the uniform phase is metastable against phase separation in this regime, and moreover, that the doping holes go into additional orbitals – in particular, the Cu $d_{xz}$ orbitals. Hence, the change in slope may be a signature of this electronic effect – experiments at higher temperatures and lower doping are clearly desirable. Again, this shows that electronic effects must be included in order to understand the structural phase transitions.

The dynamic JT model can provide at least a partial explanation of these facts. It is important to recall that the onset of the tilting instability actually occurs at $T^*$. Hence, since both the LTO and HTT phases are dynamic JT phases, the HTT-LTO crossover will be controlled by long-range strain forces, and need not involve a substantial change in the Cu-O bond length.

IV. LINEAR ELECTRON-PHONON COUPLING AND THE O-O BOND STRETCHING MODE

Figure 3 illustrates some of the phonon modes which could couple to the large O-atom valence fluctuations. To better understand the nature of the resulting electron-phonon coupling, the modification of the electronic band structure can be calculated, in the presence of a static distortion of the appropriate symmetry. It is assumed that the distorted bond lengths lead to a modulation of the Cu-O hopping parameter $t_{\text{CuO}}$, $t_{\text{CuO}} \rightarrow t_{\text{CuO}} \pm \delta t$. Assuming the standard three-band model for the CuO$_2$ planes, Figure 5 illustrates the resulting dispersions, showing that several modes can open a gap at the Fermi level. The calculations are given in Appendix C. (The figure is calculated assuming bare band parameters, $t = 1eV$, $\Delta = 4eV$; for the renormalized bands [34], the energy scale should be reduced by a factor of $\sim 4$.)

From Fig. 5, it can be seen that the largest gap is associated with the O-O bond stretching mode, Fig. 5d. The Cu-Cu bond stretching mode has a comparable gap, but with a strong $k$-dependence, and vanishes at the vHs
(5c). This difference is discussed in Appendix C. No gap is opened for the FE mode (5e) or the strains (5f), although in the latter case, the anisotropy splits the vHs degeneracy along the X and Y axes. The differences between the $q_1$ nesting (Fig. 5a,b) and $q_0$ nesting (Fig. 5c,d) lie mainly in the different zone folding associated with the doubling of the unit cell. For $q_1$ nesting, the X point is mapped into $\Gamma$, while M is mapped into $Y$; on the other hand, $q_0$ maps M into $\Gamma$ and X into Y. For ease in comparison, Figs. 5e,f are illustrated including a $q_0$-type zone folding.

The O-O bond stretching mode looks like an ordinary 1D Peierls instability cum CDW, and has the form postulated for the vHs-JT effect. Tang and Hirsch [35] had analyzed the CDW transition several years ago, and found that it did not couple to the vHs’s. However, they used a Cu-only model, so their CDW corresponds to the Cu-Cu bond stretching mode, which indeed does not split the vHs degeneracy, Fig. 5c. From Eq. C9, it can be seen that the O-O bond stretching mode, Fig. 3d and the shear strains, Fig. 3f, involve a linear electron-phonon coupling, as opposed to the quadratic coupling to the tilt-mode phonons. This linear coupling will lead to large polaronic effects, since the more localized the hole is, the closer to O$^-$ is the corresponding oxygen, with a much larger local contraction. Such polaronic effects have often been postulated to play a role in the high-T$_c$ superconductivity.

Direct evidence for anomalously strong electron-phonon coupling of the O-O bond stretching mode has been found by neutron scattering measurements, both in LSCO and in YBCO, and closely analogous results are found in Ba$_{1-x}$K$_x$BiO$_3$ (BKBO). In undoped LSCO, this one-dimensional bond stretching mode is found near 20THz, with a weak softening near the X-point. Upon doping, the softening substantially increases [29]. A similar result is found in YBCO [20].

In BKBO, it has generally been believed that the structural anomalies are associated with three dimensional breathing modes. However, in the heavily doped materials there are soft modes associated with BiO$_6$ octahedral tilts, similar to those in LSCO [14]. Moreover, no anomalous softening of the three-dimensional breathing modes is found. Instead, the one-dimensional Bi - O bond stretching mode softens, again in complete analogy to the cuprates [14]. It has proven difficult to model this softening in a lattice dynamical model, assuming the local symmetry is cubic. These results suggest that in BKBO the structural and superconducting anomalies may be associated with a 3D vHs, as in the Bilbro-McMillan model [27], which has been applied to the A15’s and BaPb$_{1-x}$Bi$_x$O$_3$ [58].

V. POLARONIC HAMILTONIAN

Let us briefly summarize the above discussion. The analysis of the doping dependence of $T_{c\text{LTO}}$ shows that, while interlayer mismatch is a dominant driving force, a purely ionic model cannot provide an adequate description of the data. Moreover, even within the ionic model, most of the accommodation of the mismatch with doping is found to be due to a large variation of the in-plane Cu-O bond length with doping (chemically, with the valence change O$^2-$ → O$^-$). This bond length change itself produces a large electron-phonon coupling, with a number of in-plane modes. The strength of coupling can be estimated from the size of the gap resulting from a CDW distortion: the largest gap is associated with the O-O bond stretching mode, Fig. 5d, due to the splitting of the vHs degeneracy. However, the symmetry of this distortion is not that of the LTO phase, so this distortion can only be present in the form of a local, short-range order, possibly dynamic. Such short range order has already been postulated in terms of the tilting modes [3]. This picture is supported by experiments, which find significant softening of the relevant modes, and LDA frozen phonon calculations, which find a significant phonon softening for this mode.

These results suggest an important modification to the earlier calculations of the LT-T-LTO-HTT transitions as a series of dynamic vHs-JT effects [3,15]. In these papers, the soft mode was identified with the experimentally observed mode, associated with octahedral tilt (plus an associated shear strain). This led to an unusual electron-phonon coupling, quadratic in the tilt angle $\theta$, and hence in the phonon creation operator – in violation of Migdal’s theorem. Nevertheless, the resulting coupling is estimated to be quite large [4,35]. The present results suggest that the tilting is a secondary effect, and the primary driving force is associated with in-plane modes (particularly the O-O bond stretching mode) that have a linear electron-phonon coupling. Hence, there are important polaronic contributions, which will be estimated below. Note that many of the predictions of the model are not sensitive to the particular phonon mode; these include the occurrence of a pseudogap [4], and of a dynamic JT effect [11], which has apparently been observed experimentally [4,11].

In this section it will be assumed that the principal electron-phonon coupling is with the planar bond stretching mode, and that the tilt mode softens first due to phonon mode-mode coupling with these planar modes. The complications due to this mode-mode coupling will here be ignored, leaving a problem with a linear electron-phonon coupling, which can be analyzed using standard techniques. It should be noted that the resulting model is essentially a vHs-driven CDW instability, and hence very similar to a number of earlier calculations [12,43]. The differences are in the identification of the dominant phonon mode (Fig. 5d), and the realization that the
Among the simplifications assumed are (1) the Fermi surface is square at half filling, since the O-O hopping term has been neglected (this was done only for simplicity, and an appropriate \( t_{OO} \) is required to move the vHs into this regime, and the extra couplings introduced by this term greatly complicate the analysis, without significantly affecting the underlying physics.

Assumption (3) restricts the analysis to a single branch of phonons, which includes the O-O bond stretching mode. The distinction between the phonons of the form of Fig. 4b and 4d lies in the direction of the phonon propagation vector, corresponding to two different cuts along this branch. For the cut of Fig. 4b, \( \vec{q} = \xi \vec{q}_0 \), where \( \vec{q}_0 = (\pi/a, \pi/a) \); and for cut 4d, \( \vec{q} = \xi \vec{q}_0 \), \( \vec{q}_0 = (\pi/a, \pi/a) \). Only the latter cut will be analyzed in detail. The corresponding phonon operators will be denoted so \( Q_{\vec{q}} = Q(\lambda, \vec{q}) \), \( P_{\vec{q}} = P(\lambda, \vec{q}) \), and \( \omega_{\vec{q}} = \omega_0(\lambda, \vec{q}) \). It should be noted that this same phonon, at \( \vec{q} = 0 \), has the character of a FE mode. In a more detailed treatment of the phonons, this should correspond to a nearly pure O-O vibration, with the xO’s and yO’s vibrating out of phase.

The analysis of Section III (Figs. 4,5) suggests that the electron-phonon coupling should be included via the dependence of \( t \) on the ionic separation \( \vec{u} \):

\[
t_{ij} = t + (\vec{u}_j - \vec{u}_i) \cdot \vec{\nabla} t_{ij},
\]

where the \( \vec{u}_i \)'s are the displacements of the \( i \)th atoms. The \( \vec{u}_i \) can be expanded in terms of the phonon normal mode coordinates as

\[
\vec{u}_i = \sum_{\lambda, \vec{q}} \frac{\vec{e}(\lambda, \vec{q})}{(mN)^{1/2}} e^{i \vec{q} \cdot \vec{R}_i} Q(\lambda, \vec{q}),
\]

with \( \vec{e}(\lambda, \vec{q}) \) the polarization vector and \( m \) the ionic mass. In the present, single branch approximation, defining \( \vec{g}_{\vec{q}} = -\vec{e}(\lambda, \vec{q}) \cdot \vec{\nabla} t/\sqrt{mN} \), the electron-phonon coupling with the O-O bond stretching mode becomes

\[
H_{e-\text{ph}} = \sum_{\vec{k}, \vec{q}} g_{\vec{q}}(\vec{k})(d_{\vec{k}\vec{x}}^\dagger p_{\vec{x}, \vec{k} - \vec{q}}^\dagger + p_{\vec{x}, \vec{k} - \vec{q}}^\dagger d_{\vec{x}}^\dagger),
\]

with

\[
g_{\vec{q}}(\vec{k}) = 2g_{\vec{q}c_x}.
\]

(To describe the Cu-Cu hopping, it is only necessary to make the substitution \( c_x \rightarrow -\cos(k_x - \pi)\pi/2 \) in Eq. 10.)

