Structural phase transitions in $La_{2-x}(Ba,Sr)_xCuO_{4-y}$ and related physical properties

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A Landau free energy for the $La_{2-x}(Ba,Sr)_xCuO_{4-y}$ family is constructed, including the coupling energy between the order parameter and strain tensor. Using group theory, it is demonstrated that the coupling energy can be expressed as a sum of terms linear in the strain and quadratic in the order parameter and should contain a coupling term bilinear in the two order-parameter components. The structural phase transitions (SPT's) in $La_{2-x}(Ba,Sr)_xCuO_{4-y}$ are discussed on this basis. It is shown that several SPT's may occur in this system under different conditions. The observations of the influences of applied pressure, doping concentration x, and oxygen deficiency y on the SPT temperature are interpreted quantitatively. Relations connecting spontaneous strain, soft-mode vibrational frequencies, heat capacity, and elastic constants of the lower-temperature phases are derived. The mean-field results of the elastic properties and the results of the scaling analysis are also given. The results of ultrasonic measurements on a $La_{1.88}Sr_{0.12}CuO_4$ single crystal are reported. The present and other relevant experimental observations are compared with the obtained theoretical results. The possible effects of structural phase transitions or structural instabilities on the superconductivity of the system are discussed.

I. INTRODUCTION

The high-temperature structure of $La_{2-x}(Ba,Sr)_xCuO_{4-y}$ compounds has been determined by neutron powder and x-ray-diffraction measurements[1-5] to be body-centered tetragonal with space group $I4/mmm$. On cooling, they undergo a structural phase transition (SPT) at a temperature T_0, depending on the concentration of the Sr or Ba dopant as well as on oxygen contents. This transition is induced by the softening of the optical phonons associated with the tilting of CuO_6 octahedra with wave vectors[6,7] $(2\pi/a)[\frac{1}{2},\frac{1}{2},0]$ and $(2\pi/a)[\frac{1}{2},-\frac{1}{2},0]$, denoted as $Q(\mathbf{q}_1)$ and $Q(\mathbf{q}_2)$, respectively. These phonons are degenerate modes at the X point of the Brillouin-zone boundary of the body-centered tetragonal Bravais lattice. The low-temperature phase is usually taken to be the *Cmca* phase with two formula units in the primitive unit cell. However, some reports have claimed that their data could not be fitted completely using the *Cmca* group.[8,9] Interestingly, recent measurements have shown[10,11] other SPT's in $La_{2-x}Ba_xCuO_{4-y}$ (LBCO) and structural instabilities[12,13] in $La_{2-x}Sr_xCuO_{4-y}$ (LSCO) at low temperatures. These experimental results need to be explained and understood, since the structural varieties may have great influence on the physical properties of the compounds. This is especially important in the low-temperature region, where the superconducting transition also takes place. In the past few years, considerable effort has been devoted to this aim, and analyses based on Landau theory have been put forward.[10,11,14-18] However, a systematic study is still lacking.

Various SPT's in $La_{2-x}(Ba,Sr)_xCuO_{4-y}$ are expected to have great influence on, among others, the elastic properties of the compounds. Particularly from the elastic measurements of single crystals, by the proper choice of polarization and propagation directions of ultrasonic waves a soft phonon mode of a SPT can be detected. In this paper some results of our latest ultrasonic measurements on a $La_{1.88}Sr_{0.12}CuO_4$ single crystal are reported together with the presentation of a systematic Landau theoretical study of SPT's and related physical properties in the $La_{2-x}(Ba,Sr)_xCuO_{4-y}$ family.

The format of this paper is as follows: In Sec. II we show explicitly how to construct a suitable Landau free energy for the $La_{2-x}(Ba,Sr)_xCuO_{4-y}$ system, including the strain energy, the energy expanded in a power series in the order parameter components, as well as the coupling energy due to the interaction between the strain tensor and the order parameter. In Sec. III a prediction of the possible structural phase transitions in the $La_{2-x}(Ba,Sr)_xCuO_{4-y}$ systems is given. A temperature-dependent Landau theory is developed. Relations connecting spontaneous strains, soft-mode vibrational frequencies, heat capacity, and elastic constants of the lower-temperature phases are derived. The mean-field results of elastic properties are also presented. Scaling analysis is performed in the hydrodynamic limit in Sec. IV. In Sec. V, we use the Landau theory to examine the effects of the external constraints, doping, and oxygen deficiency on the phase transition temperature in $La_{2-x}(Ba,Sr)_xCuO_{4-y}$. Section VI reports the results of ultrasonic measurements on a $La_{2-x}Sr_xCuO_{4-y}$ single crystal. Section VII contains a discussion and a comparison between experiments and calculated results. Possible effects of SPT or structural instability on superconducting properties of $La_{2-x}(Ba,Sr)_xCuO_{4-y}$ compounds are discussed. A summary is given in Sec. VIII.

II. CONSTRUCTION OF THE LANDAU FREE ENERGY

One of the main tasks of this paper is to develop explicitly an appropriate Landau free energy for the system un-

der study. Before doing so, let us first address the choice of coordinates.

A. The coordinates

Usually the choice of unit-cell axes for a body-centered tetragonal lattice is as shown in Fig. 1 with corresponding coordinates $\{x,y,z\}$. The SPT from tetragonal to orthorhombic structure, for instance in D_yVO_4,[19] may be described as an expansion of one of the two equal lattice parameters, while contracting the other one. However, in the present case of $La_{2-x}(Ba,Sr)_xCuO_{4-y}$ compounds, the SPT from the tetragonal ($I4/mmm$) to the orthorhombic ($Cmca$) structure may be expressed in terms of the unit-cell transformation

$$\begin{bmatrix} a_0 \\ b_0 \\ c_0 \end{bmatrix} = \begin{bmatrix} 2\sin\left[\frac{\pi}{4}+\frac{\theta}{2}\right] & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 2\cos\left[\frac{\pi}{4}+\frac{\theta}{2}\right] & 0 \end{bmatrix} \begin{bmatrix} a_t \\ b_t \\ c_t \end{bmatrix}, \tag{1}$$

where θ is the change of angle between the a_t and b_t directions caused by the tilting of CuO_6 octahedra about the [1,1,0] or [1,−1,0] directions. It will be seen later that it is advantageous for the development of the Landau free energy if we choose the unit-cell axes with corresponding coordinates $\{x',y',z'\}$ (see Fig. 1).

B. The order parameter

The symmetry of the order parameter places this system in the universality class $d=3$ XY with cubic anisotropy.[7] The order parameter $\mathbf{Q}$ has two components, $Q(\mathbf{q}_1)$ and $Q(\mathbf{q}_2)$, associated with the two orthogonal tilting modes of the CuO_6 octahedra, representing the tilting angles. $\mathbf{q}_1$ and $\mathbf{q}_2$ are the two arms of the K-star vector at the X point of the first Brillouin-zone boundary of the body-centered tetragonal structure. It can be easily verified that both amplitudes of $Q(\mathbf{q}_1)$ and $Q(\mathbf{q}_2)$ are real. For simplicity, we denote $Q(\mathbf{q}_1)$ as Q_1 and $Q(\mathbf{q}_2)$ as Q_2.

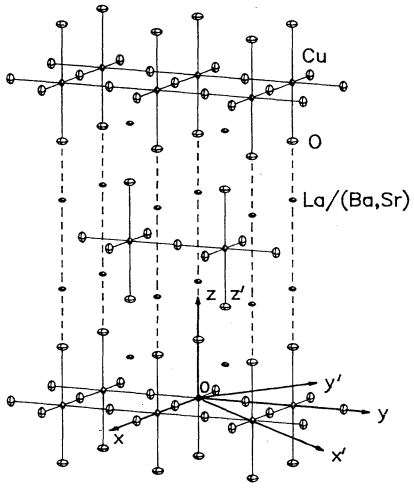

FIG. 1. The structure of $La_{2-x}(Sr,Ba)_xCuO_{4-y}$ at high temperature with space group $I4/mmm$.

C. Landau free energy

A Landau free energy normally comprises three parts: (a) a free-energy contribution, F_s, from the strain fields, (b) a free energy, F_0, expanded in a power series in the order parameter, and (c) a free-energy contribution, F_c, from the coupling between strains and the order parameter. The inclusion of these three parts is usually sufficient for a system without any external constraints as long as only the structural and elastic properties are considered. The Landau free energy may be extended to take into account possible magnetic or piezoelectric effects.

For the present case, the strain energy can be obtained directly from the following general expression:

$$F_s=\tfrac{1}{2}C^t_{mn}e_me_n\ , \tag{2}$$

where C_{mn} are the elastic moduli and e_m,e_n are the corresponding strains. Summation over repeated indices is understood. The superscript t denotes the $I4/mmm$ phase. Since we already know that our system belongs to the $d=3$ XY universality class, the standard free-energy expansion in the power series of the order parameter reads[20]

$$F_0=\tfrac{1}{2}K(T)(Q_1^2+Q_2^2)+u(Q_1^2+Q_2^2)^2 +v(Q_1^4+Q_2^4)+\cdots\ . \tag{3}$$

The last contribution comes from the coupling between strains and the order parameter. Generally such contributions are constructed using group theory. It is required that the Landau free energy must be invariant under the symmetry operations of the space group $I4/mmm$. First, let us consider the invariant functions for the corresponding point group $4/mmm$. An important and useful group theoretical result often being used for this purpose is the generalized Unsöld theorem, which states that[21] the quantity

$$\sum_{k=1}^{1_j}|\varphi_k^{(j)}|^2 \tag{4}$$

is invariant under all operations of the point group for which $\varphi_k^{(j)}$ are the basis functions of an irreducible representation j of dimension 1_j. Applying this theorem to our case results in the conclusion that a coupling term between a particular combination of strain tensors and a given power of the order parameter can exist only if they belong to the same irreducible representation of the point group $4/mmm$. Also, from group theory we know that after the transformation from $\{x,y,z\}$ to $\{x',y',z'\}$, the space group $I4/mmm$ and the irreducible representations of the point group $4/mmm$ remain the same. Therefore, the symmetrized strains and symmetrized elastic constants can be obtained straightforwardly from the character table[22] of $4/mmm$ as listed in Table I. It

TABLE I. Symmetrized elastic moduli and strains in $\{X',Y',Z'\}$ and $\{XYZ\}$ coordinates.