The resulting Hamiltonian, Eqs. 4-7,9, is almost exactly of the form analyzed in Ref. [4] (after Balseiro and Falicov [17]) to study the competition between Peierls instability and superconductivity. The differences are (1) the Fermi surface is square at half filling, since the O-O hopping term has been neglected (this was done only for simplicity, and an appropriate \( t_{OO} \) may readily be reintroduced); and (2) the electron-phonon coupling \( g(\vec{k}) \) now has an important wave number dependence.
B. Link Operator Formalism

The electron-phonon coupling term can be eliminated by a canonical transformation [46, 48–50]:

\[ \hat{H} = e^{-iS/h}He^{iS/h} \approx H + \frac{i}{\hbar}[H, S]. \] (11)

In the usual small polaron theory (e.g., Ref. [50]), this transformation must be carried out to all orders in \( S \) to correctly describe the polaronic band narrowing. However, in the present problem, the function \( S \) is quite complicated, due to the 2D nature of the problem. Hence, in what follows, I introduce the following approximation scheme. I first find an \( S \) which exactly eliminates the electron-phonon coupling in first order, Eq. 11. I then show that in the transformed Hamiltonian \( \hat{H} \), the hopping parameter is renormalized to \( t \to t(1 - S) \). This is precisely the form of the lowest order band narrowing found in conventional small polaron theory, and \( S \) can be shown to have exactly the same interpretation. Hence, it will be assumed that the role of higher order terms is essentially the same in the present model, to transform the renormalization to \( (1 - S) \to e^{-S} \). The results are given in Section V.C.4.

\( S \) can be expressed in terms of the (generalized) link operators as

\[ S = i \sum_{\vec{k}, \vec{q}} (Q_{\vec{k}, \vec{q}} A_{\vec{k}, \vec{q}} - iP_{\vec{k}, \vec{q}} B_{\vec{k}, \vec{q}}), \] (12)

where

\[ A_{\vec{k}, \vec{q}} = \sum_{i=1,9} f_{\vec{i}, \vec{q}} \rho_{i, \vec{k}, \vec{q}} \] (13a)

\[ B_{\vec{k}, \vec{q}} = \sum_{i=1,9} h_{\vec{i}, \vec{q}} \rho_{i, \vec{k}, \vec{q}} \] (13b)

\[ \rho_{1, \vec{k}, \vec{q}} = d_{\vec{i}, \vec{q}}^d \rho_{x, \vec{k}, \vec{q}} \pm p_{x, \vec{k}, \vec{q}}^d d_{\vec{i}, \vec{q}}^d, \] (14a)

\[ \rho_{2, \vec{k}, \vec{q}} = p_{x, \vec{k}, \vec{q}}^d d_{\vec{i}, \vec{q}}^d \pm d_{\vec{i}, \vec{q}}^d p_{x, \vec{k}, \vec{q}}^d, \] (14b)

\[ \rho_{3, \vec{k}, \vec{q}} = d_{\vec{i}, \vec{q}}^d \rho_{y, \vec{k}, \vec{q}} \pm d_{\vec{i}, \vec{q}}^d \rho_{y, \vec{k}, \vec{q}} \] (14c)

\[ \rho_{4, \vec{k}, \vec{q}} = p_{y, \vec{k}, \vec{q}}^d d_{\vec{i}, \vec{q}}^d \pm d_{\vec{i}, \vec{q}}^d p_{y, \vec{k}, \vec{q}}^d \] (14d)

\[ \rho_{5, \vec{k}, \vec{q}} = d_{\vec{i}, \vec{q}}^d \rho_{z, \vec{k}, \vec{q}} \pm d_{\vec{i}, \vec{q}}^d \rho_{z, \vec{k}, \vec{q}} \] (14e)

\[ \rho_{6, \vec{k}, \vec{q}} = p_{z, \vec{k}, \vec{q}}^d d_{\vec{i}, \vec{q}}^d \pm d_{\vec{i}, \vec{q}}^d p_{z, \vec{k}, \vec{q}}^d \] (14f)

These link operators are the generalization of the operators introduced by Halperin and Rice [51] into the problem of density wave instabilities of an electron gas, and first applied to the cuprates by Schulz [52]. They also bear a close resemblance to the valence bond operators studied by Affleck and Marsden [53].

A few technical points about these operators should be noted. First, the Hamiltonian, Eq. 4, can be rewritten in terms of these operators:

\[ H_e = \sum_{\vec{k}} \left( \frac{\epsilon_d \rho_{5, \vec{k}, \vec{q}} + \epsilon_p (\rho_{6, \vec{k}, \vec{q}} + \rho_{7, \vec{k}, \vec{q}})}{2} \right. \]

\[ \left. + t_{xz} \rho_{1, \vec{k}, \vec{q}}, \rho_{3, \vec{k}, \vec{q}}, \rho_{4, \vec{k}, \vec{q}} \right), \] (15a)

\[ H_{e-ph} = \sum_{\vec{k}, \vec{q}} Q_{\vec{k}, \vec{q}} \tilde{\gamma} (\vec{k}) \rho_{1, \vec{k}, \vec{q}} \] (15b)

with \( t_{x, \vec{k}} = 2it_{s, \vec{i}, \vec{q}}, \) \( s_{\vec{i}, \vec{q}} = \sin(k_i a/2). \) Secondly, the sign change in Eq. 14e-i arises because the hopping term in \( H_e \) is imaginary (i\( s_{\vec{k}, \vec{q}} \)). Finally, the set of \( \rho \)'s is actually overcomplete, since, e.g., \( \rho_{3, \vec{k}, \vec{q}} = \pm \rho_{1, \vec{k}, \vec{q}} \). Because of the 2D nature of the problem, finding the \( f_i \)'s and \( h_i \)'s requires inverting an 18 \( \times \) 18 matrix. The solution is given in Appendix D.

C. Polaronic Effects

1. Effective Interaction

Once the linear electron-phonon coupling is eliminated, we are left with a complicated Hamiltonian involving electron-electron and quadratic electron-phonon interactions, describing a rich variety of phenomena, including phonon softening, structural instability (CDW formation), and superconductivity. In this paper, no attempt is made to sort out all of these effects, but only to summarize the various phenomena which are expected. For this purpose, two simpler, approximate solutions are also presented in Appendix D: one is a three-band, but quasi-1D solution, in which coupling terms involving only the \( x \) direction are retained. The second approximate solution is an effective one-band solution, in which the three-band electronic Hamiltonian is diagonalized, and only transitions within the antibonding band are retained. The resulting equations are qualitatively similar to standard results for polaronic calculations. However, there are some
subtleties, involving band mixing and a potential \( k \) dependence of the couplings.

The qualitative nature of the resulting polaronic Hamiltonian can be seen by ignoring all the link operators except \( \rho_1 \) in Eqs. 12-14, and approximating

\[
f_{\vec{k}, \vec{q}} \approx \frac{\hbar \tilde{g}_q(\vec{k}) \beta_{\vec{q}}}{\hbar^2 \omega_{\vec{q}}^2 - (E_{\vec{k}} - E_{\vec{k}-\vec{q}})^2},
\]

(16a)

\[
\beta_{\vec{q}} \approx \frac{\hbar^2 \omega_{\vec{q}}^2 \Delta}{\Delta^2 + 16\beta^2}.
\]

(16b)

\[
h_{\vec{k}, \vec{q}} \approx \frac{f_{\vec{k}, \vec{q}} A t^2}{\Delta \hbar \omega_{\vec{q}}^2}
\]

(16c)

(see Eq. D11). The commutator of \( S \) with \( H_{e-ph} \) gives the residual interaction terms,

\[
\frac{i}{\hbar} [H_{e-ph}, S] = H_{e-e} + H_{e-ph}^{(2)},
\]

(17)

with (Eq. D9)

\[
H_{e-e} = - \sum_{\vec{k}, \vec{k}'} h_{\vec{k}, \vec{q}} \tilde{g}(\vec{k}) \rho_{\vec{k}+\vec{q}} \rho_{\vec{k}'+\vec{q}}
\]

(18)

The remaining term, \( H_{e-ph}^{(2)} \), is complicated in the three-band model, because it mixes in different link operators, \( \rho \) (see Eq. D13). However, it simplifies in the one-band model, to

\[
H_{e-ph}^{(2)} = - \sum_{\vec{k}} \frac{f_{\vec{k}, \vec{q}} Q^2}{\hbar} (\alpha_{\vec{k}+\vec{q}} \psi_{\vec{k}+\vec{q}} - \alpha_{\vec{k}-\vec{q}} \psi_{\vec{k}-\vec{q}}^\dagger),
\]

(19)

where \( \psi \) is the wave function of the antibonding band, \( f_\vec{k} \) (Eq. D20) is closely related to \( f_{\vec{k}, \vec{q}} \) above, and \( \alpha_{\vec{k}} \) is given by Eq. D18b.

2. Polaron Binding Energy

The polaron binding energy can be defined from Eq. 18 as

\[
E_P = \lim_{\Delta E \to 0} \sum_{\vec{k}} h_{\vec{k}, -\vec{q}} \tilde{g}(\vec{k})
\]

\[
= \sum_{\vec{k}} |\tilde{g}_q(\vec{k})|^2 \eta \frac{2}{2\omega_{\vec{q}}}
\]

\[
= \frac{4\beta^2 a^2}{ma^2 \omega_{\vec{q}}^2},
\]

(20)

where \( \Delta E = E_k - E_{k-\vec{q}} \), \( \eta = 1/2(1 + (\Delta/4t)^2) \), and the electron-phonon coupling constant can be roughly estimated as \( |g_{\vec{q}}| \sim -\hbar \gamma / \sqrt{mN} \), where \( \beta \) is a dimensionless parameter, \( \sim 3 - 5 \) [32]. This estimate relies on a simple tight-binding model. A better way to estimate \( g \) would be via an LDA frozen phonon calculation [13].

Using numerical estimates of \( t = 0.25 eV \), \( \beta = 3.5 \), and \( \hbar \gamma \approx 50 meV \), a modest value \( E_P \approx 6 meV \) is found. However, since \( \Delta E \ll \hbar \gamma \), Grilli and Castellani [34] showed that correlation effects should not reduce \( g \). This would correspond to using a bare value \( t \approx 1.3 eV \) in the above estimate, leading to \( E_P \approx 70 meV \).

3. Phonon Softening

In a mean field decoupling, \( H_{e-ph}^{(2)} \) leads to a phonon mode softening,

\[
\omega_0^2 = \omega_0^2 + \sum \gamma_k \frac{(n_k - n_{k-\vec{q}})(E_k - E_{k-\vec{q}})}{(E_k - E_{k-\vec{q}})^2 - \hbar^2 \omega_0^2}
\]

(21)

where \( n_k = \langle \psi_{\vec{k}}^\dagger \psi_{\vec{k}} \rangle \), and the precise form of \( \gamma_k \) is not important for present purposes (see Eq. D22). In a self-consistent calculation, the bare \( \omega_0 \) in the denominator of Eq. 21 would be replaced by \( \omega_0 \). Making this substitution, a phase transition occurs when \( \omega_0 \) is renormalized to zero, or

\[
\omega_0^2 = - \sum \gamma_k \frac{n_k - n_{k-\vec{q}}}{E_k - E_{k-\vec{q}}}
\]

(22)

In Eq. 22, the \( E \)'s can be replaced by \( E' = E - E_F \). Now if the Fermi energy falls at the vHs, then \( E_{k-\vec{q}} = -E_k \), so the transition temperature \( T_0 \) is given by

\[
\omega_0^2 = \gamma_k > \int_{-B}^{B} \frac{N^*(E) dE}{2E tanh(\frac{E}{2k_B T_0})},
\]

(23a)

where \( \gamma_k \) is the average of \( \gamma_k \) over angles, \( B \) is the half bandwidth, and \( N^*(E) \) is an effective density of states (dos)

\[
N^*(E) = \frac{1}{\pi} \sum_{k, \epsilon} \frac{\gamma_k}{|\partial E / \partial k_x|}
\]

(23b)

The integral in Eq. 23 must be evaluated numerically, but certain general features can be directly extracted. The result is sensitive to the angle dependence of \( \gamma_k \). If \( \gamma_k \) is a constant, then the results are the same as found earlier [4]. \( N^*(E) \) is the actual dos, which diverges logarithmically at the vHs, greatly enhancing \( T_0 \). This appears to be consistent with the gap found for the O-O bond stretching mode, Fig. 5d. However, the approximation of retaining only one pair of link operators is too
crude to reproduce this feature, and the model γ’s are found to have a more complicated angular dependence. Indeed, it is expected, on analogy with the results of Appendix C, that extreme care must be taken to derive the correct angle-dependence of the gap.

For other phonon modes, however, γ_E is expected to have an important angle dependence. Thus, for the Cu-Cu bond stretching mode, γ_E γ ≈ γ0 sin^2 k_a a (see the discussion below Eq. C8). In this case, N*(E) ≈ 16πB^2 - E^2/πB^2, remaining finite at the vHs, E = 0, and

\[ k_B T_0 \simeq 1.14 \frac{B}{\lambda} e^{-1/\lambda}, \quad (24a) \]

with

\[ \lambda = 4 < \gamma_E > N_1 / \omega_q^2, \quad (24b) \]

with N_1 = 16/\pi^2 B. Thus, for the Cu-Cu bond stretching mode, the CDW has a logarithmic instability, and not the ln^2 instability expected for a vHs-related singularity, due to the fact that the CDW gap for this mode vanishes at the vHs, Fig. 5c. This is consistent with earlier work [35].

4. Polaronic Band Narrowing

The term H_2^{(2)} also induces a polaronic reduction of the bandwidth [39]. In the Appendix, this reduction is calculated to lowest order in S as t → t (1 - S), Eq. D15, with

\[ S \simeq \sum_q \left( \frac{\bar{g}_q(\bar{k}) h_1 \bar{E}_q - \bar{q}}{\hbar \omega_q^2} \right) (N_q + \frac{1}{2}), \quad (25a) \]

where the Bose function is

\[ N_q = \frac{1}{e^{\hbar \omega_q / k_B T} - 1}. \quad (25b) \]

In conventional polaron theory, inclusion of higher order commutators in S leads to an exponential bandwidth reduction. Hence, I hypothesize that the main effect of including higher order commutators with S in Eq. 11 would be the renormalization

\[ t \rightarrow t e^{-S}. \]

However, since S can have either sign, a more appropriate approximation would be

\[ t \rightarrow \frac{2t}{1 + e^{2S}}. \quad (25c) \]

By comparing Eq. 25a and Eq. 20, it can be seen that at low temperatures (N_q ≈ 0) S ≈ E_p / \hbar \omega_q, so using the above estimate for E_p, exp(S) ≈ 5.

In all of the above expressions, the Fermi energy enters only through the Fermi-Thomas function, n^-1. The polaronic band narrowing, Eq. 25, however, is independent of n^-1, and hence of E_p! It depends only on the details of the band structure; in particular, there is a significant band narrowing only when

\[ \hbar \omega_{ph} > |E_{\bar{k} + \bar{q}/2} - E_{\bar{k} - \bar{q}/2}|. \quad (25d) \]

When this condition is satisfied, the bandwidth reduction is similar to the usual phonon renormalization, 1/(1 + λ), with λ ~ e^S.

The condition, Eq. 25d, is discussed in more detail in the following section. It is found that this condition can be satisfied only in the immediate vicinity of the vHs! This may explain the presence of ‘extended vHs’s’ [3] in the cuprates. Figure 6 illustrates a calculation of the modified band structure of Bi-2212, if it is assumed that there is a phonon renormalization of the energy bands by a factor λ = 3 within ω = 40 meV of the Fermi level. The value λ = 3 is in satisfactory agreement with the renormalization factor exp(S) found above. Moreover, a similar band narrowing is found near the vHs in YBa_2Cu_3O_6 [1], even though the vHs is ~ 19 meV away from the Fermi level.

If terms in t_{OO} are retained, the parameters t and t_{OO} are renormalized by different factors, so polaronic effects could lead to a change in the shape of the Fermi surface. Analogous effects found in the f-electron problem [50] suggest that direct O-O hopping may be more seriously affected than Cu-O hopping.

In ordinary small polaron theory [51], the higher order commutators play two roles: for the coherent hopping, they lead to a polaronic band which becomes increasingly narrow as temperature is raised, as in Eq. 25. However, they also lead to an incoherent hopping due to nondiagonal transitions (in which the number of phonons bound to the electron changes during the hopping process). This latter effect is not accounted for in the present calculation, which treats S to lowest order.

5. CDW vs. Superconductivity

The CDW and superconducting instabilities can also be studied in terms of H_{e-e}. For the CDW instability, only the term in \bar{q} = \bar{q}_0 is retained [17,4]. With this approximation, H_{e-e} becomes, in mean field,

\[ H_{CDW} = -G_0 \sum_{\bar{k}} \bar{c}_e \rho_{1 + \bar{k}, \bar{q}_0}. \quad (26) \]

Since H_e + H_{CDW} is quadratic, it can be diagonalized by the Bogoliubov-Valatin transformation. The resulting dispersion satisfies Eq. C6, if G_0 = 2δt. Again, the present approximate models lead to a G_0 with a more complicated angular dependence.
VI. DISCUSSION

A. Ionic-Covalent Crossover and the vHs

In their discussion of electron-phonon coupling induced by valence fluctuations in f-electron metals, Sherrington and Riseborough (SR) introduced a Hamiltonian with a somewhat different form of $H_{e-ph}$. SR assumed a direct coupling to the valence fluctuation, which in the present context would give

$$H_{e-ph}^{SR} = \sum_{\vec{k}, \sigma} g_{\vec{q}} p_{\vec{k}+\vec{q}, \sigma}^\dagger p_{\vec{k}, \sigma} Q_0.$$  (27)

Here, while the tight-binding electron-phonon coupling has a different form, Eq. 9, the resulting Hamiltonian automatically includes a term like Eq. 27, but with quadratic phonon coupling, Eq. D13.

The present calculation sheds some light on a feature that SR were attempting to describe: the competition between covalency and ionicity. They pointed out that earlier theories of electron-phonon coupling in f metals ranged from strongly covalent, with each rare earth ion having average values of ionic size and f-electron occupation number, to strongly ionic, with well-defined $f^n$ and $f^{n-1}$ ions. SR suggested that this competition is represented by terms describing hopping, $t$, and electron-phonon coupling, $H_{e-ph}$: $H_{e-ph} < t$ represents the covalent limit, with the valence that can freely fluctuate, while the opposite limit, $H_{e-ph} > t$, is the ionic limit, in which each ion has a well defined valence.

This can be restated: the strong electron-phonon coupling is associated with valence fluctuations: a hole hops onto an O$^2-$, causing its radius to collapse, leading to an enhanced local value of $t$. For the collapse to occur, the phonon must be able to follow the electronic motion, $\omega_{ph} \sim (hopping rate)$. For an ‘isolated CuO molecule’, this hopping rate is $\sim t/h > \omega_{ph}$. Near half filling, strong correlations reduce the hopping, but the inequality still holds, $J \approx 130meV > \hbar \omega_{ph} \approx 30 – 70meV$.

In a band, however, the electronic motion is restricted by the motion of other electrons, and the relevant frequency becomes $\vec{q} \cdot \vec{v}_F$, where $q$ is the phonon wave number and $v_F$ the Fermi velocity. At an arbitrary point on the Fermi surface, this quantity is of comparable magnitude to $t/h$, but $v_F$ *vanishes at a vHs*! Figures 7a,b show a map of the $v_F$ surface for a variety of different Fermi levels, while Fig. 7c (solid line) shows the minimum value of $\vec{q}_0 \cdot \vec{v}_F$, as a function of Fermi energy. What is plotted is the velocity normalized to a zone boundary phonon, $v_i^r = \hbar v_{Fi}/a$; for a phonon away from the zone boundary, the curves should be scaled by the ratio $qa/\pi$. (In this plot, the renormalized band dispersion parameters are used, $t = 0.25eV$, $\Delta = 1eV$.) From these figures, it is clear that there is only a narrow range of energies for which $\vec{q} \cdot \vec{v}_F \leq \omega_{ph}$, particularly near the zone boundary. Moreover, the slowest velocities are associated with hopping in directions near X and Y – i.e., towards the Cu’s. For these directions, and sufficiently close to the vHs, the electronic motion is slow enough that the molecular distortions can keep up.