Coordinates $\{x'y'z'\}$		$\{xyz\}$		
Symmetrized strains	Symmetrized elastic moduli	Symmetrized strains	Symmetrized elastic moduli	Transforms under
$\varepsilon_1+\varepsilon_2,\varepsilon_3$	$D_{11}+D_{12}$	e_1+e_2,e_3	$C_{11}+C_{12}$	A_{1g}
$\varepsilon_1-\varepsilon_2$	$D_{11}-D_{12}$	$2e_6$	$2C_{66}$	B_{1g}
ε_6	D_{66}	$(1/2)(e_2-e_1)$	$(1/2)(C_{11}-C_{12})$	B_{2g}

may be demonstrated that $Q_1^2+Q_2^2$, $Q_1^2-Q_2^2$, and Q_1Q_2 are the symmetry-adapted basis functions of the irreducible representations of A_{1g}, B_{1g}, and B_{2g}, respectively, by using the following formula for creating symmetry-adapted functions:[23]

$$F^j(Q)\propto\sum_r \chi^j(G_r)^*G_r f(Q)\ , \tag{5}$$

where $f(Q)$ is some chosen function of the general type of interest, G_r is the rth symmetry operation of the jth irreducible representation, and $\chi^j(G_r)^*$ is the corresponding complex conjugate character. In the cases of one-dimensional irreducible representations, such as A_{1g}, B_{1g}, and B_{2g} in the $4/mmm$ point group, if $f(Q)$ is chosen to be the symmetry-adapted basis function, Eq. (5) becomes

$$f(Q)=\frac{1}{g}\sum_r \chi^j(G_r)^*G_r f(Q)\ . \tag{6}$$

Here g is the order of the point group $4/mmm$. Indeed, $Q_1^2+Q_2^2$, $Q_1^2-Q_2^2$, and Q_1Q_2 do satisfy Eq. (6) for the A_{1g}, B_{1g}, and B_{2g} irreducible representations respectively. This provides the coupling energy as

$$[a_1(\varepsilon_1+\varepsilon_2)+a_2\varepsilon_3](Q_1^2+Q_2^2) +b_1(\varepsilon_1-\varepsilon_2)(Q_1^2-Q_2^2)+b_2\varepsilon_6Q_1Q_2 \tag{7}$$

where a_1,a_2,b_1,b_2 are coupling constants. By performing a coordinate transformation from the $\{x',y',z'\}$ system to the $\{x,y,z\}$ system, we may express the coupling energy in terms of the strain tensors e_i in the $\{x,y,z\}$ system as

$$F_c=[a_1(e_1+e_2)+a_2e_3](Q_1^2+Q_2^2) +2b_1e_6(Q_1^2-Q_2^2)+\tfrac{1}{2}b_2(e_2-e_1)Q_1Q_2\ . \tag{8}$$

D. The coupling term bilinear in order parameter components

Before we subject the coupling energy to the examination of the translational operations of the $I4/mmm$ phase, we must be aware of the fact that for a given system, the possible low-temperature phases are fixed as soon as the universality class and the order parameter are known. The effect of the coupling between strains and order parameter leads only to a change of the conditions for a particular SPT to take place and possibly alters the SPT from a second-order transition to a first-order transition.[20] For the $d=3$ XY universality class, there are three possible low-temperature phases:[20] (a) $Q_1\neq0$, $Q_2=0$ or $Q_1=0$, $Q_2\neq0$, (b) $Q_1=Q_2\neq0$, and (c) $Q_1\neq Q_2\neq0$ (see Sec. III for details). In the first case, the bilinear coupling term vanishes and therefore produces no influences on the macroscopic properties of the system. However, in the second and third cases the bilinear coupling does not give a zero contribution and is invariant under all symmetry operations of the $I4/mmm$ group. The latter point can be demonstrated as follows: Let us consider case (b) to be specific. The $Q_1=Q_2\neq0$ phase is understood as the coherent superposition[10] of the tiltings of the $Q_1\neq0$, $Q_2=0$ and $Q_1=0$, $Q_2\neq0$. It is easily shown graphically that the resulting tilting is along the [1,0,0] or [0,1,0] directions (see Fig. 3). Therefore, here the real physical meanings of Q_1 and Q_2 are the clockwise tiltings around the [1,0,0] and [0,1,0] directions, respectively. The verification of the invariance of the coupling energy under the symmetry operations of the point group $4/mmm$ is the same as before. If we perform translational symmetry operations using Seitz operator,[23] we get the following results:

$$\{E/[n_1/2,n_2/2,n_3/2]\}Q_1=\begin{cases}\begin{bmatrix}-Q_2 & \text{When } n_1,n_2 \text{ are odd integers}\\ Q_1 & \text{otherwise}\end{bmatrix} & \text{when } n_1>0,\ n_2>0 \text{ or } n_1<0,\ n_2<0\\ \begin{bmatrix}Q_2 & \text{when } n_1,n_2 \text{ are odd integers}\\ Q_1 & \text{otherwise}\end{bmatrix} & \text{when } n_1>0,\ n_2<0 \text{ or } n_1<0,\ n_2>0\ ,\end{cases} \tag{9a}$$

$$\{E/[n_1/2,n_2/2,n_3/2]\}Q_2=\begin{cases}\begin{bmatrix}-Q_1 & \text{when } n_1,n_2 \text{ are odd integers}\\ Q_2 & \text{otherwise}\end{bmatrix} & \text{when } n_1>0,\ n_2>0 \text{ or } n_1<0,\ n_2<0\\ \begin{bmatrix}Q_1 & \text{when } n_1,n_2 \text{ are odd integers}\\ Q_2 & \text{otherwise}\end{bmatrix} & \text{when } n_1>0,\ n_2<0 \text{ or } n_1<0,\ n_2>0\ .\end{cases} \tag{9b}$$

Here n_1,n_2,n_3 are integers satisfying $|n_1|=|n_2|=|n_3|\neq 0$, and

$$\{E/[n_1,0,n_3] \text{ or } [0,n_2,n_3]\}Q_1=\begin{cases}-Q_1 \text{ when } n_1,n_2 \text{ are odd integers}\\ Q_1 \text{ otherwise},\end{cases} \tag{9c}$$

$$\{E/[n_1,0,n_3] \text{ or } [0,n_2,n_3]\}Q_2=\begin{cases}-Q_2 \text{ when } n_1,n_2 \text{ are odd integers}\\ Q_2 \text{ otherwise}.\end{cases} \tag{9d}$$

Here n_1,n_2,n_3 are integers or zero. In this case, the term $2b_1e_6(Q_1^2-Q_2^2)$ gives a zero contribution. We see, therefore, that the bilinear term is invariant under all symmetry operations of the $I4/mmm$ group.

It has been argued that the bilinear term should be omitted, since the Q_1Q_2 term transforms as a K vector at a point of the first Brillouin-zone boundary.[24] Therefore, it cannot couple to the long-wavelength quantities. This argument is correct only under the assumption that there is only one possible SPT, namely, the SPT from $I4/mmm$ to *Cmca*. This assumption is, however, not true in the present case due to the multicomponent nature of the order parameter. On the other hand, even if this assumption were correct, the inclusion of the bilinear term could not have altered the total free energy of the system, since one of the order-parameter components must be zero. The important idea here is that there are two other possible SPT's in addition to the $I4/mmm$ to *Cmca*. For the other two cases, which are at least theoretically allowed, the order parameter is the coherent superposition of the tilting around the [1,1,0] and [1,−1,0] directions. Therefore, the Q_1Q_2 term will transform as a zone-center K vector instead of zone boundary. It is evident then that if one wants to construct a Landau free-energy density, which can account for all three possible SPT's, the bilinear term must be included. We will show later that the importance of this bilinear term is clearly reflected in explaining experimental data.

Finally, we obtain the total Landau free energy F, which is suitable for describing the structural phase transitions in $La_{2-x}(Ba,Sr)_xCuO_{4-y}$ as the sum

$$\begin{aligned}F=F_c+F_s+F_0=&[a_1(e_1+e_2)+a_2e_3](Q_1^2+Q_2^2)+2b_1e_6(Q_1^2-Q_2^2)+\tfrac{1}{2}b_2(e_2-e_1)Q_1Q_2\\&+\tfrac{1}{2}C_{11}^t(e_1^2+e_2^2)+\tfrac{1}{2}C_{33}^te_3^2+C_{12}^te_1e_2+C_{13}^t(e_1e_3+e_2e_3)+\tfrac{1}{2}C_{44}^t(e_4^2+E_5^2)+\tfrac{1}{2}C_{66}^te_6^2\\&+\tfrac{1}{2}K(T)(Q_1^2+Q_2^2)+u(Q_1^2+Q_2^2)^2+v(Q_1^4+Q_2^4)+\cdots .\end{aligned} \tag{10}$$

The symmetrized elastic constants expressed with respect to both $\{x,y,z\}$ and $\{x',y',z'\}$ coordinates are listed in Table I.

III. MEAN-FIELD CALCULATION, PHASE DIAGRAM

On cooling, the system will be unstable at $K(T)<0$. The equilibrium states of a $La_{2-x}(Ba,Sr)_xCuO_{4-y}$ crystal in the absence of external constraints are obtained by minimizing F with respect to all Q_i and e_k ($i=1,2$, $k=1-6$). The range of possibilities is conveniently visualized by minimizing F first with respect to all e_k, while keeping all Q_i arbitrary. Setting $\partial F/\partial e_k=0$, we get a set of equations from which we may express e_k as a function of Q_i. Then substituting the obtained $e_k(Q_i)$ into Eq. (10), the free energy now (denoted as $\tilde{F}$) can be rewritten as a function of the order parameter alone,

$$\begin{aligned}\tilde{F}&=F[Q_i,e(Q_i)]\\&=\tfrac{1}{2}K(T)(Q_1^2+Q_2^2)+Y(Q_1^2+Q_2^2)^2+v'Q_1^2Q_2^2 .\end{aligned} \tag{11}$$

Here, Y, v', and α are defined as follows:

$$\begin{aligned}&\alpha=\{2[p^2(C_{11}^t+C_{12}^t)+2pa_1k]C_{33}^t-(2C_{13}^tp+a_2k)^2\}/2k^2C_{33}^t\\&Y=u+\alpha+v-(2b_1^2/C_{66}^t),\quad v'=(8b_1^2/C_{66}^t)-\{b_2^2/[4(C_{11}^t-C_{12}^t)]\}-2v ,\\&s=\tfrac{1}{2}C_{33}^t(C_{11}^t+C_{12}^t)-C_{13}^{t2},\quad k=2(C_{11}^t-C_{12}^t)s,\quad p=(C_{11}^t-C_{12}^t)(a_2C_{13}^t-a_1C_{33}^t) .\end{aligned} \tag{12}$$

From the expression of $\tilde{F}$, one can see that the transition temperature does not change due to the coupling between the order parameter and the strain tensors in the absence of external constraints. However, if the system is subjected to an external stress field, the transition temperature will be modified greatly by the coupling.[25,26] The discussion of this situation will be given in Sec. V. Here we restrict ourselves to the case of free cooling.

Before performing the minimization, we first normalize the eigenvector

$$Q_i=\xi_i Q, \quad \sum_i \xi_i^2=1, \quad i=1,2 \ .$$

By minimizing $\tilde{F}$ with respect to Q_i, we have the following solutions.