The condition

$$\omega_{ph} \simeq \vec{q} \cdot \vec{v}_F.$$  (28a)

can be reinterpreted in a number of ways. First, for acoustic phonons the sound velocity is $c_s = \omega_{ph}/q$, and Eq. 28a becomes

$$c_s \simeq v_F.$$  (28b)

– the ‘surf riding’ condition that signals the onset of Landau damping. Finally, for large $q$, the electronic dispersion should be treated more carefully, and Eq. 28a should be replaced with

$$\hbar \omega_{ph} \simeq E_{\vec{k}+\vec{q}/2} - E_{\vec{k}-\vec{q}/2},$$  (28c)

for some electronic wave number $k$, where $E_{\vec{k}}$ is the electronic energy dispersion. Equation 28c should be compared to the resonant denominators of Eqs. 16a and 21.

The right-hand side of Eq. 28c is plotted as the dashed line in Fig. 7c, and it can be seen that use of this condition broadens the range of energies over which the inequality is satisfied. This last equation is the condition for a resonant electron-phonon interaction – i.e., both energy and momentum are conserved. Such a coupling will lead to large modifications of both the electronic and phononic dispersions.

This suggests a new interpretation for the vHs. Away from a vHs, electronic hopping is very fast, and it is hard to say just which atom the electron is on instantaneously. The band is a mixture of Cu and O, with both at an intermediate valence – i.e., the coupling is covalent. The Born-Oppenheimer (adiabatic) approximation is valid: the electronic motion is so fast that it responds instantaneously to any nuclear motions. Near a vHs, the opposite, anti-adiabatic limit is valid. The electronic motions are slow compared to the nuclear motions – for at least some of the electrons, $v_F = 0$. In this limit, the valence of an individual atom is much more definite. For instance, in the fast hopping regime, the local distortions associated with O$^-$ vs O$^{2-}$ do not have a chance to develop, so all O’s have a common, intermediate value of radius. Near the vHs, on the other hand, Cu-O hopping is slowed down, allowing local distortions to develop, so that an O$^-$ can be clearly distinguished from an O$^{2-}$ by its smaller radius. In short, near a vHs the nuclear
motion can ‘instantaneously’ follow the electronic motion, and the bonding goes from covalent to substantially more ionic. This leads to the strong enhancement of the electron-phonon coupling.

Since correlation effects also act to slow down the Cu-O hopping, this may be an explanation for why correlation effects act to pin the vHs nearer to the Fermi level at half filling.

B. Future Work

The present paper is the second of a projected series of papers whose aim is to provide a firm basis for analyzing the vHs-JT model within the three-band model of the cuprates. The first paper (XA) had two purposes: the main purpose was to extend the slave boson calculation of correlation effects to the full 3-band model; the second, to explore a possible linear electron-phonon coupling induced by spin-orbit coupling. The present paper (XB) further explores electron-phonon coupling in the Peierls regime, when correlation effects are expected to be weak. A strong, linear component is found to contribute to the dynamic JT fluctuations, leading to important polaronic effects.

A related paper (XIA) presently under preparation, analyzes electron-phonon coupling in the spin-Peierls regime, where correlation effects are strong – in the 2D Heisenberg limit near half filling. In future papers, I hope to extend these results to the three-band model. At this point, I should be able to study both Peierls and spin-Peierls regimes in parallel. Only then will I be able to give a detailed calculation of the doping dependence of the structural transitions, including the ‘pseudogap’, and to better understand the possible nanoscale phase separation in these materials.

A brief mention should be made about spin-orbit coupling, discussed in XA. Spin-orbit coupling leads to interesting modifications of Fermi surfaces, and, since it leads to a linear electron-phonon coupling, it could play a role in driving structural instabilities. This effect competes with the dynamic JT effect (a competition well known in molecular JT problems). It has been suggested that spin-orbit coupling is too small to drive any structural instabilities. However, a simple estimate (Appendix E) shows that, near a vHs, this suggestion may not be correct.

VII. CONCLUSIONS

The present calculations clarify the nature of electron-phonon coupling in the HTT-LTO-LTT phase transitions in LSCO, LBCO. First, the dominant effect in the transition is the change of Cu-O bondlength with doping. This large valence dependence of the oxygen ion radius is a signature of a strong, linear electron-phonon coupling. However, as the corresponding phonon modes soften, they interact with the very soft tilt modes, driving them unstable. Thus, although the dominant coupling is linear, the final instability involves quadratically coupled phonons.

Therefore, the full theory involves both holes and two types of phonons – the stretch modes and the tilt modes. However, the main effects on the holes are produced by the stretch modes, and including only these leads to a major simplification within the vHs-JT model, in that the earlier, quadratic phonon coupling to electrons is replaced by a linear coupling. This linear, in-plane coupling can now be treated by conventional techniques, providing a possible microscopic basis for the many polaronic models of superconductivity. A striking prediction of the model is a significant band narrowing, only in the immediate vicinity of the vHs, thereby providing a plausible explanation for the existence of ‘extended vHs’.

The reason the band narrowing is localized near the vHs is connected with a special property of the vHs. Near a vHs, the material is in the ‘ionic limit’, in that the electronic motion is slow compared to phonon motion, so valence fluctuations are well defined.

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APPENDIX A: DOPING DEPENDENCE OF LTO TRANSITION

Figure 3 of Ref. showed that the phonon softening associated with the LTO transition in La$_2$CuO$_4$ could be modelled in terms of a microscopic picture involving phonon anharmonicity and electron-phonon coupling. The data were insufficient to fix values for all the parameters, and in particular the electron-phonon interaction parameter could be varied over a large range, including zero. The same model can be applied to explaining the doping dependence of the transition temperature, $T_{LTO}$, for either Sr or Nd doping, Figure 2.

From Eq. 35 of Ref., $T_{LTO}$ is the solution of

$$\omega_0^2 + [9\Gamma_1 + \Gamma_2 - \alpha_e^2 N(0)]\Delta_1 = 0. \quad (A1)$$

Here, $\omega_0$ is the ‘bare’ phonon frequency, the $\Gamma_i$’s represent anharmonic (quartic) phonon-phonon couplings, $\alpha_e$ is an electron-phonon coupling parameter, and $\Delta_1 \propto \coth(\omega_1/2k_BT)$ is proportional to the fluctuations of the tilt amplitude (the frequency $\omega_1$ is defined in Ref.). In the absence of electron-phonon coupling, Eq. A1 has a solution only if $\omega_0^2$ is negative. Such negative values
can be caused by strains due to interlayer mismatch, and to explain the doping dependence of $T_{LTO}$, it will be assumed that Eq. 2 holds, which can be rewritten as
\[ \omega_0^2 = \omega_0^2 + \Gamma (a - a_2). \] (A2)
(Since $n_h$ only varies from 1 to $\sim 1.2$, the main effect of the middle term in Eq. 2 can be absorbed into a renormalized value of $\tilde{\omega}_0$.)

The temperature dependence of Eq. A1 comes from that of $\Delta_1$ and that of $N(0)$, whereas the doping ($x$) dependence is assumed to come from that of the lattice mismatch, $(a - a_2)$, and that of $N(0)$. The lattice mismatch is estimated in Appendix B. The hardest factor to quantify is the dos, $N(0)$, due to the important role of correlation effects. In the absence of correlation effects, assuming a rigid-band doping dependence and a $vH$s shifted away from half filling, $N(0)$ can be written as
\[ N(0) = \frac{1}{2B} \ln \left( \frac{B}{\sqrt{\mu^2 + (k_B T)^2}} \right), \] (A3)
where $B$ is the bandwidth, and $\mu(x)$ is the distance in energy between the $vH$s and the Fermi level. This equation should hold in the doped materials near optimum $T_c$, but near half filling correlation effects become important.

Correlation effects reduce the electron-phonon coupling, $\alpha_e$, for the usual Peierls interaction [1][4], but there is also a spin-Peierls coupling, for electron-phonon coupling stronger than a critical threshold [3][5]. The strength of this effect is comparable at half filling and at the $vH$s: while nesting is better at half filling (the pseudofermions having a square Fermi surface), $vH$s nesting is suppressed by matrix element effects [4]. Hence, the conventional nesting at half filling will be of comparable strength to the $vH$s nesting in the doped material. Therefore, for the calculations of $T_{LTO}$ in Fig. 2, a simplifying assumption is made – that the $vH$s is pinned to the Fermi level, but that the strength of coupling (represented by $N(0)$) is independent of doping.

In analyzing the $T$-dependence of the soft mode frequency in the undoped La$_2$CuO$_4$ [3], it was found that the transition could be equally well fit by either a purely anharmonic model or one with a strong component of electron-phonon coupling. In analyzing the doping dependence, it is found that the same ambiguity of parameter values remains, and Fig. 2a-c correspond to essentially the same parameters as Fig. 3a-c of Ref. [3]. Identical parameters cannot be used, since the transition temperature at zero doping is considerably higher for the present data than for the earlier (the fits in Ref. [3] found $T_{LTO}$ between 455-508K). There is no unique technique for adjusting the parameter values to the new $T_{LTO}$ without fitting the entire transition, for which data are not available. However, $T_{LTO}$ is directly related to the ‘bare’ phonon frequency, $\omega_0$, so this parameter was increased slightly (by $\sim 4-8\%$) to correct for the higher $T_{LTO}$ values (corresponding to fit values of $T_{LTO} \approx 540 - 576K$ at $x = 0$).

The parameters $i\omega_0$, $\tilde{\omega}_0$, and $\tilde{\Gamma}$ are listed in Table I. The other parameters are the same as in the respective parameter sets of Table II of Ref. [3]. Note that the lattice mismatch is clearly responsible for the instability: whereas $\omega_0^2$ is negative, signalling an instability, the bare parameter $\tilde{\omega}_0$ is large and positive.

One feature should be noted: the renormalized Nd parameter, $(a - a_2)^+$ from Appendix B, had to be used, to get good fits. This is directly related to the fact that the electron-phonon coupling term was assumed to be doping independent. If $a_2^+N(0)$ is assumed to be smaller at $x = 0$, then electron-phonon coupling would favor a higher $T_{LTO}$ in the doped material, a trend that would have to be compensated by a larger value of $\tilde{\Gamma}$. To explain the Nd-doping results then would require a smaller value of $(a - a_2)$ when $y$ is varied. Contrariwise, if $a_2^+N(0)$ increases as half filling is approached, a larger value of the $y$-coefficient of $(a - a_2)$ is needed. This result can be turned around: if we knew perfectly the theoretical form of $(a - a_2)$, we could determine from experiment the precise doping dependence of the electron-phonon coupling coefficient. Unfortunately, the uncertainty in parameters is too large to determine whether $a_2^+N(0)$ increases or decreases with doping.

**APPENDIX B: ATOMIC RADII**

In testing an ionic model for the LTO transition, it is necessary to estimate the effective ionic radii in the various layers as a function of doping. This will be done in two ways: by using tabulated values of radii [30] and via valence bond sums [31]. Exact agreement with experiment should not be expected, since the tabulated values are averages over many compounds. Nevertheless, an approximate agreement is found.

**1. On the LaO Plane**

Commensurability strains will arise in LSCO whenever the tolerance factor, Eq. 1, is different from unity. It should be noted that, in this equation, both $d_{LaO}$ and $d_{CuO_2}$ are functions of doping. In undoped La$_2$CuO$_4$, the CuO$_2$ planes are under compression, $t < 1$. The atoms in the LaO layer are easier to discuss, since they can be treated in the ionic limit. The radii will first be estimated from Shannon’s tables [30], assuming the La site to be 9-fold coordinated [62]. In this case, assuming the conventional $O^2-$ radius, $r_{O^2-} = 1.40\AA$, the relevant radii are $r_{La^{3+}} = 1.216\AA$, $r_{Nd^{3+}} = 1.163\AA$, $r_{Ba^{2+}} = 1.07\AA$, $r_{Sr^{2+}} = 1.31\AA$, and $r_{Ca^{2+}} = 1.18\AA$. Thus, for undoped La$_2$CuO$_4$, $d_{LaO} = 2.616\AA$, while in an Sr and Nd co-doped material, La$_2-x$-Sr$_x$Nd$_y$CuO$_4$, $d_{LaO} = (2.616 + 0.047x - 0.027y)\AA$. Thus, Sr doping reduces the interlayer strains, while Nd substitution makes them worse.
In the $T'$ structure, the rearrangement of the apical O's to interstitial positions expands the lattice, and leaves the CuO$_x$ layers under tension [20], and leading to materials which can be electron doped. These structures will not be further discussed here.

2. On the CuO$_2$ Plane

Shannon’s tables list $r_{Cu^{1+}} = 0.77 \text{Å}$, $r_{Cu^{2+}} = 0.73 \text{Å}$, and $r_{Cu^{3+}} = 0.54 \text{Å}$. Assuming the Cu is all in the 2+ state, this yields $d_{CuO_2} = 2.13 \text{Å}$, to be compared with $a_2 \equiv d_{LaO}/\sqrt{2} = 1.850 \text{Å}$ in La$_2$CuO$_4$. This severe mismatch is largely corrected for by a large molecular LT effect in the CuO$_x$ octahedra: the electronic degeneracy of the Cu d levels ($d_{x^2-y^2}, d_{z^2}$) is split by a molecular distortion in which the planar CuO distance becomes much smaller than the apical distance. A rough estimate of the effect can be made from the Shannon values. For Cu$^{2+}$, the one hole in the Cu d-shell is generally an equal mix of the $d_{x^2-y^2}$ and the $d_{z^2}$ orbitals. In the JT state, the hole is completely taken from the $d_{z^2}$ orbital. Hence, for in-plane lengths, the relevant orbital has the same occupation as in the isotropic Cu$^{3+}$ ion, with a corresponding length $d_{CuO_2}^{\text{in-plane}} \simeq 1.94 \text{Å}$. For the apical lengths, the $d_{x^2}$ orbital has the same length as Cu$^{1+}$, or $d_{CuO_2}^{\text{apical}} \simeq 2.17 \text{Å}$. Experimentally, these lengths are found to be $d_{CuO_2}^{\text{in-plane}} = 1.905 \text{Å}$ and $d_{CuO_2}^{\text{apical}} = 2.421 \text{Å}$ in La$_2$CuO$_4$ at 10K. For the apical O, the agreement could be further improved by noting that screening is very weak along the c-axis, so the Pauling value [5] $r_{Cu^{1+}} = 0.96 \text{Å}$ is more appropriate, yielding $d_{CuO_2}^{\text{apical}} \simeq 2.36 \text{Å}$.

To extend the above picture to the doped regime, it is necessary to understand where the doped holes go. Experimentally, it is found that hole occupation of the Cu $d_{z^2}$ orbital only becomes apparent for $x > 0.15$ -- i.e., just above the optimal doping for superconductivity. Hence, in the low-doping regime it can be assumed that the holes go primarily onto the in-plane O’s. Chemically, this would correspond to the appearance of the species $O^{1-}$. This is a rare species, and its ionic radius is not well established. The present analysis will provide an estimate of its value.

3. Doping Dependence of $T_{LT0}$

Using the above estimates, in La$_2$CuO$_4$, $a_2 = 1.850 \text{Å}$, $a_1 \equiv d_{CuO_2} = 1.94 \text{Å}$, and $a = 1.905 \text{Å}$, for a reasonably consistent picture. The doping dependence of $a_2$ is

$$a_2 = (1.850 + 0.033x - 0.019y) \text{Å}, \quad (B1)$$

while, experimentally [64]

$$a = (1.901 - 0.085x + 0.0y) \text{Å} \quad (B2)$$

so

$$a - a_2 = (0.051 - 0.118x + 0.019y) \text{Å} \quad (B3)$$

at room temperature. Note that there are additional small corrections, which are neglected. In particular, no correction is made for the fact that the La and the O are not strictly coplanar (and similarly for the Cu and O). Also, there is no temperature dependence of the lattice constants, and all 9 La-O distances are assumed to be the same.

The above model predicts too small a change of $a - a_2$ with $y$ to agree with experiment. Empirically, the ratio of the coefficients of $y$ and $x$ can be estimated from the change in $T_c$ with these parameters. Now

$$T_{LT0} = T_0 - T_xx + T_yy, \quad (B4)$$

with $T_0 \simeq 546 \text{K}, T_x \simeq 2456 \text{K}$ (from Ref. [65]), and $T_y \simeq 560 \text{K}$ (Ref. [28]). This yields $T_x/T_y = 4.39$, compared to the predicted value, 0.118/0.019 = 6.21. In the following subsection, we will see that this lattice mismatch can also be estimated from valence bond sums, and here the $y$-coefficient is found to be too large. In the present paper, an effective average value will be assumed, to give better agreement with experiment:

$$(a - a_2)^* = (0.051 - 0.118x + 0.027y) \text{Å}. \quad (B5)$$

4. Valence Bond Sums

In view of the importance of the above results, it is preferable to recalculate $a_2$ by another technique. The method of valence bond sums [61] has been applied by several authors to the high-$T_c$ superconductors [6] [8]. In this model, the valence associated with a bond between atoms A and B is written as

$$V_{AB} = cexp\left(\frac{r_{AB0} - r_{AB}}{r_0}\right), \quad (B6)$$

where $r_0 = 0.37 \text{Å}$ is a constant, $r_{AB0}$ is tabulated for over a hundred possible pairs [61], and $r_{AB}$ is the measured AB distance. The total valence of atom A is then

$$V_A = \sum_i V_{AB_i}, \quad (B7)$$

where the sum is over all close neighbor atoms, $B_i$. This can be rearranged to give the ideal radius for a given atom:

$$r_{AB} = r_{AB0} + r_0 \ln \left(\frac{N_A}{V_A}\right), \quad (B8)$$

14
where $N_A$ is the coordination of atom $A$ ($N_{La} = 9$). Taking $V_{La} = V_{Nd} = 3$ and $V_{Sc} = 2$, and using tabulated values \[ \text{[61]} \] for $r_{AB0}$, it is found that

$$a_2_{\text{val.bond}} = (1.823 + 0.069x - 0.047y)\AA, \quad (B9)$$

so

$$(a - a_2)_{\text{val.bond}} = 1.31(0.060 - 0.118x + 0.036y)\AA. \quad (B10)$$

The coefficient of $y$ is here found to be much larger than that estimated from the Shannon tables, and even larger than the experimental value.

5. The Radius of $O^-$

Now, from Eq. 3b,

$$(a_1 - a) = \frac{2C_2}{C_1} (a - a_2). \quad (B11)$$

Since $a_1$ should be independent of $y$, the experimental observation that $a$ is approximately independent of $y$ requires that $C_2 << C_1$. For example, if $2C_2/C_1 \approx 0.1$, then $a$ would have to include a term $\approx 0.003y$. This would then yield

$$a_1 \approx (1.904 - 0.097x)\AA. \quad (B12)$$

(Note that, at $x = 0$, this yields a smaller value of $a_1$ than the chemical estimate, $a_1 \approx 1.94\AA$, made above.) Combining this with Eq. B1 yields a tolerance factor

$$t = \frac{a_2}{a_1} \approx 0.972 + 0.069x - 0.010y,$$

or $t = 1$ at $x = 0.42$, when $y = 0$.

If all the doping is assumed to go into the oxygens, then setting $x = 2$ is equivalent to converting both planar O’s to O$^-$, yielding $r_{O^-} = (1.40 - 0.194) = 1.206\AA$. Grenier \[ \text{[69]} \] has postulated that O$^2-$ is too large to readily diffuse, and that the diffusing species in YBCO and the other cuprates is probably O$^-$. He estimates its radius to be $\sim 1.1\AA$, comparable to the present estimate. From the valence bond sums, a similar estimate can be made, $r_{O2^-} - r_{O^-} \approx r_{O}ln2 \approx 0.256\AA$.

The large increase in radius on going to O$^2-$ is consistent with the suggestion that O$^2-$ is inherently unstable, being stabilized in a lattice by the Madelung potential \[ \text{[67]} \]. This near instability leads to a large, nonlinear polarizability which has been hypothesized to lead to ferroelectricity in the perovskites \[ \text{[77]} \].