A. Orthorhombic phase

Under the conditions $v'>0$ and $Y>0$, the stable phase has one of four domains ($\xi_1=\pm 1$, $\xi_2=0$ or $\xi_1=0$, $\xi_2=\pm 1$). Here $\pm$ denotes tilting of the CuO_6 octahedra in anticlockwise and clockwise directions, respectively. This phase corresponds to the *Cmca* structure with a doubling of the volume of the crystallographic unit cell of the high-temperature tetragonal phase (see Fig. 2). First,

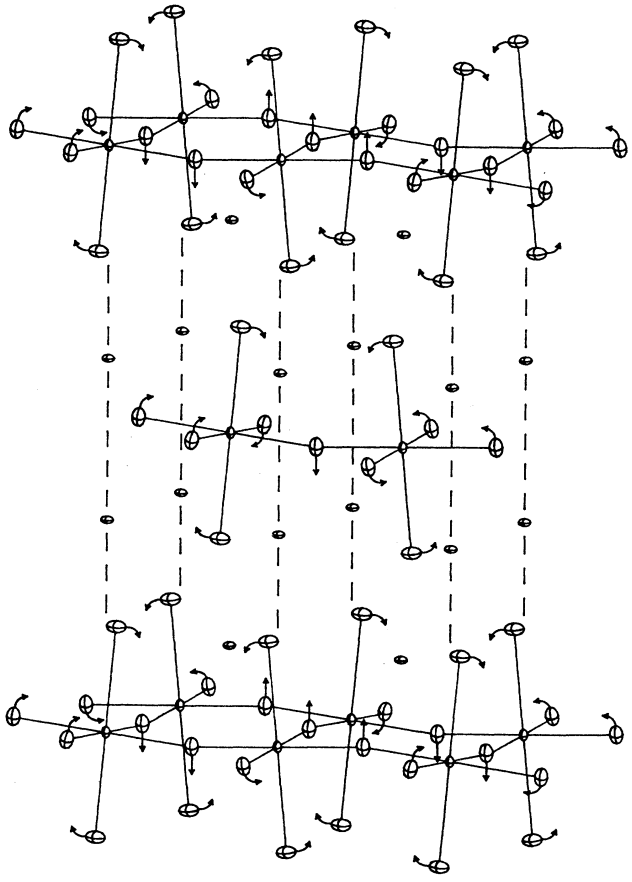

FIG. 2. The MO phase of $La_{2-x}(Sr,Ba)_xCuO_{4-y}$ with space group *Cmca* ($\xi_1=\pm 1$, $\xi_2=0$). Each arrow indicates the direction of tilting.

let us calculate the changes in elastic moduli due to this SPT. Usually the elastic moduli are measured under the condition that the order parameter can change freely in the presence of applied ultrasonic strain. Its conjugate force $\partial F/\partial Q_i$ is kept zero during the measurements. Therefore, in the calculation of the elastic moduli of this low-temperature phase, we may first take the partial derivatives of F with respect to Q_i, while keeping e_k arbitrary. Then setting $\partial F/\partial Q_i=0$ ($i=1,2$), we can express Q_i in terms of e_k ($k=1-6$). It is known that the elastic moduli entering the expression for the purely elastic free energy are those determined under the condition $Q_i=0$. The changes of the elastic moduli due to SPT's are created by the motion of the order parameter. So the elastic tensor C_{jt} in the low-temperature phase is given by

$$C_{jt}=\frac{\partial^2 \bar{F}(Q_i(e_k),e_k)}{\partial e_j \partial e_t} = C_{jt}^t-\sum_{il}\frac{\partial^2 F}{\partial e_j \partial Q_i}R_{il}\frac{\partial^2 F}{\partial Q_l \partial e_t} \ , \tag{13}$$

where C_{jt}^t are the tetragonal elastic constants appearing in the expression of F. Using the relations[27]

$$\sum_l R_{il}\frac{\partial^2 F}{\partial Q_l \partial Q_m}=\delta_{im} \quad \text{and} \quad I\omega_i^2\delta_{ij}=\frac{\partial^2 F}{\partial Q_i \partial Q_j} \ , \tag{14}$$

where I is a generalized mass, we get

$$C_{jt}=C_{jt}^t-I^{-1}\sum_i \frac{\partial^2 F}{\partial e_j \partial Q_i}\omega_i^{-2}\frac{\partial^2 F}{\partial Q_i \partial e_t} \ . \tag{15}$$

It is easily seen that C_{jt} are equal to C_{tj} because of the symmetry of the Landau free energy. For $T>T_0$, the order parameter is zero. Therefore,

$$C_{jt}=C_{jt}^t \ .$$

For $T<T_0$, we get

$$\begin{aligned}
&C_{11}^0=C_{22}^0=C_{11}^t-I^{-1}Q_0^2\left[4a_1^2\omega_2^{-2}+\frac{b_2^2}{4}\omega_1^{-2}\right] \ , \\
&C_{12}^0=C_{12}^t-I^{-1}Q_0^2\left[4a_1^2\omega_2^{-2}-\frac{b_2^2}{4}\omega_1^{-2}\right] \ , \\
&C_{13}^0=C_{23}^0=C_{13}^t-4a_1a_2I^{-1}Q_0^2\omega_2^{-2} \ , \\
&C_{33}^0=C_{33}^t-4a_2^2I^{-1}Q_0^2\omega_2^{-2} \ , \\
&C_{66}^0=C_{66}^t-16b_1^2I^{-1}Q_0^2\omega_2^{-2}, \quad C_{36}^0=8a_2b_1I^{-1}Q_0^2\omega_2^{-2} \ , \\
&C_{16}^0=C_{26}^0=8a_1b_1I^{-1}Q_0^2\omega_2^{-2} \ , \\
&C_{44}^0=C_{55}^0=C_{44}^t, \quad C_{45}^0=C_{46}^0=C_{56}^0=0 \ .
\end{aligned} \tag{16}$$

These relations clearly show that C_{11}, C_{22}, C_{33}, and C_{66} will exhibit a steplike decrease at the transition temperature when the temperature is lowered, while C_{44} and C_{55} remain unchanged. For C_{13}, C_{23}, and C_{12}, either a step decrease or increase is possible, depending on the relative magnitudes and signs of the coupling constants a_1, a_2, and b_2. From Eq. (16) we see that several spontane-

ous elastic tensor components appear in the low-temperature *Cmca* phase. This is because we do our calculation in the high-temperature tetragonal coordinates. They could be removed by making a coordinate transformation from the $\{x,y,z\}$ coordinates to the $\{x',y',z'\}$ coordinates. Perhaps the most important information obtained from such relations is that they show how to determine the coupling constants a_1,a_2,b_1,b_2, and the generalized mass I experimentally by measuring the elastic tensors, the soft-mode vibrational frequencies and the order parameter, and generally a way of testing the range of validity of the mean-field theory. The changes in other physical properties due to this phase transition is summarized in Table II.

B. New tetragonal phase

Under the condition of $v'<0$, $Y+(1/4)v'>0$, the stable phase has one of four domains $[\xi_1=\xi_2=\pm\sqrt{2}/2]$. This corresponds to a new tetragonal phase with a volume of the primitive unit cell four times larger than that of the original tetragonal phase. Symmetry considerations show that the space group of the new phase may be $P4_2/ncm$ (see Fig. 3). This structure is developed by coherent superposition of the tilted CuO_6 octahedra around [1,1,0] and [1,−1,0] directions.

Following the same procedure as the *Cmca* phase, we get the changes in elastic moduli as

$$
\begin{aligned}
C_{11}^{l}&=C_{11}^{t}-2I^{-1}Q_0^2\omega_1^{-2}\left[2a_1-\frac{b_2}{2}\right]^2,\\
C_{22}^{l}&=C_{11}^{t}-2I^{-1}Q_0^2\omega_1^{-2}\left[2a_1+\frac{b_2}{2}\right]^2,\\
C_{13}^{l}&=C_{13}^{t}-2a_2I^{-1}Q_0^2\omega_1^{-2}(4a_1-b_2),\\
C_{23}^{l}&=C_{13}^{t}-2a_2I^{-1}Q_0^2\omega_1^{-2}(4a_1+b_2),\\
C_{12}^{l}&=C_{12}^{t}-2I^{-1}Q_0^2\omega_1^{-2}\left[4a_1^2-\frac{b_2^2}{4}\right],\\
C_{33}^{l}&=C_{33}^{t}-8a_2^2I^{-1}Q_0^2\omega_1^{-2},\\
C_{66}^{l}&=C_{66}^{t}-36b_1^2I^{-1}Q_0^2\omega_1^{-2}.
\end{aligned}
\tag{17}
$$

TABLE II. Several physical quantities in the MO and LT phases, calculated by employing the standard procedure.

	Cmca	$P4_2/ncm$
Order parameter Q_0	$[-K(T)/4Y]^{1/2}$	$[-K(T)/(4Y+v')]^{1/2}$
Spontaneous strains[a]	$e_1=e_2=PQ_0^2/k$	$e_1=\left[P+\frac{b_2}{2}S\right]Q_0^2/k$
	$e_3=-(2C_{13}^tP+a_2k)Q_0^2/C_{33}^tk$	$e_2=\left[P-\frac{b_2}{2}S\right]Q_0^2/k$
	$e_4=e_5=0$	$e_3=-(2C_{13}^tP+a_2k)Q_0^2/C_{33}^tk$
	$e_6=2b_1Q_0^2/C_{66}^t$	$e_4=e_5=e_6=0$
Ground-state energy	$-K^2(T)/16Y$	$-K^2(T)/(16Y+4v')$
Change in specific heat ΔC[b]	$\frac{a^2T}{8Y}$	$\frac{a^2T}{8Y+2v'}$
Soft-mode vibrational frequencies	$T>T_0$	$T>T_0$
	$\omega_1^2=\omega_2^2=I^{-1}K(T)$	$\omega_1^2=\omega_2^2=I^{-1}K(T)$
	$T<T_0$	$T<T_0$
	$\omega_1^2=I^{-1}K(T)\left[\frac{v+\alpha}{Y}-\frac{a_1P}{kY}+a_2\frac{2C_{13}^tP+a_2k}{2C_{33}^tKY}-\frac{4b_1^2}{C_{66}^tY}\right]$	$\omega_1^2=\omega_2^2=2I^{-1}K(T)\left[\frac{-2u-v+\alpha}{4Y+v'}+a_2\frac{2C_{13}^tP+a_2k}{2C_{33}^tk(4Y+v')}-\frac{2a_1P}{k(4Y+v')}\right]$
	$\omega_2^2=I^{-1}K(T)\left[\frac{-2(u+v)+\alpha}{Y}-\frac{a_1P}{kY}+a_2\frac{2C_{13}^tP+a_2k}{2C_{33}^tKY}\right]$	

[a]Parameters Y, v', P, S and k are defined in expressions (12).
[b]Here, we have assumed $K(T)=\frac{1}{2}a(T-T_0)$.

So the degeneracy of the pairs of elastic constants C_{11}, C_{12} and C_{13}, C_{23} of the high-temperature tetragonal phase will be lifted in the ordered phase. The reason why the calculated elastic moduli here differ from the standard tetragonal form is the same as that for *Cmca* case [see Eqs. (16) and the following discussion]. The calculated changes in other physical quantities due to the SPT are listed in Table II.

C. Intermediate phase

When $v' \to 0$, which is possible in these systems,[20] the ordered phase may take up any orientation in the order parameter space. In order to determine what is the stable phase now, the next order in the expansion should be taken into account. Unlike Ref. 10, which includes the eighth-order term as the next approximation, here we suggest instead that the sixth-order terms should be included. This is simply due to the fact that the sixth-order terms are the terms, which give the largest contribution to the Landau free energy among those terms we have neglected so far in this study.

The sixth-order terms may be divided into two types. One type, such as $(Q_1^2+Q_2^2)^3$, is isotropic, which does not help in determining the favorable orientation of the order parameter in the order parameter space and therefore will not be included for consideration. The other type is anisotropic, which may be formally expressed as $w(Q_1^2+Q_2^2)(Q_1^4+Q_2^4)$. This expression can be rewritten as $w(Q_1^2+Q_2^2)Q_1^2Q_2^2+w(Q_1^6+Q_2^6)$. It is easily seen now that the first term is not an independent term. It has already been considered in the v' term in expression (11), and v' is now supposed to approach to zero. Thus, here we need only to include $w(Q_1^6+Q_2^6)$ into expression (11) for the following discussion. It is important now to study the consequences of this term. It is known that v' is temperature dependent.[28] One crucial question, which cannot be answered at the phenomenological level, is how the parameter v' varies with temperature. On cooling, v' may first take a positive value and then at a certain temperature change its sign gradually or abruptly depending on the sign of w. Or it may occur in the opposite order. As a result, several possible SPT's may take place as listed in Table III. Note that the *Pccn* phase appears when $Q_1 \neq Q_2 \neq 0$ (see Fig. 4). The initial conditions imposed on the parameters v', Y, w in Table III refer to $T > T_0$. The physical quantities involved in each SPT can be calculated by a similar procedure as before. We shall not now pursue this line of development in further detail.