APPENDIX C: IN-PLANE MODE COUPLING IN A TIGHT BINDING MODEL

In this Appendix, the electron-phonon coupling associated with the various structural distortions will be estimated in a tight-binding model, assuming that the coupling arises from the bond-length dependence of the hopping parameter, $t_{CuO}$. In the standard three-band model, assuming $t_{OQ} = 0$ for simplicity, a very general case can be handled. Assume that the distortions have led to a $\sqrt{2} \times \sqrt{2}$ unit cell, with alternating hopping parameters $t_1$, $t_2$, $t_3$, and $t_4$ along the $x$-axis (Fig. 3a,c), and $t$ along $y$. Then four possible distortion modes are (1) Cu-Cu bond stretching mode, $t_1 = t_2 = t = t\delta$; (2) O-O bond stretching mode, $t_1 = t_2 = t = t\delta$; (3) ferroelectric (FE) mode, $t_1 = t_3 = t = t\delta$; (4) shear strain, $t_1 = t_2 = t_3 = t = t\delta$. For the shear strain mode, the $y$-hopping must be reset to $t_y = t + \delta t$, and for comparable distortions, $\delta t$ must be smaller by a factor of $\sqrt{2}$ than for models 1-3.

For these distortions, the energy dispersion is given by the solutions

$$(W - W_k)(W - W_{\vec{q}-\vec{q}}) = \Gamma, \quad (C1)$$

with $W = E(E - \Delta),$

$$W_k = 4t^2s_y^2 + \frac{\sum_{i=1,4} t_i^2}{2} - (t_1t_2 + t_3t_4)c_z, \quad (C2)$$

$$\Gamma = \frac{1}{4}[(t_1^2 - t_3^2)^2 + (t_2^2 - t_4^2)^2 + 2(t_1t_4 - t_2t_3)^2 + 2(t_1t_2 - t_3t_4)^2(1 - 2c_z^2)], \quad (C3)$$

and $s_i = \sin(k_ia/2)$, $c_i = \cos(k_ia/2)$, $c_z = \cos(k_xa)$. The values of $W_{\vec{k}-\vec{q}}$ are also given by Eq. C2, with the substitution $\vec{k} \rightarrow \vec{k} - \vec{q}$ in the arguments of the trig functions. In particular, for $\vec{q} = \vec{q}_0$ (Fig. 3c-f) $s_i \rightarrow -c_i$, $c_i \rightarrow s_i$, $i = x,y$. The same dispersion relations also hold for the distortions of Fig. 3a,b, but with $\vec{q} = \vec{q}_1$. In this case, the terms in $s_y$ remain unchanged in $W_{\vec{k}-\vec{q}}$. The calculated energy dispersions are illustrated in Fig. 5, assuming $t = 1eV$, $\Delta = 4eV$, and $\delta t = 0.1eV$. Note that the Cu-Cu and O-O bond stretching modes give identical dispersions for a $\vec{q}_1$ distortion (Fig. 5a,b – this can be shown analytically from Eq. C1) but very different dispersions for the $\vec{q}_0$ distortion (Fig. 5c,d).

In Eq. C3, $\Gamma$ is the square of an umklapp scattering gap. For the four various modes, it can be simplified to

$$\Gamma_i = \begin{cases} 64t^2\delta t^2s_z^2c_z^2 & \text{if } i = 1; \\ 16t^2\delta t^2 & \text{if } i = 2; \\ 0 & \text{if } i = 3,4. \end{cases} \quad (C4)$$

Note that there is no gap for the FE mode, but a large gap $\sim \delta t$ opens up for the other modes, although it vanishes at the vHs for the Cu-Cu bond stretching mode. When $\gamma = 0$, the dispersion becomes $E = E_k$, with

$$E_k = \frac{\Delta}{2} + \sqrt{\left(\frac{\Delta}{2}\right)^2 + W_k}. \quad (C5)$$
For $\Gamma \neq 0$, by defining $F(E) = E - \Delta / 2$, Eq. C1 can be rewritten

$$F^2(E) = \frac{F^2(E_k) + F^2(E_{k-\vec{q}})}{2} + \Gamma. \quad (C6)$$

Explicitly, for either the O-O bond stretching mode or the FE mode,

$$W_k = 4t^2(s_x^2 + s_y^2) + 4\delta t^2 c_r^2, \quad (C7a)$$

for the Cu-Cu bond stretching mode:

$$W_k = 4(t^2 + \delta t^2) s_x^2 + 4t^2 s_y^2, \quad (C7b)$$

and for the strain:

$$W_k = 4(t - \delta t)^2 s_x^2 + 4(t + \delta t)^2 s_y^2. \quad (C7c)$$

When $E_k - E_{k-\vec{q}}$ is large, the dispersion is essentially given by Eq. C5. However, when $E_k = E_{k-\vec{q}}$, the excitation spectrum is gapped. For the O-O bond stretching mode,

$$E \simeq E_k \pm \frac{2t \delta t}{\sqrt{(\frac{\delta t}{\delta})^2 + 4t^2(s_x^2 + s_y^2)}}. \quad (C8)$$

to lowest order in $\delta t$. Since $s_x^2 + s_y^2 = 1$ everywhere on the Fermi surface, the gap is isotropic, as seen in Fig. 5d. Similar equations hold for the remaining two distortions, except that the factor $2t$ in the numerator becomes $8t s_r c_r$ for case 1 (Cu-Cu hopping) and $2\sqrt{2}t( s_x^2 - s_y^2)$ for case 4 (shear strain). Even though there is no gap in the FE band, the distortion still leads to a net energy lowering, but it is $\sim \delta t^2$. This is a 2D version of the model discussed by Egami, et al. \[10\].

The gap at the vHs can be calculated as

$$\Delta E_i = \frac{2\beta_i \delta t}{\sqrt{1 + (\frac{\delta t}{\delta})^2}}, \quad (C9)$$

$i = 1, 4$ labelling the four modes, with $\beta_1 = \beta_3 = 0, \beta_2 = 1,$ and $\beta_4 = \sqrt{2}$. For the strain mode, this represents a splitting of the vHs degeneracy at the X and Y points.

**APPENDIX D: POLARONIC CALCULATIONS**

1. Canonical Transformation: Full Three Band Model

The complete, fully 2D solution to Eqs. 11-14 involves a system of 18 equations in 18 unknowns, the $f$’s and $h$’s. Ten unknowns can immediately be eliminated by direct substitution. Defining $\tilde{f}_i = f_i / \omega_q$, these are

$$h_9 = \frac{t_{x_k - \vec{q}} \tilde{f}_1 + t_{y_k} \tilde{f}_1}{\hbar \omega_q}, \quad (D1a)$$

$$h_8 = \frac{t_{x_k} \tilde{f}_3 + t_{y_k - \vec{q}} \tilde{f}_2}{\hbar \omega_q}, \quad (D1b)$$

$$h_7 = \frac{t_{y_k} \tilde{f}_1 + t_{y_k} \tilde{f}_4}{\hbar \omega_q}, \quad (D1c)$$

$$h_6 = \frac{t_{x_k} \tilde{f}_1 + t_{x_k - \vec{q}} \tilde{f}_2}{\hbar \omega_q}, \quad (D1d)$$

$$h_5 = \frac{[t_{x_k - \vec{q}} \tilde{f}_1 + t_{x_k} \tilde{f}_2 + t_{y_k - \vec{q}} \tilde{f}_3 + t_{y_k} \tilde{f}_4]}{\hbar \omega_q}, \quad (D1e)$$

with the five equations formed by interchanging $h_i \leftrightarrow \tilde{f}_i$.

Solution of the remaining eight equations is more involved. Defining column matrices

$$\hat{H} = \begin{pmatrix} h_1 \\ h_2 \\ h_3 \\ h_4 \end{pmatrix}, \quad (D2a)$$

$$\hat{F} = \begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \end{pmatrix}, \quad (D2b)$$

$$\hat{G} = \begin{pmatrix} \hbar^2 g(q, \vec{k}) \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad (D2c)$$

then the remaining equations become

$$\hat{A}\hat{H} + \hat{B}\hat{F} = \hat{G}, \quad (D3a)$$

$$\hat{A}\hat{F} + \hat{B}\hat{H} = 0, \quad (D3b)$$

with solution

$$\hat{H} = \frac{1}{2}[(\hat{A} + \hat{B})^{-1} + (\hat{A} - \hat{B})^{-1}]\hat{G}, \quad (D4a)$$

$$\hat{F} = \frac{1}{2}[(\hat{A} + \hat{B})^{-1} - (\hat{A} - \hat{B})^{-1}]\hat{G}. \quad (D4b)$$
Introducing the notations \( a = t_{x\xi - \varrho} \), \( b = t_{x\xi} \), \( c = t_{y\xi - \varrho} \), \( d = t_{y\xi} \), and \( e = \hbar \omega_q \Delta \), the matrices \( \tilde{A} = \tilde{P} \tilde{R} \tilde{P} \) and \( \tilde{B} \) can be written

\[
\tilde{B} = \begin{pmatrix}
e & 0 & 0 & 0 \\
0 & -e & 0 & 0 \\
0 & 0 & e & 0 \\
0 & 0 & 0 & -e
\end{pmatrix}, \quad (D5a)
\]

\[
\tilde{P} = \begin{pmatrix}
a & 0 & 0 & 0 \\
0 & b & 0 & 0 \\
0 & 0 & c & 0 \\
0 & 0 & 0 & d
\end{pmatrix}, \quad (D5b)
\]

\[
\tilde{R} = \begin{pmatrix}
\alpha & 2 & 1 & 2 \\
2 & \beta & 1 & 2 \\
1 & 2 & \gamma & 2 \\
1 & 2 & 1 & \delta
\end{pmatrix}, \quad (D5c)
\]

with

\[
\alpha = \frac{W - d^2}{b^2}, \quad (D6a)
\]

\[
\beta = \frac{W - c^2}{a^2}, \quad (D6b)
\]

\[
\gamma = \frac{W - b^2}{d^2}, \quad (D6c)
\]

\[
\delta = \frac{W - a^2}{c^2}, \quad (D6d)
\]

and \( W = \hbar^2 \omega_q^2 + a^2 + b^2 + c^2 + d^2 \).