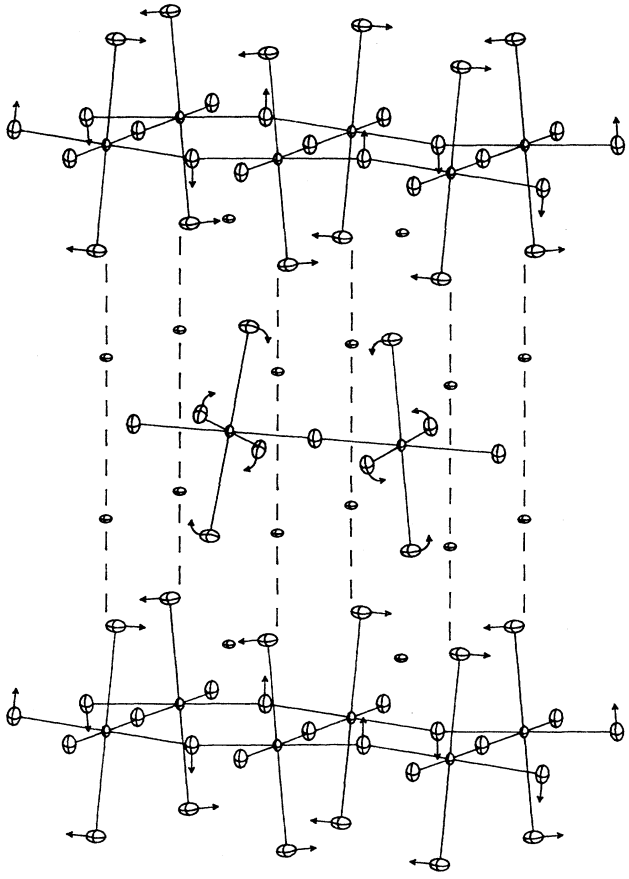

FIG. 3. The LT phase of $La_{2-x}(Sr,Ba)_xCuO_{4-y}$ with space group $P4_2/ncm$ ($\xi_1=\sqrt{2}/2$, $\xi_2=-\sqrt{2}/2$ and $\xi_1=-\sqrt{2}/2$, $\xi_2=\sqrt{2}/2$). Each arrow indicates the direction of tilting.

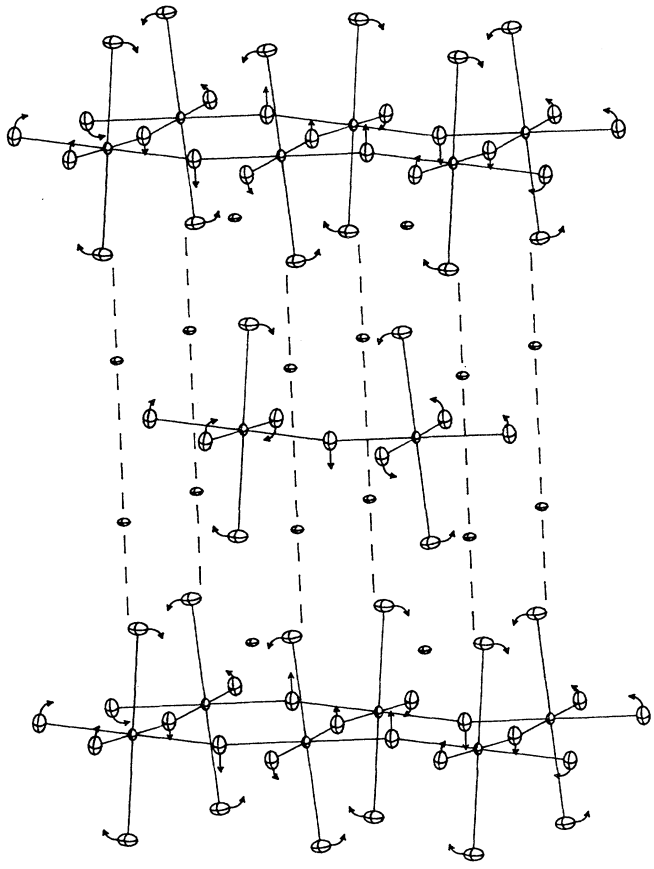

FIG. 4. The PO phase of $La_{2-x}(Sr,Ba)_xCuO_{4-y}$ with space group $Pccn$ ($\xi_1=2\sqrt{5}/5$, $\xi_2=-\sqrt{5}/5$ and $\xi_1=-2\sqrt{5}/5$, $\xi_2=\sqrt{5}/5$). Each arrow indicates the direction of tilting and the length of the arrow is proportional to magnitude of tilting.

TABLE III. In this table, we list the various possibilities for second- or first-order transitions. The symbols HT, MO, PO, and LT refer to the $I4/mmm$, $Cmca$, $Pccn$, and $P4_2/ncm$ phases, respectively.

$v'>0,\ Y>0$	$\mathrm{HT} \xrightarrow[\text{order}]{\text{second}} \mathrm{MO}$
$v'>0,\ Y>0,\ w<0$	$\mathrm{HT} \xrightarrow[\text{order}]{\text{second}} \mathrm{MO} \xrightarrow[\text{order}]{\text{first}} \mathrm{LT}$
$v'>0,\ Y>0,\ w>0$	$\mathrm{HT} \xrightarrow[\text{order}]{\text{second}} \mathrm{MO} \xrightarrow[\text{order}]{\text{second}} \mathrm{PO}^{a} \xrightarrow[\text{order}]{\text{second}} \mathrm{LT}$
$v'<0,\ Y+(1/4)v'>0$	$\mathrm{HT} \xrightarrow[\text{order}]{\text{second}} \mathrm{LT}$
$v'<0,\ w>0$ $Y+(1/4)v'>0$	$\mathrm{HT} \xrightarrow[\text{order}]{\text{second}} \mathrm{LT} \xrightarrow[\text{order}]{\text{first}} \mathrm{MO}$
$v'<0,\ w<0$ $Y+(1/4)v'>0$	$\mathrm{HT} \xrightarrow[\text{order}]{\text{second}} \mathrm{LT} \xrightarrow[\text{order}]{\text{second}} \mathrm{PO}^{b} \xrightarrow[\text{order}]{\text{second}} \mathrm{MO}$

[a]This phase is stable in the region $-3wQ^2<v'<3wQ^2$.
[b]This phase is stable in the region $3wQ^2<v'<-3wQ^2$.

Let us only point out here that the energy contributions from the strain field and the coupling between trains and the order parameter to the Landau free energy should always be constructed in the high-temperature phase. For instance, if the SPT is the MO→LT [which has been observed in $La_{2-x}Ba_xCuO_4$ (Refs. 10 and 11)], instead of using the strain field and coupling energy like F_s and F_c, we should use F_s' and F_c' given by

$$F_s'=\tfrac{1}{2}C_{mn}e_m e_n=\tfrac{1}{2}C_{11}^0\varepsilon_1^2+\tfrac{1}{2}C_{22}^0\varepsilon_2^2+\tfrac{1}{2}C_{33}^0\varepsilon_3^2+C_{12}^0\varepsilon_1\varepsilon_2+C_{13}^0\varepsilon_1\varepsilon_3+C_{23}^0\varepsilon_2\varepsilon_3+\tfrac{1}{2}C_{44}^0\varepsilon_4^2+\tfrac{1}{2}C_{55}^0\varepsilon_5^2+\tfrac{1}{2}C_{66}^0\varepsilon_6^2 \quad (18)$$

and

$$F_c'=(a_1'\varepsilon_1+a_2'\varepsilon_2+a_3'\varepsilon_3)(Q_1^2+Q_2^2)+b_2'\varepsilon_6 Q_1 Q_2 \ . \quad (19)$$

Note here that we are using $\{x',y',z'\}$ coordinates (see Fig. 1). The Landau free energy proper for describing this transition is now (here we assume that the discontinuity in the order parameter at phase-transition temperature is small so that Landau analysis is still valid)

$$F'=F_c'+F_s'+F_0 \ . \quad (20)$$

After performing the same mathematic treatment as before, we could express F' in the same form as Eq. (11). The coefficients Y and v' now have changed their values (since they are temperature-dependent functions). For example, v' has changed from a previous positive value to a negative value $-\frac{1}{2}(b_2'^2/C_{66}^0)-2v$ as expected (see Fig. 5).

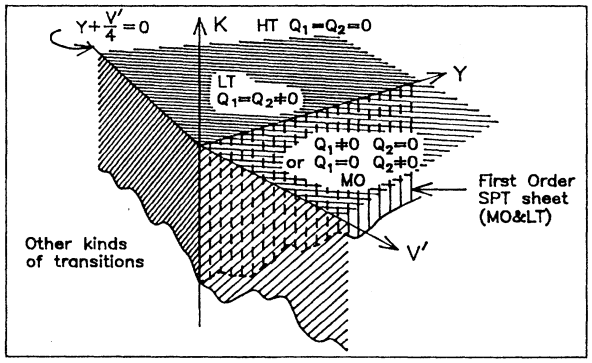

FIG. 5. The phase diagram of $La_{2-x}(Sr,Ba)_xCuO_{4-y}$ resulted from calculations.

IV. SCALING ANALYSIS

In the previous section, we presented the results of mean-field calculations which are expected to be valid in the region where the correlated fluctuations are small on a length scale larger than the interaction range in the system. Once the system approaches the region very close to the SPT temperature, fluctuation effects are no longer negligible. In this region the critical behavior will dominate. Some basic critical exponents for $d=3$, XY model have been calculated.[29] Here we want to see how elastic moduli behave in this region.

Proceeding in a similar way as for the case of $d=3$, Heisenberg model,[30,31] we start from the effective Landau-Ginzberg-Wilson Hamiltonian[32]

$$H=\int d\mathbf{r}\left[\tfrac{1}{2}\gamma|\mathbf{Q}|^2+\tfrac{1}{2}|\nabla\mathbf{Q}|^2+u_0|\mathbf{Q}|^4+v_0\sum_a Q_a^4-\tfrac{1}{2}f\sum_a\left[\frac{\partial Q_a}{\partial X_a}\right]^2+\sum_i\sum_j a_i e_i Q_j^2\right], \quad (21)$$

where e_i, Q_j^2 are symmetrized elastic strains and corresponding Q^2 representations respectively. The free energy of the system can be written as

$$F=-\frac{kT}{V}\ln Z \ . \tag{22}$$

Here V is the volume and Z is the partition function

$$Z=\sum_{Q} e^{-H/kT} \ . \tag{23}$$

The summation runs over all relevant configurations of the order parameter, which are allowed by the symmetry of the system. According to the definition of elastic moduli, we get the isothermal change of elastic constants ΔC_{mn} as

$$\Delta C_{ij}=-\frac{1}{kTV}\left[\left\langle\frac{\partial H}{\partial e_i}\frac{\partial H}{\partial e_j}\right\rangle-\left\langle\frac{\partial H}{\partial e_i}\right\rangle\left\langle\frac{\partial H}{\partial e_j}\right\rangle\right] \ . \tag{24}$$

The thermal average of some quantity P is now found as $\langle P\rangle=(1/Z)\sum_Q Pe^{-H/kT}$. Note here that higher order terms have been dropped. After inserting Eq. (21) into Eq. (24), we obtain

$$\Delta C_{33}=-\frac{a_2^2}{kTV}\int d\mathbf{r}\int d\mathbf{r}'\{\langle|\mathbf{Q}(\mathbf{r})|^2|\mathbf{Q}(\mathbf{r}')|^2\rangle-\langle|\mathbf{Q}(\mathbf{r})|^2\rangle\langle|\mathbf{Q}(\mathbf{r}')|^2\rangle\} \ , \tag{25}$$

$$\Delta C_{66}=-\frac{4b_1^2}{kTV}\int d\mathbf{r}\int d\mathbf{r}'\{\langle[Q_1^2(\mathbf{r})-Q_2^2(\mathbf{r})][Q_1^2(\mathbf{r}')-Q_2^2(\mathbf{r}')]\rangle\} \tag{26}$$

$$\begin{aligned}\Delta(C_{11}+C_{12})=-\frac{1}{kTV}\int d\mathbf{r}\int d\mathbf{r}'\Bigg[&\left\langle\left[a_1|\mathbf{Q}(\mathbf{r})|^2-\frac{b_2}{2}Q_1(\mathbf{r})Q_2(\mathbf{r})\right]\left[a_1|\mathbf{Q}(\mathbf{r}')|^2-\frac{b_2}{2}Q_1(\mathbf{r}')Q_2(\mathbf{r}')\right]\right\rangle\\&-\left\langle\left[a_1|\mathbf{Q}(\mathbf{r})|^2-\frac{b_2}{2}Q_1(\mathbf{r})Q_2(\mathbf{r})\right]\right\rangle\left\langle\left[a_1|\mathbf{Q}(\mathbf{r}')|^2-\frac{b_2}{2}Q_1(\mathbf{r}')Q_2(\mathbf{r}')\right]\right\rangle\\&+\text{antisymmetric terms}\Bigg] \ .\end{aligned} \tag{27}$$

The expression for $\Delta(C_{11}-C_{12})$ is similar to expression (27) except for the minus sign in antisymmetric terms. Two important conclusions could be drawn from the expressions given above.

(1) Although C_{33} and $C_{11}+C_{12}$ belong to the same irreducible representation as can be seen from the model Hamiltonian, they will behave differently in the critical region.

(2) The expression for ΔC_{33} is essentially the same as that for the change of specific heat. Therefore, ΔC_{33} will vary with the reduced temperature $t-|(T-T_c)/T_c|$ as $t^{-\alpha}$.

The behavior of ΔC_{66}, $\Delta(C_{11}-C_{12})$, and $\Delta(C_{11}+C_{12})$, on the other hand, is more complicated and will depend on the properties of a particular SPT. We will discuss this in Sec. VII.

Without loss of generality, we discuss the behavior of the symmetry-breaking elastic constant. The exponents for such elastic constants can be derived from the scaling hypothesis,[28]

$$F=t^{2-\alpha}Y_f\left[\frac{h}{t^{\Delta}},\frac{e_m}{t^{\phi}}\right] \ , \tag{28}$$

where the symmetrized strain e_m has been taken as a relevant field. Δ is the gap exponent and ϕ is the crossover exponent. For $T<T_c$ the mean value of the order parameter $\langle Q\rangle\neq 0$. The coupling energy can be written as

$$H_c\sim e_m(Q_0+\delta Q)^2=e_m(Q_0^2+2Q_0\delta Q+\delta Q\delta Q) \ . \tag{29}$$

Here Q_0 is the thermal average of Q and δQ is the fluctuation relative to Q_0. It is easily seen from Eq. (29) that there is one "field" $e_m Q_0$ coupled linearly to the order parameter fluctuations in addition to the quadratic coupling. This field $e_m Q_0$ can be regarded as representing the field h. Hence, we may write

$$F=t^{2-\alpha}Y_f\left[\frac{e_m Q_0}{t^{\Delta}},\frac{e_m}{t^{\phi}}\right] \ . \tag{30}$$

Therefore,

$$\Delta C_m\sim\partial^2F/\partial e_m^2\sim t^{2\beta-\gamma}+t^{-\mu}+t^{2\beta-\phi} \ . \tag{31}$$

In writing the expression like this, we have used the relation $Q_0\propto t^{-\beta}$ and the scaling laws[27] $\alpha+2\beta+\gamma=2$, $\gamma=\alpha+2\Delta-2$, and $\mu=\alpha+2(\phi-1)$. For $T>T_c$, $\langle Q\rangle=0$. So

$$F=t^{2-\alpha}Y_f\left[\frac{e_m}{t^{\phi}}\right] \tag{32}$$

and

$$\Delta C_m\sim\partial^2F/\partial e_m^2\sim t^{-\mu} \ . \tag{33}$$

For our purpose, we have discussed here only the behavior of the elastic constants in the hydrodynamic limit. In the region where the correlation length is com-

parable or larger than the sound wavelength, the calculations should be performed using the classical fluctuation-dissipation theorem.[33] The detailed treatment is lengthy and the resulting expressions for real and imaginary parts of the elastic constant are expected to depend on many exponents. Since large and good-quality single crystals of high-temperature superconductors (HTSC's) are still not available, no reliable data so far could be used to extract meaningful exponents in this region. Thus we will not discuss it here. The interested reader is referred to Ref. 34.

V. THE EFFECTS OF EXTERNAL CONSTRAINTS, DOPING CONCENTRATION, AND OXYGEN DEFICIENCY ON THE STRUCTURAL TRANSITION TEMPERATURE T_0

A treatment of this problem was proposed in a recent paper.[18] For the sake of completeness, we outline the main ideas and results here.

A. Effects of applied pressure

From the preceding section we see that the interaction between the strain field and the order parameter in the absence of external constraints only renormalizes the parameters u and v resulting in different SPT's and without any effects on the transition temperature T_0. However, in the case of applying a pressure to the system there is, of course, a nonzero strain field above T_0. This strain field (denoted as d_i, $i=1-6$) is different from the spontaneous strains e_i caused by the SPT. As shown previously[18] it is the coupling between the applied strain field and the order parameter, which creates a change of T_0 rather than the coupling between the e_i and the order parameter. As an example, let us look at the transition HT$\rightarrow$MO. When the system is subjected to a hydrostatic pressure P, a strain field d_i is produced. d_i are related to P through Hooke's law

$$d_1=-(S_{11}^t+S_{12}^t+S_{13}^t)P=d_2,\quad d_3=-(2S_{13}^t+S_{33}^t)P\ . \tag{34}$$

Here S_{ij}^t are the elastic compliances in the HT phase. We replace the e_i by e_i+d_i in the coupling part of the Landau free energy in Eq. (10). Collecting the $(Q_1^2+Q_2^2)$ terms and taking the derivative of the $(Q_1^2+Q_2^2)$ coefficient with respect to P, we obtain

$$dT_0/dP=2[2a_1(S_{11}^t+S_{12}^t+S_{13}^t)+a_2(2S_{13}^t+S_{33}^t)]/a\ . \tag{35}$$

The generalization to other ways of applying pressure or stress, or to other SPT's is straightforward.

B. Effects of doping concentration x and oxygen deficiency y

We suggest that the dependences of T_0 on the doping concentration and oxygen deficiency are closely related to the pressure effect. The influence of partial substitution of La by Sr or Ba on the T_0 is physically equivalent to introducing an average internal static strain field, which can be expressed in terms of d_1, d_2, and d_3 formulated by the following consideration: Let us look at one unit cell in $La_{2-x}(Ba,Sr)_xCuO_4$. The ratio of Sr or Ba to La is $x/2$. There is one La in the [1,0,0] or [0,1,0] direction, and two in the [0,0,1] direction. If we use R and r to denote the radii of Sr or Ba and La, respectively, and x for the Sr or Ba concentration, the average strains may be expressed as

$$d_1=d_2=-x(R-r)/a_1,\quad d_3=-2x(R-r)/c_t\ . \tag{36}$$

Here a_t and c_t are the lattice parameters. In this way we obtain the relation

$$dT_0/dx=4(R-r)[(a_1/a_t)+(a_2/c_t)]/a\ . \tag{37}$$

The influence of oxygen deficiency can be formulated similarly.[18] Therefore, we expect that the SPT temperature T_0 decreases with increasing oxygen content. So for the $La_{2-x}(Ba,Sr)_xCuO_{4-y}$ system, the SPT temperature $T_0(P,x,y)$ from the HT phase to the MO phase is determined completely by the following relation[18]

$$T_0(P,x,y)=\frac{2}{a}\left\{P[2a_1(S_{11}+S_{12}+S_{13})+a_2(2S_{13}+S_{33})]+\left[\frac{a_1}{a_t}+\frac{a_2}{c_t}\right][2(R-r)x-r_0y]\right\}+T_0(0)\ . \tag{38}$$

Here r_0 is the covalent radius of oxygen and $T_0(0)$ is the SPT temperature of pure La_2CuO_4 at $P=0$.

It should be pointed out that the above discussion is valid only in the region where the applied pressure does not exceed the elastic limit of the samples. For a polycrystalline sample, this elastic limit is defined as the applied force which creates the first deformed grain inside the sample.

VI. ULTRASONIC MEASUREMENTS ON A $La_{1.88}Sr_{0.12}CuO_4$ SINGLE CRYSTAL

In the preceding sections of this paper, the results of mean-field theory as well as scaling analysis have been ob-

TABLE IV. Elastic constants C_{11}, C_{33}, and C_{44} at 297 K for single-crystals $La_{1.88}Sr_{0.12}CuO_4$, $La_{1.86}Sr_{0.14}CuO_4$, and La_2CuO_4 in 10^{12} dyn/cm^2.

Sample \ Mode	C_{11}	C_{33}	C_{44}	Reference
$La_{1.88}Sr_{0.12}CuO_4$	2.33	1.94	0.677	This work
$La_{1.86}Sr_{0.14}CuO_4$	2.48	2.05	0.674	39
La_2CuO_4	1.72	2.00	0.656	39

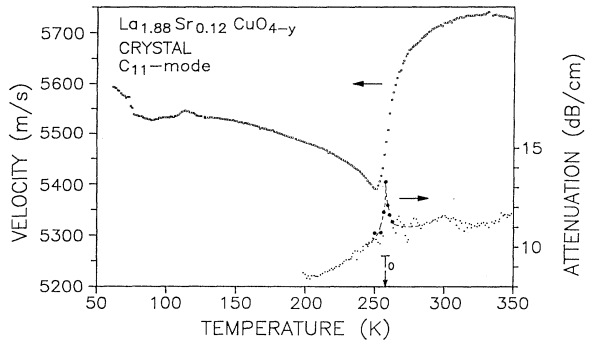

FIG. 6. The temperature dependence of C_{11} mode in $La_{1.88}Sr_{0.12}CuO_4$ single crystal.

tained. As is clearly seen from the expressions given above, in this mean-field theory we introduce only six independent parameters, namely a_1, a_2, b_1, b_2, u, and v. Once these six parameters are determined, the behavior of various physical quantities near T_0 is fixed. Therefore, the next task is then to try to evaluate these six constants experimentally. Ultrasonic measurement on single crystals is one of the obvious choices for this purpose.