Defining \( \tilde{H}_\pm = (\tilde{A} \pm \tilde{B})^{-1} \tilde{G} \), \( W_\pm = W \pm e \), \( A = a^2 + c^2 \), \( B = b^2 + d^2 \), the explicit solution is

\[
h_{i \pm} = \frac{\hbar^2 \tilde{g}_q(\tilde{k})}{(W_\mp W_\pm - 4AB)(W_\pm - A)}, \quad (D7a)
\]

\[
\hat{h}_{1 \pm} = W_\mp(W_\pm - A) + c^2(W_\mp - 4B), \quad (D7b)
\]

\[
\hat{h}_{2 \pm} = -2ab(W_\pm - A), \quad (D7c)
\]

\[
\hat{h}_{3 \pm} = -ac(W_\mp - 4B), \quad (D7d)
\]

\[
\hat{h}_{4 \pm} = -2ad(W_\pm - A). \quad (D7e)
\]

The most important factor in the above expressions is the first factor in the denominator of Eq. D7a, which can be rewritten

\[
W_\pm W_\mp - 4AB = \hbar^2 \omega_q^2[h^2 \omega_q^2 + 2(A + B) - \Delta^2] + (A - B)^2
\]

\[
= [h^2 \omega_q^2 - (E_{\tilde{k}} - E_{\tilde{k} - \varrho})^2][h^2 \omega_q^2 - (E_{\tilde{k}} + E_{\tilde{k} - \varrho} - \Delta)^2]. \quad (D7f)
\]

Here, the first term in brackets contains the essential \( \omega \)-dependence of the problem, and \( \omega_q \) can essentially be set to zero in all remaining terms.

The residual interaction terms are given by Eq. 17, with

\[
H_{e - e} = - \sum_{\tilde{k}, \tilde{k}', \varrho} \tilde{g}_q(\tilde{k}) \rho_{1+ \tilde{k}, \varrho} B_{\tilde{k}' \varrho} \rho_{1+ \tilde{k}', \varrho}, \quad (D8)
\]

and

\[
H_{e - ph}^{(2)} = - \sum_{\tilde{k}, \tilde{k}', \varrho} Q_\varrho Q_{\varrho} \tilde{g}_q(\tilde{k}) \times
\]

\[
\times (f_1 \tilde{k}, \varrho) \rho_{6 - \tilde{k} - \varrho, \varrho} - f_2 \tilde{k} + \varrho, \varrho \rho_{6 - \tilde{k} - \varrho, \varrho} - \tilde{q} - \tilde{q}
\]

\[
+ f_3 \tilde{k} - \tilde{q}, \rho_{8 - \tilde{k} - \varrho, \varrho} - \tilde{q} - \tilde{q}
\]

\[
+ f_5 \tilde{k}, \varrho \rho_{2 - \tilde{k} - \varrho, \varrho} - \tilde{q} - \tilde{q} + f_5 \tilde{k} + \varrho, \varrho \rho_{2 - \tilde{k} - \varrho, \varrho} - \tilde{q} - \tilde{q}
\]

\[
+ f_2 \tilde{k} - \varrho, \rho_{5 - \tilde{k} + \varrho, \varrho} - \tilde{q} - \tilde{q} - \tilde{q} - \tilde{q}
\]

\[
+ f_6 \tilde{k} - \varrho, \rho_{1 - \tilde{k}, \varrho} + f_6 \tilde{k} + \varrho, \varrho \rho_{1 - \tilde{k}, \varrho}
\]

\[
+ f_8 \tilde{k} - \varrho, \rho_{3 - \tilde{k}, \varrho} + f_9 \tilde{k} - \varrho, \rho_{3 - \tilde{k}, \varrho} \), \quad (D9)
\]

where it is assumed that the terms linear in \( Q_{\varrho} P_{\varrho} \) will average to zero.

### 2. Canonical Transformation: Quasi-1D Approximation

Due to the complicated nature of the solution, Eqs. D1.7, this subsection introduces a simpler, quasi-1D approximation: the commutator of \( S \) with the hopping Hamiltonian along the \( y \)-direction will be neglected. The next subsection gives a different, effective mass type approximation.

In the quasi-1D case, only the \( f_i \)'s and \( h_i \)'s with \( i = 1, 2, 5, 6 \) are non-vanishing. When \( c = d = 0 \), Equations D7 reduce to \( \hat{h}_{3 \pm} = \hat{h}_{4 \pm} = 0 \), \( f_2 = 0 \),

\[
\hat{f}_1 = \frac{-eh_1}{W}, \quad (D10a)
\]

\[
h_{2} = \frac{-2abh_{1}}{W}, \quad (D10b)
\]

and

\[
h_{1} = \frac{\hbar^2 \tilde{g}_q(\tilde{k}) W}{W_{\mp} W_{\pm} - 4AB}. \quad (D10c)
\]
Equation D10a can be rewritten in the suggestive form

\[ f_{1\vec{k},\vec{q}} = \frac{\hbar \tilde{g}(\vec{k}) \beta_{\vec{k},\vec{q}}}{\hbar^2 \omega_{\vec{q}}^2 - (E_{\vec{k}} - E_{\vec{k} - \vec{q}})^2}, \]  

(D11a)

with

\[ \beta_{\vec{k},\vec{q}} = \frac{\hbar^2 \omega_{\vec{q}}^2 \Delta}{(E_{\vec{k}} + E_{\vec{k} - \vec{q}} - \Delta)^2 - \hbar^2 \omega_{\vec{q}}^2}, \]  

(D11b)

and

\[ E_{\vec{k}} = \Delta + \sqrt{\frac{\Delta^2}{4} - t_{x\vec{k}}^2}. \]  

(D11c)

The effective electron-electron interaction \( H_{ee}^{(2)} \) can still be written in the form of Eq. D8, while the residual electron-phonon interaction becomes

\[ H_{e-\text{ph}}^{(2)} = - \sum_{\vec{k},\vec{q},\vec{q}'} Q_{\vec{q}} \frac{\tilde{g}(\vec{k})}{\hbar} \times \]

\[ \times \left( f_{1\vec{k},\vec{q}} \rho_{6\vec{k},\vec{q},\vec{q}' - \vec{q}} - f_{1\vec{k} + \vec{q},\vec{q},\vec{q}'} \rho_{5\vec{k},\vec{q},\vec{q}' - \vec{q}} + f_{5\vec{k},\vec{q}} \rho_{2\vec{k},\vec{q},\vec{q}'} - f_{5\vec{k} + \vec{q},\vec{q}' - \vec{q}} \rho_{5\vec{k},\vec{q},\vec{q}' - \vec{q}} \right). \]  

(D12)

Equation D12 can be further simplified, by noting that in the most important case, \( \vec{q}' = -\vec{q} \) and \( 2\vec{q} \) is a reciprocal lattice vector, and hence equivalent to zero. In this case,

\[ H_{e-\text{ph}}^{(2)} = - \sum_{\vec{k},\vec{q}} Q_{\vec{q}} \frac{\tilde{g}(\vec{k})}{\hbar} \times \]

\[ \times \left( f_{1\vec{k},-\vec{q}} \rho_{6\vec{k},-\vec{q},0} - f_{1\vec{k} + \vec{q},-\vec{q},0} \right) + f_{5\vec{k},-\vec{q}} \rho_{2\vec{k},-\vec{q},0} - f_{5\vec{k} + \vec{q},-\vec{q},0} \rho_{5\vec{k},-\vec{q},0} \]

\[ - f_{5\vec{k},-\vec{q},0} \rho_{1\vec{k},-\vec{q},0} + f_{5\vec{k} + \vec{q},-\vec{q},0} \rho_{5\vec{k},-\vec{q},0} \right). \]  

(D13)

Note that the term in \( \rho_6 \) is of the form of Eq. 27, but with a quadratic \( Q \) dependence.

In mean field theory, the four-operator terms are split up according to

\[ AB \simeq A < B > + < A > B - < A > < B >, \]  

(D14)

where \( A, B \) are products of two operators, and \( < \cdots > \) denotes a thermal equilibrium average. At sufficiently high temperatures, only \( Q \tilde{g}(\vec{q}) < \tilde{g}(\vec{k}) > \tilde{g}(\vec{k} + \vec{q}) \) have non-zero averages. As the temperature is lowered, other quantities may develop nonvanishing averages, signaling a phase transition. A discontinuous change in \( \rho_6 - \rho_5 \) would signal an ionic-to-covalent transition.

This canonically transformed Hamiltonian contains information on many physical processes, not all of them relevant to the present discussion. Here, I will briefly survey some of the terms which arise at mean field level. From \( H_{e-\text{ph}}^{(2)} \), the term in \( < \tilde{g}(\vec{q}) \tilde{g}(\vec{k}) > \) \( f_1 \) leads to a polaronic renormalization of the Cu-O \( x \) hopping:

\[ t_{x\vec{k}} \rightarrow t_{x\vec{k}} \left( 1 - \sum_{\vec{q}} \frac{< \tilde{g}(\vec{q}) \tilde{g}(\vec{k}) >}{\hbar^2} \right) \]  

(D15a)

(neglecting terms in \( \vec{k} - \vec{q} \)). The average over \( Q^2 \) is given by

\[ \omega_{\vec{q}}^2 < \tilde{g}(\vec{q}) \tilde{g}(\vec{k}) > \tilde{g}(\vec{k}) h_{\vec{k},\vec{q}} \]  

where \( N_{\vec{q}} \) is given by Eq. 25b. There is also a renormalization of the phonon frequency,

\[ \omega_{\vec{q}}^2 = \frac{\omega_{\vec{q}}^2}{2} - \sum_{\vec{k}} 2 f_{\vec{k},\vec{q},-\vec{q}} \rho_{\vec{k},\vec{q},-\vec{q},0} - \rho_{\vec{k} + \vec{q},-\vec{q},0}. \]  

(D16)

The presence of \( \rho_6 - \rho_5 \) indicates that this softening is associated with charge transfer effects, and will be modified by correlation effects: in the insulating phase at half filling, \( \rho_5 \) is constrained to be unity.