We have performed ultrasonic measurements on a

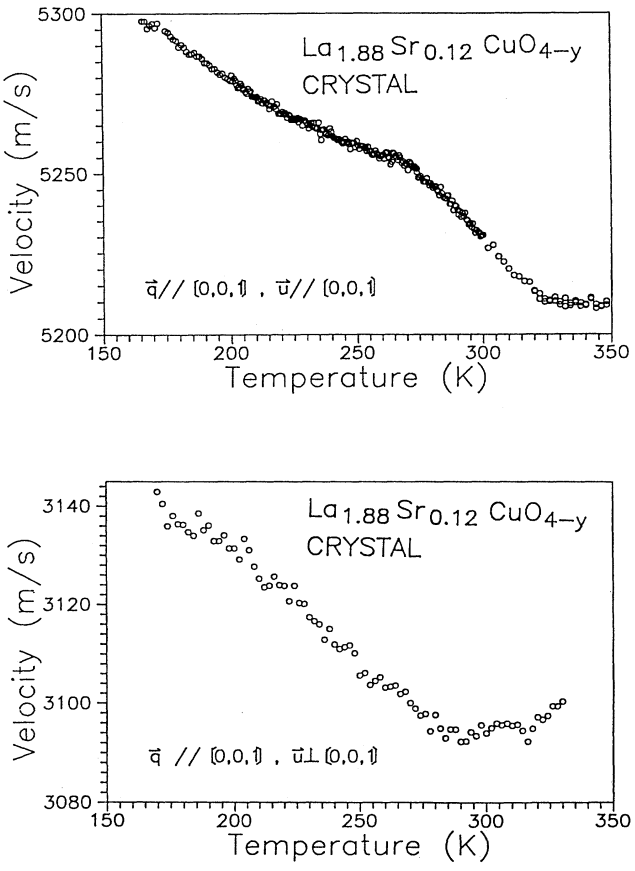

FIG. 7. The temperature dependence of C_{33} (upper curve) and C_{44} modes in $La_{1.88}Sr_{0.12}CuO_4$ single crystal.

$La_{1.88}Sr_{0.12}CuO_4$ single crystal. The superconducting onset temperature of the sample was 12 K, measured by ac susceptibility. A standard pulse-echo method with time-of-flight technique was used for the measurements.

As a by product of this study, the values of elastic constants C_{11}, C_{33}, and C_{44} at 297 K were determined and are given in Table IV. Included also in the Table IV for comparison are the reported corresponding values for La_2CuO_4 and $La_{1.86}Sr_{0.14}CuO_4$ single crystals.

Results for the temperature dependence of the C_{11} mode are shown in Fig. 6. These results were confirmed later by other groups.[35,36] The large anomalies in both velocity and attenuation were tentatively attributed to the HT→MO SPT.[12] However, it was noted that the observations could also be well explained if we suppose the SPT was of HT→LT type.[17]

Further measurements of C_{33} and C_{44} modes were done recently as shown in Fig. 7. Measurement below 165 K was impossible due to serious distortion of the reflection signal and overlap of echos. Nevertheless, the data at temperatures above 165 K are reliable, since during the measurements more than a dozen echoes could always be clearly separated and detected. As expected, the C_{44} mode shows no change in velocity in passing through the high-temperature SPT, regardless of whether the SPT is HT→MO or HT→LT.

VII. COMPARISON WITH EXPERIMENTS AND DISCUSSION

In this study, we have proposed several alternative ways in which successive SPT's may occur in $La_{2-x}(Ba,Sr)_xCuO_{4-y}$. A comparison with available structural data has been made in a previous paper.[17] In order to compare the calculated results with experiments, we need to know the value of the coupling constants. In Ref. 17, we have estimated the three coupling parameters a_1, a_2, and b_2 in the case of the HT→MO SPT for $La_{1.88}Sr_{0.12}CuO_4$ by employing the La_2CuO_4 elastic moduli of the HT phase calculated by Allan and Mackrodt.[37] These calculated elastic moduli, however, have turned out to be different from those determined by later measurements.[38] Therefore the estimated coupling parameters need to be corrected. Recently measurements on the $La_{1.86}Sr_{0.14}CuO_4$ single crystal done by Migliori *et al.*,[39] giving a complete determination of all elastic moduli in the HT phase, enabled us to calculate the coupling parameters more accurately.

A. Evaluation of the coupling constants a_1, a_2, b_1, and b_2

The evaluation is performed in the following way: From Sec. V, we know that the coupling parameters a_1 and a_2 can be obtained from the measurements of pressure and Sr or Ba concentration dependences of the high-temperature SPT T_0. In order to do so, first we need to know the value of the parameter a, which is calculated to be 1.83×10^{25} N/m^{4}K from the measurement of the soft-mode vibrational frequency above T_0 (Ref. 40) (Table II) and taking I^{-1}—the inverse of the mass densi-

ty of oxygen atoms participating in each vibrational mode to be 8.78×10^{-4} m^3/kg. The radii of Sr and La are easily found from the Periodic Table to be 1.91 Å and 1.69 Å, respectively. Q_0^2,ω_1,ω_2 were taken from the inelastic neutron-scattering measurement[40] as $Q_0^2=8.23\times10^{-23}$ m^2, $\omega_1=1.06\times10^{12}$ rad/sec, and $\omega_2=2.20\times10^{12}$ rad/sec at 150 K. For the $La_{2-x}Sr_xCuO_{4-y}$ system, if we choose the lattice parameters a_t,c_t to be 3.7709 Å and 13.2009 Å, respectively,[41] taking $dT_0/dP=-10$ K/kPa (see Fig. 8) and $dT_0/dx=-2454$ K (see Fig. 9), and adopting the elastic moduli of the $I4/mmm$ phase from Ref. 39, the coupling constants a_1 and a_2 can be evaluated quantitatively by resolving Eqs. (35) and (37). The results are

$$a_1=-2.10\times10^{29}\ \text{N/m}^4,\quad a_2=6.52\times10^{28}\ \text{N/m}^4\ .$$

The other two coupling constants b_1 and b_2 are expected to vary with x and y of different specimens. Therefore, each set of b_1 and b_2 corresponds to a particular system and has to be calculated for each sample. Here we take $La_{1.88}Sr_{0.12}CuO_4$ as an example to show how to evaluate them from experimental results.

The absolute value of b_2 can be evaluated by using Eq. (16). The jump of C_{11} is determined from Fig. 6 to be 2.6×10^{10} N/m^2 after subtracting a linear background. The result is $|b_2|=1.21\times10^{30}$ N/m^4. Measurements of C_{66} vs temperature provide a way to obtain the value of b_1. Due to the limited size of single crystal, however, so far only one measurement of C_{66} above T_0 using a resonant ultrasound technique has been reported.[38] Below T_0 the signal disappears because of relaxation effects.[39] This prevents an accurate determination of the softening of C_{66}. If we use the difference between the value at T_0 and the value at room temperature as the reduction due to the SPT, we get $|b_1|=3.12\times10^{29}$ N/m^4.

Since we have to use data from different groups and different specimens, the Sr concentration and oxygen deficiency may differ somewhat between these measurements. This affects the accuracy of the determination of the coupling constants, particularly the b_1,b_2 values,

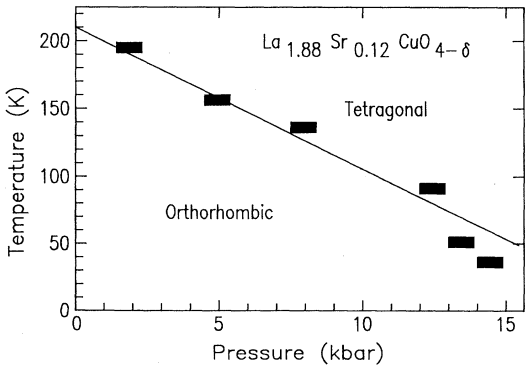

FIG. 8. Transition temperature vs pressure for $La_{1.88}Sr_{0.12}CuO_{4-y}$. The line shows the value $dT_0/dP=-10$ K/kPa. The size of the rectangles corresponds to the uncertainties (data taken from Ref. 26).

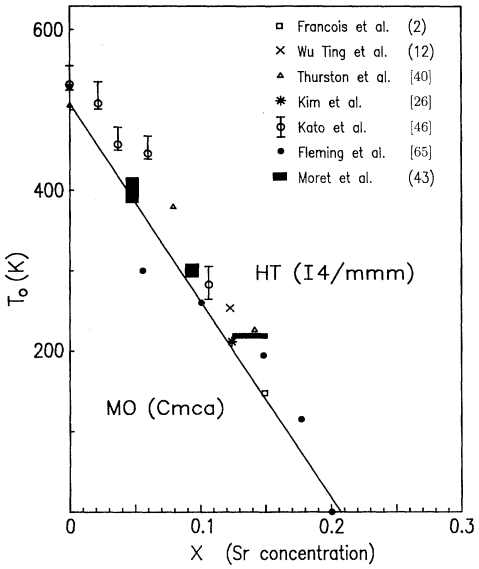

FIG. 9. Transition temperature vs Sr concentration for $La_{2-x}Sr_xCuO_4$. The line shows the value $dT_0/dx=-2454$ K. The size of the symbols shows the uncertainty.

which are expected to be sensitive to Sr or Ba concentration and oxygen deficiency. a_1 and a_2, on the other hand, will not change from sample to sample as long as they have the same SPT sequence.[18]

B. Anomalies of elastic moduli near T_0

Having determined the four coupling parameters, we are now able to predict the elastic moduli vs temperature curves in the MO phase by resolving Eq. (16) (see Fig. 10). The values of Q_0^2,ω_1,ω_2 at each temperature are taken from Ref. 39. Figure 10 shows that in the $La_{1.88}Sr_{0.12}CuO_4$ single crystal below about 200 K all elastic moduli except C_{11} and C_{12} are almost independent of temperature, which is a feature of the mean-field behavior, indicating that Q_0^2 and ω_1,ω_2 have the same temperature dependent character below 200 K. The calculated jump of C_{33} is compared with the measured one as shown in Fig. 11. We can see that the theory predicts a correct direction of the jump, and the predicted magnitude of the jump agrees with the experimental data within a factor of 2 in the temperature region 10 K below T_0. The difference can be explained by the uncertainty in the determination of b_1 and b_2. For C_{44}, no noticeable change was observed near T_0 in our measurements as expected (see Fig. 7), since there is no coupling between e_4 and the structural order parameter.

Close to the SPT, critical behavior will dominate. This effect is expected to be quite significant for the symmetry-breaking elastic moduli, in agreement with observation for C_{11} (Ref. 12) and C_{66} (Ref. 39). But for non-symmetry-breaking elastic constants such as C_{33}, the elastic behavior very close to T_0 is still governed by mean-field behavior. In fact, the agreement between experiment and theoretical prediction is almost perfect within around 3 K of T_0 (see Fig. 11). From the data of

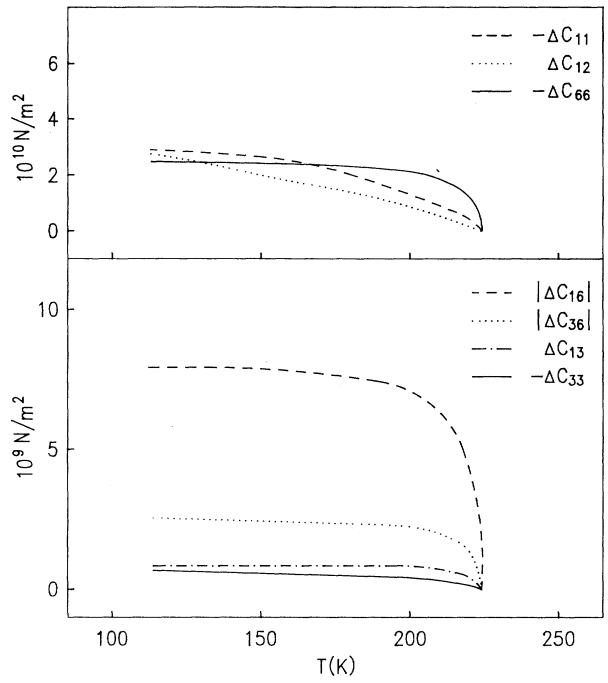

FIG. 10. The predicted elastic moduli vs temperature curves in the MO phase for $La_{1.86}Sr_{0.14}CuO_4$ using Eq. (34). The corresponding values of $Q_0^2, \omega_1, \omega_2$ are taken from Ref. 40.

Ref. 12, a critical exponent μ near 0.5 is deduced after subtracting a linear background, which is consistent with the scaling analysis.[12] X-ray and neutron diffraction experiments on the same crystal were also carried out. An order parameter exponent value $\beta=0.34\pm0.02$ was obtained[42] again in quite good agreement with expected β value for the $d=3$, XY model.[29] The C_{66} mode exhibited severe damping[38,35] below T_0 due to the formation of domain structure. This prevents us from making a conclusive determination of critical exponent. In Ref. 38, attempts were made to extract the critical exponent from the data above T_0 alone. Three different values 0.37, 0.5, and 1 were obtained depending on the way of subtracting a background.

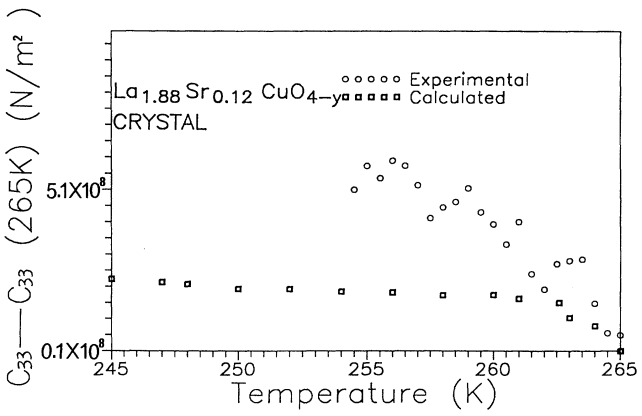

FIG. 11. The comparison between the measured (open circle) and the calculated changes of C_{33} mode at T_0 in $La_{1.88}Sr_{0.12}CuO_4$ single crystal.

Furthermore, elastic data also gives strong evidence for the necessity of including the bilinear coupling energy in the Landau free energy. Recent experimental data on $La_{1.85}Sr_{0.15}CuO_4$ single crystal[36] showed that C_{33} and C_{11}-C_{12} displayed exactly the same feature at T_0, namely, a step down jump during cooling. This behavior would not have appeared without the bilinear coupling term in the Landau free energy [see Eqs. (16)]. Besides, that study revealed that the behavior of $C_{11}+C_{12}$ was totally different from that of C_{33} as expected from the scaling analysis in Sec. IV. This result again proves that the bilinear term must be included in the Landau free energy. However, this is not the only important information provided from the measurements. The most important consequence is that it implies that the tilting axis of CuO_6 octahedra does not lie exactly on the [1,1,0] or [1,$\bar{1}$,0] direction. The reason is rather obvious if we rewrite Eq. (27) in the following form:

$$\Delta(C_{11}+C_{12}) = -\frac{a_1}{kTV}\int d\mathbf{r}\int d\mathbf{r}'\{\langle[Q_1'(\mathbf{r})Q_2'(\mathbf{r})][Q_1'(\mathbf{r}')Q_2'(\mathbf{r}')]\rangle + \text{antisymmetric terms}\} \quad (39)$$

where $Q_1'(\mathbf{r})$ and $Q_2'(\mathbf{r})$ are defined as $|\mathbf{Q}(\mathbf{r})|-[(b_2/2a_1)Q_1(\mathbf{r})Q_2(\mathbf{r})]^{1/2}$ and $|\mathbf{Q}(\mathbf{r})|+[(b_2/2a_1)Q_1(\mathbf{r})Q_2(\mathbf{r})]^{1/2}$, respectively. A similar definition will be applied to $Q_1'(\mathbf{r}')$ and $Q_2'(\mathbf{r}')$ too. Since $\langle[Q_1'(\mathbf{r})Q_2'(\mathbf{r})][Q_1'(\mathbf{r}')Q_2'(\mathbf{r}')]\rangle$ is equivalent to $\langle[Q_1^2(\mathbf{r})-Q_2^2(\mathbf{r})][Q_1^2(\mathbf{r}')-Q_2^2(\mathbf{r}')]\rangle$,[30] this explains why both $C_{11}+C_{12}$ and C_{66} showed critical fluctuation very close to T_0. The key point in this discussion is that neither Q_1 nor Q_2 must be strictly zero in the low-temperature phase. Consequently, it means that at least in that specimen the low-temperature structure deviates a little from the *Cmca* symmetry. It may modify the *Cmca* structure in the sense that the tilting axis of CuO_6 octahedra deviate from the [1,1,0] or the [1,$\bar{1}$,0] direction clockwise and anticlockwise by very small angle. This small deviation could be smeared out in the structural measurements, such as neutron or x-ray measurements, where only an average of atomic positions in a large sample are probed.

C. Behavior of specific heat near T_0

Heat-capacity measurements[44] on single crystal La_2CuO_4 and polycrystalline $La_{2-x}Sr_xCuO_4$ ($0\le x\le 0.20$) revealed that the magnitudes of the jumps in heat capacity for different Sr concentration were not simply proportional to T_0. This was suggested[44] to be in disagreement with Landau theory. Note, however, that in the formulation of the Landau free energy of Ref. 44 the energy contributions from the strain field and the interaction between the strain field and the order parameter were neglected. Looking at Table II, however, we see that ΔC due to the SPT depends not only on T_0, but also on Y, which is a function of b_1, u, and v. In the region of

Sr concentration where all samples have the same low-temperature phase, the u and v will not change much with different Sr content but rather with temperature. The dependence is expected to be weak. Therefore, these factors cannot account for the rapid change in the magnitude of the jump of the specific heat with different Sr concentrations. An alternative source is presumably a large change in b_1. This idea is supported by the vibrating reed measurements[45] on ceramic LSCO samples, where a different magnitude of decrease in Young's modulus for different Sr concentrations near the HT→MO SPT was observed, also being controlled by the changes in b_1 and b_2. Since ΔC decreases with increasing Sr-doping concentration, b_1 is expected, therefore, to decrease as well. This implies that the jumps in the elastic moduli C_{66}, C_{36}, and C_{16} are smaller for the samples with higher Sr concentration. This prediction needs to be checked.

D. Doping concentration and pressure dependence of T_0

Theoretically we predict (see Sec. V) that the SPT temperature will change linearly with pressure and Sr- or Ba-doping concentration. This has indeed been observed in the $La_{2-x}(Sr,Ba)_xCuO_{4-y}$ family.[26,46] We have used the experimental data to calculate the coupling constants a_1 and a_2 as given in Sec. VII A. Using these two constants and Eq. (38), we now predict dT_0/dx for LBCO as shown in Fig. 12 without any adjustable parameters. It should be pointed out that we have used covalent radii of Ba, Sr, and La in order to get a good fit to the experimental data. Attempts to use metallic radii gave less good agreement and even worse when trying ionic radii. Therefore, in reality, a mixture of covalent and metallic character may be the correct description. In fact, this situation has been elucidated in a "Wigner-Seitz local environment" study of the structure of the La 2:1:4 family made by Melamud, Bennett, and Watson,[47] where they used the atomic radii (either ionic or metallic) to construct generalized space-filling Wigner-Seitz cells and the same conclusion was drawn.

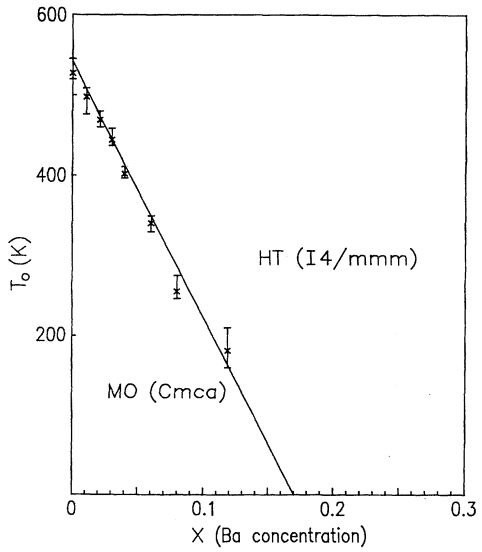

FIG. 12. Predicted transition temperature vs Ba concentration for $La_{2-x}Ba_xCuO_4$. The line represents the prediction based on analysis of data in Figs. 8 and 9 with T_0 taken as 546 K (data taken from Ref. 46).

The measurement of oxygen-deficiency dependence of T_0,[48] agrees with our calculation within a factor of 2.[18] Since only a few data points were available for the analysis, we therefore conclude that the agreement is satisfactory. It is expected also from the present model that upon substituting Sr for Ba in $La_{2-x}Ba_xCuO_4$ the T_0 will increase with increasing Sr concentration. The variation should not be so drastic in comparison with dT_0/dx due to the smaller difference in covalent radii of Sr and Ba than in that of Ba and La. This expectation was in fact verified experimentally in a recent report,[49] which found that $dT_0/dz = 2.5\times10^2$ K in $(La_{0.9375}Ba_{0.0625-z}Sr_z)_2CuO_4$ compounds. What is expected from our calculation using Eq. (38) is $dT_0/dz = 3.88\times10^2$ K. The validity of our model can be checked further by several proposed measurements as described in our previous paper.[18]

E. Comparison with the results of x-ray and neutron-diffraction measurements

Recently Crawford *et al.*,[50] have studied the SPT's in $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$ compounds using synchrotron x-ray and neutron-diffraction. They confirmed the three possible sequences of SPT's as listed in the upper half of Table III.

The HT→MO SPT also induces some spontaneous strains, which are linked to the order parameter (see Table II). Powder x-ray diffraction measurement of lattice parameters on ceramic $La_{1.85}Sr_{0.15}CuO_4$ (Ref. 41) provides a means to evaluate e_3 caused by the SPT and then to compare it with the calculated e_3. Q_0^2 values are taken from Ref. 40. The two results are plotted in Fig. 13. We see that the two results agree qualitatively. But the result obtained from the x-ray measurement is one order of magnitude larger than the calculated one. We ascribe the discrepancy to the fact that in our calculation using measured lattice parameters, we did not take the thermal expansion into consideration, since no such data are available in the literature.

The critical exponent for the order parameter obtained from the measurements of powder neutron diffraction[51] on La 1:2:4 is $\beta=0.372$, which is in reasonably good agreement with the calculated value for the $d=3$ XY model.[29] However, the critical exponents obtained from measurements[7] of inelastic neutron scattering on Li-doped La 1:2:4 deviate remarkably from the expected values for the $d=3$, XY universality class as pointed out by Sokolov.[52] It was noted that the critical exponents were closer to those of a tricritical point rather than the $d=3$ XY model. Recalling the form of Eq. (11), the condition for the existence of a tricritical point is the disappearance of the fourth-order invariant terms of the order parameter. This may suggest that the low-temperature structure could possibly be *Pccn* in the Li-doped La 1:2:4 samples.

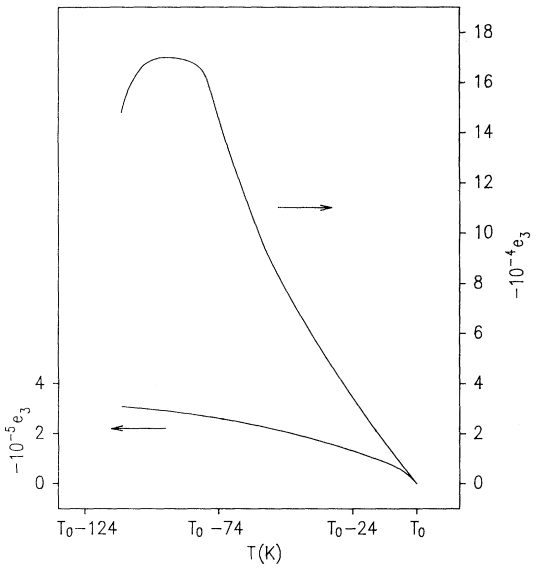

FIG. 13. The lower curve is the calculated e_3 employing Eq. (24). The corresponding Q_0^2 values are taken from Ref. 40. The other curve is the e_3 obtained from the powder x-ray diffraction measurement of lattice parameters (Ref. 41). (See text for more detail.)