In \( H_{e-c} \), the mixed terms will lead to additional interference effects. However, the most important term is given by Eq. 18 in the main text.

### 3. Canonical Transformation: One Band Approximation

An alternative approximate solution to Eq. 11 can be found by assuming that only the antibonding band is populated by holes, and projecting the electron-phonon Hamiltonian onto this band. The electronic Hamiltonian is

\[ H_e = \sum_{\vec{k}} E_{\vec{k}} \psi_{\vec{k}}^\dagger \psi_{\vec{k}}. \]  

(D17)

with \( E_{\vec{k}} \) given by Eq. 6,

\[ H_{e-\text{ph}} = \sum_{\vec{k}} Q_{\vec{q}} \alpha_{\vec{k},\vec{q}} \psi_{\vec{k},\vec{q}}^\dagger \psi_{\vec{k}}, \]  

(D18a)

and, at the Fermi surface,

\[ \alpha_{\vec{k}} \simeq \frac{i \tilde{g}(\vec{k}) t (s_x - s_y)}{\sqrt{(s_x)^2 + 4t^2(s_x^2 + s_y^2)}}. \]  

(D18b)

In this case, by the same calculations as for the quasi-1D case, we find

\[ S = i \sum_{\vec{k}} \left[ f_{1\vec{k}} \psi_{\vec{k}} - i f_{2\vec{k}} \psi_{\vec{k}} \right] \psi_{\vec{k}}. \]  

(D19)
where the primed sum means that only states which satisfy the conditions $|E_{k} - E_{F}| < \hbar \omega$, and $|E_{k} - \bar{q}_{0} - E_{F}| < \hbar \omega$, are included. In the present problem, $E_{F} = 0$.

The resulting Hamiltonian, $H_{e} + H_{C,DW}$ can be diagonalized by the Bogoliubov-Valatin transformation, yielding quasiparticle energies

$$\mathcal{E}_{k}^{\pm} = \frac{E_{k} + E_{k} - \bar{q}}{2} \pm \sqrt{\left(\frac{E_{k} - E_{k} - \bar{q}}{2}\right)^{2} + G_{k}^{2}W_{k}^{2}}, \quad (D27a)$$

with

$$G_{k} = \begin{cases} G_{0} + G_{1} & \text{if } |E_{k} - E_{F}| < \hbar \omega, \\ G_{0} & \text{otherwise}. \end{cases} \quad (D27b)$$

When $E_{k} = E_{k} - \bar{q}$, this reduces to

$$\mathcal{E}_{k}^{\pm} \simeq E_{k} \pm |G_{k}W_{k}|, \quad (D27c)$$

which should be compared to Eq. C8.

### APPENDIX E: SPIN-ORBIT ELECTRON-PHONON COUPLING

Earlier suggestions involving charge density waves (CDWs) in the cuprates were largely abandoned when it was pointed out that the orthorhombic splitting in the low-temperature orthorhombic (LTO) phase of LSCO leaves the two in-plane oxygens in symmetrically equivalent positions, and hence should not split the vHs degeneracy [71]. In fact, there are actually two independent mechanisms which can lead to a splitting of the vHs degeneracy in the LTO phase: a dynamic Jahn-Teller effect, where the local symmetry is not orthorhombic, or spin-orbit coupling, even in a uniform orthorhombic phase [72]. It would be useful to be able to simplify the analysis by definitively ruling out one of the other effects. This has proven to be a non-trivial task, as the present estimate makes clear.

Spin-orbit coupling can profoundly change the shape of the Fermi surfaces, by opening gaps where the bands cross, and thereby splitting the vHs degeneracy in the dos. This spin-orbit coupling also leads to a linear coupling to the tilt modes [72,73]. However, the magnitude of these effects is expected to be small, and hence the effect would be unimportant for driving either the structural or magnetic transitions.

Here, a simple estimate of $\lambda_{p} = NV_{0}$ is presented, which reveals an underlying subtlety. The dos can be estimated as

$$N = \frac{16}{\pi^{2}B} n(B/\epsilon), \quad (E1)$$

where $B$ is the electronic bandwidth and $\epsilon$ is an energy scale, $\sim T$. For the three-band model, $B \simeq 8t^{2}/\Delta$. Assuming the renormalized parameters are $\epsilon \approx 0.25eV$, $\Delta \approx 1eV$, then $B \approx 0.5eV$, $\epsilon \approx 10meV$, and $N \approx 13eV^{-1}$.
The electron-phonon interaction \( V_0 \) can be estimated as follows. The interaction Hamiltonian can be written

\[
H_{e-ph} \simeq \sum d^\dagger p_x \lambda,
\]

where the spin-orbit coupling term is \( \lambda = \gamma \theta \), with \( \theta \) the octahedral tilt angle,

\[
\theta \simeq \frac{2z}{a_0} \equiv \eta(a + a^\dagger).
\]

Here, \( a_0 \) is the in-plane lattice constant, \( z \) the displacement of the O out of the CuO plane, \( a^\dagger \) the phonon creation operator, and

\[
\eta = \left( \frac{2\hbar}{m\omega a_0} \right)^{1/2} \simeq 0.18,
\]

with \( m \) the mass of an O ion and the bare tilt-mode phonon frequency \( \hbar \omega \sim 5\text{meV} \). The parameter \( \gamma \) is, approximately \([73]\)

\[
\gamma \simeq \frac{\Delta g}{g} t \simeq 25\text{meV}
\]

with \( \Delta g / g \sim 0.1 \) the relative \( g \)-shift. Finally,

\[
V_0 = \frac{(\gamma \eta)^2}{\omega} \simeq 4\text{meV},
\]

so

\[
\lambda_{ep} = V_0 N \simeq .05. \quad (E2)
\]

This is too small to drive either the structural or superconducting transition. However, \( \gamma \sim t \), and, up to logarithmic corrections, \( N \propto t^2 \), so \( \lambda_{ep} \sim t^4 \). Grilli and Castellani \([22]\) have suggested that, in the present circumstances, \( \lambda_{ep} \) should not be renormalized by correlation effects. This would mean that the bare value \( t = 1.3\text{eV} \) should be used in Eq. E2, leading to \( \lambda_{ep} \simeq 36 \), a surprisingly large value.

| Data Set | \( \omega_0 \) | \( \tilde{\omega}_0 \) | \( \Gamma \) |
|----------|----------------|----------------|------|
| (1)      | 11.3           | 8.9            | 4060 |
| (5)      | 11.0           | 8.8            | 3880 |
| (10)     | 8.8            | 7.3            | 2550 |
| (11)     | 6.5            | 8.9            | 1500 |

**Figure Captions**

**Fig. 1** Phase diagram of LSCO, including the pseudo-gap transition at \( T = T^* \). Symbols from Hwang, et al. \([17]\), short-dashed line = twice the LTO transition temperature.

**Fig. 2** Doping dependence of LTO transition in \( \text{La}_{2-x-y}\text{Sr}_x\text{Nd}_y\text{CuO}_4 \). Open symbols from Fig. 1 of \([27]\); filled circles from \([23]\). Lines = theory; solid lines correspond to \( y = 0 \); dashed to \( x = 0.15 \). Frames a, b, and c correspond to fit data sets 1, 5, and 10 respectively in Table I (set 11 is indistinguishable from set 10).

**Fig. 3** Phonon modes in LSCO: (a) \( \vec{q} = \vec{q}_1 \equiv (\pi/a, 0) \) Cu-Cu bond stretching mode; (b) \( \vec{q} = \vec{q}_1 \) O-O bond stretching mode; (c) \( \vec{q} = \vec{q}_0 \equiv (\pi/a, \pi/a) \) Cu-Cu bond stretching mode; (d) \( \vec{q} = \vec{q}_0 \) O-O bond stretching mode; (e) FE mode; (f) shear strain; (g) possible mixed O-O bond stretching, octahedral tilt mode.

**Fig. 4** In-plane Cu-O bond length vs doping, after Radaelli, et al. \([33]\). Open circles = 10K data; filled circles = 295K data; +'s = locations of the HTT-LTO transition. Dot-dashed line = Eq. A12; other lines = guides to the eye.

**Fig. 5** Electronic dispersion associated with static distortions of the symmetry of the phonon modes in Fig. 3. The dashed lines show the dispersion along \( \Gamma - Y - M \), whenever this differs from that along \( \Gamma - X - M \), while the dot-(dot-)dashed lines are the dispersion along the line \( X(Y) - M \equiv (\pi/2a, \pi/2a) \). For ease in comparison, frames e and f are shown zone-folded into the same \( \sqrt{2} \times \sqrt{2} \) supercell as in frames c,d (beaded lines show original bands).

**Fig. 6** Effect of correlations and polaronic effects on the CuO2 band dispersion in Bi-2212. Solid circles = data of Dessau, et al. \([1]\). Fig. 6a: Dotted line = bare parameters (data for LSCO); solid line = parameters renormalized by correlation effects \([34]\); dashed lines = ghost Fermi surfaces, due to orthorhombic superlattice. Fig. 6b: solid and dashed lines = correlated bands, with additional band narrowing due to polaronic effects.

**Fig. 7** Normalized Fermi velocity, \( v_F^* = \hbar v_F / a \) at a series of Fermi levels. (Renormalized band parameters: \( t = 0.25\text{eV}, \Delta = 1\text{eV} \).) Fig. 7a: energies below the vHs, \( E_{vHs} \simeq 1.207\text{eV} \). Dashed lines, with increasing \( v_F^* \): \( E = 1.01, 1.02, 1.04, 1.06, 1.08\text{eV} \); solid lines, with decreasing \( v_F^* \): \( E = 1.10, 1.12, 1.14, 1.16, 1.18, 1.20\text{eV} \), and \( E = E_{vHs} \). Fig. 7b: energies above the vHs. Solid lines, with increasing \( v_F^* \): \( E = E_{vHs} + 0.25, 0.5, 0.75, 1, 1.25, 1.5\text{eV} \); dashed lines, with decreasing \( v_F^* \): \( E = 1.30, 1.32, 1.33\text{eV} \). Fig. 7c: \( v_F^* \) (solid line) and \( E_k^* - E_{k-\vec{q}_0} \) (dashed line) plotted vs. \( E_k^* \).

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