F. Structural instabilities and superconductivity

The present study has shown that the high-temperature $I4/mmm$ phase of the $La_{2-x}(Sr,Ba)_xCuO_{4-y}$ system is unstable against the various collective tilting of the CuO_6 octahedra upon cooling. The change of structure has a large effect on many physical quantities, and the relations between these physical quantities have been derived. However, so far we have not touched upon one of the most attractive questions: What is the interplay, if any, between these structural instabilities and superconductivity? In which structure can the highest T_c appear and why? Clearly answering this question is beyond the reach of the Landau theory used above. Still, it might be worthwhile, although quite laborious, to make some valuable calculations and predictions by including the superconducting Ginzburg-Landau free energy, and the interaction between the order parameter of the superconductor and the order parameter of the SPT into our Eq. (11). Here we would like only to make a few comments on the existent experimental results from the structural point of view.

The $La_{2-x}(Sr,Ba)_xCuO_{4-y}$ system has been a popular system for studying the physical properties of high-T_c superconductors because it possesses almost all the characteristics of high-T_c compounds. By varying the Sr- or Ba-doping concentration, the system could exist in various phases: antiferromagnetic, semiconducting, superconducting metal, and nonsuperconducting metal. The superconducting-metal phase[53] appears in the region $0.06 \lesssim x < 0.25$, where the upper boundary is still debated. Inside the superconducting region of the $T_c - x$ diagram, T_c exhibits two peaks and a local minimum at around $x = 0.125$ for LBCO while only one peak at around $x = 0.15$ and a kink near $x = 0.12$ are seen for LSCO. The location of the minimum in T_c in LBCO has been observed[54] to coincide with the maximum in the SPT temperature from the MO phase to the LT phase. Large anomalies in magnetic susceptibility,[55] resistivity,[56] specific heat,[57] thermal expansion coefficients,[58] sound velocity and attenuation,[59] and thermal conductivity[60] were detected near the MO$\rightarrow$LT SPT temperature for samples with Ba concentration close to $\frac{1}{16}$. This SPT was claimed to be responsible also for anomalous behavior in the isotope effect,[61] Hall coefficient,[55] and pressure dependence of T_c.[62] For LSCO compounds, no clear experimental evidence from neutron or x-ray measurements indicates the existence of a low-temperature SPT in $La_{2-x}Sr_xCuO_4$. However, there are reports from the elastic measurements[12,35,36] on several single crystals pointing to the onset of an intrinsic lattice instability at a temperature a few tens of degrees above T_c.

Unfortunately, there are insufficient experimental data in the literature to permit calculations of temperature, x, and y dependences of the parameters v' and Y. Therefore, we are unable at the present moment to make predictions on what structural instabilities could occur for a certain sample on cooling. Such a study could be highly relevant for the discussion of the interplay between structural instabilities and superconductivity. We believe the present experimental knowledge of the phase diagram of the $La_{2-x}(Sr,Ba)_xCuO_{4-y}$ system is still inadequate, particularly near the locations where superconductivity starts, is suppressed, or disappears. The following two aspects may contribute to this situation.

(1) The conventional experimental methods, such as x ray or neutron diffraction, cannot resolve sufficiently the change of local structure in this system. It has been suggested[63] that it is the local structure that affects superconductivity. Moreover, since the structure of a certain phase could always be regarded as a coherent superposition of the two domains of another phase, it is very difficult to make a right justification for the structure, especially when the system is located on the phase boundaries. In this regard, it may be advantageous to use elastic measurements instead. Indeed elastic measurements have made important contributions to the understanding of the superconducting properties in $A15$ compounds.[64]

(2) The existence of the possible structural instabilities for a certain sample depends on many intrinsic and extrinsic factors, such as Sr or Ba concentrations, oxygen deficiency, dislocations, stacking faults, etc. For instance, it is not always true that all samples with a common Sr concentration would have the same structural variations on cooling. Inhomogeneities of the sample and the uncertainty in the determination of doping and oxygen deficiency concentration also contribute to the complications.

Keeping the above ideas in mind, now let us consider three effects induced by Sr or Ba doping. The first one is the suppression of antiferromagnetic correlations. The second one is the introduction of mobile charge carriers into the system. The final one is the possible changes in the variations of the structures on cooling. It is likely

that it is the mixture of all these three changes that governs the variation of T_c with x. This issue deserves further study. Here we attempt only to discuss the structural effect on superconductivity.

The question regarding whether the HT phase is superconducting is still unclear. In an early study[65] superconductivity was found to disappear along with the suppression of the HT→MO SPT. However later careful study,[66,67] paying special attention to the oxygen vacancies introduced by heavy doping, revealed that superconductivity could be retained up to $x=0.26$, and the HT→MO SPT ended at around $x=0.19$.[66] The latter results implied only that the orthorhombic distortion was not a necessary condition for the onset of superconductivity in the system and did not rule out the possibility that the SPT was from the HT phase to the LT phase. Recently, Takagi *et al.*[68] reexamined this problem and found evidence that both the HT→MO SPT and superconducting phase transition terminated near $x=0.2$. Thus until more careful experiments are done, this question remains open.

Among the remaining three possible structures, the MO phase has been investigated mostly and is found to be superconductive. Recently Crawford *et al.*[50] have demonstrated that the other two phases are superconductive too. They also showed that T_c is slightly higher in the PO phase than in the LT phase. The order of T_c values from high to low for the three phases is MO, PO, and LT. What are the microscopic origins of this order is a challenging question. Since the conduction layers are responsible for superconductivity, it is natural to look at the changes in the CuO_2 planes caused by the three possible modifications. In the MO phase, the tilting of CuO_6 octahedra around the [1,1,0] or the [1,$\bar{1}$,0] direction makes half of the in-plane oxygen atoms move towards positions below the plane and the other half above the plane (see Fig. 2). The distance of the deviation in both directions is equal. Therefore the in-plane oxygen sites are equivalent. In contrast, in the LT phase in-plane oxygen sites have two distinctive locations. One is the location in the plane, the other the location above or below the plane (see Fig. 3). If we define the distance of deviation of the oxygen atom from the conduction plane as X_a in the x direction, as X_b in the y direction, and the degree of inequivalence of in-plane oxygen sites (abbreviated as "the degree of inequivalence") as $D=|X_a-X_b|$, then we can easily see that the degree of inequivalence increases in the order MO, PO, and LT.

Experimental results seem to indicate that the HT→MO SPT does not affect T_c too much except perhaps it provides the necessary environment for the emergence of superconductivity. An obvious fact supporting this idea is that no superconductivity is observed in pure La 1:2:4 without extra oxygen, although there is a HT→MO SPT at around 500 K. Nor will the normal electronic properties of the system be altered by the SPT. It is interesting to note that the degree of inequivalence is not changed either. Band-structure calculations[69] on La 2:1:4 have demonstrated that no energy gap is opened by the CuO_6 tilt mode. Neither is the transition driven by Fermi-surface nesting.

Recently, careful elastic measurements[36] have been done on a $La_{1.86}Sr_{0.14}CuO_4$ single crystal. The onset of a remarkable softening in C_{11}-C_{12} was observed at a temperature a few degrees above T_c. The temperature interval of the softening was widened by applying a magnetic field, which implied that a possible SPT below T_c was stopped by the appearance of superconductivity. This is very similar to $A15$ compounds,[63] where it was noticed that the existence of the Batterman-Barrett instability had a positive effect on T_c. Releasing the structural instability by a SPT was shown to decrease T_c.[70] This information should be considered along with the fact that the MO→LT SPT in $La_{2-x}(Ba,Sr)_xCuO_{4-y}$ at around $x=\frac{1}{8}$ suppresses superconductivity almost entirely. The question is then whether the possible SPT below T_c in that $La_{1.86}Sr_{0.14}CuO_4$ single crystal is from the MO phase to the LT phase. From the elastic data in the high-temperature region, we could rule out the possibilities that the transition is of LT→MO or LT→PO type. Since the SPT is a second-order type, the MO→LT is excluded. The only possible SPT satisfying both high-temperature and low-temperature elastic data is the PO→LT transition (see also Sec. VII 13) by assuming that $D\approx 0$. This analysis implies that a lattice instability associated with the structural deformation in the conduction planes is important for superconductivity. This lattice instability may generate a compressional strain in the basal plane of the structure. Phenomenologically one could say that the facilitation of this lattice instability could have a positive effect on T_c as in $A15$ compounds. This idea is supported by high-pressure experiments. It has been shown that applying hydrostatic pressure on LSCO could bring T_c up to 50 K. This increase of T_c results mainly from the compressional pressure applied along the basal plane, since it has been shown that the pressure along the c direction had a negative effect on T_c.[71] Once this view is accepted, it is straightforward to show that the application of a pressure on the basal plane may facilitate the lattice instability associated with the structural deformation in the conduction planes and thus lead to the enhancement of T_c. Clearly, more measurements are needed to test this idea. In particular, elastic measurements on a series of well-characterized single crystals should be performed, so that one could check (1) in which range of Sr or Ba concentration the shear instability exists and (2) how the individual elastic mode varies with applied magnetic field. As a by product of this study, one could check the validity of our mean-field theory and use the data to extract information about v'. Furthermore, one could extend this mean-field scheme to take into account the interaction between superconductivity and the structural order parameter and compare the elastic behavior near T_c with the calculated results.

What the microscopic origin of the strong suppression of T_c due to the MO→LT SPT is still unknown now. Many researchers believe that the SPT is triggered by an electronic instability. An oxygen-oxygen in-plane charge-density wave coupled to the CuO_6 tilting mode has been shown to give a negative contribution to v' and therefore tends to stabilize the LT phase.[72] Maeno

et al.[73] suggested that the MO→LT SPT is driven by a band instability, leading to the creation of additional gap structure with reduced $N(E_f)$ in the LT phase. Band-structure calculation[74] indeed found a partially gapped Fermi surface in the LT phase. The enhanced isotope effect in the LT phase was explained in terms of an electron-phonon pairing mechanism.[74] Currently this issue is drawing more and more attention from both experimentalists and theoreticians.

VIII. SUMMARY

This paper shows that although $La_{2-x}(Sr,Ba)_xCuO_{4-y}$ are high-T_c materials, their structural properties in the normal state can still be very well explained by means of Landau theory, just like other perovskite compounds such as $SrTiO_3$. Besides, in this paper the following results are obtained.

(1) We demonstrate explicitly that the Landau free-energy density for the $La_{2-x}(Sr,Ba)_xCuO_{4-y}$ system must include the coupling term bilinear in the two order-parameter components.

(2) The phase diagram of the $La_{2-x}(Sr,Ba)_xCuO_{4-y}$ system is obtained based on the constructed Landau free energy. It is shown that several different consecutive SPT's can occur in this system under different conditions. Most of the predictions have been verified experimentally, while others may account for the reported anomalous structural data.

(3) The changes of the various physical properties, such as strain, specific heat, soft-mode vibrational frequencies, and elastic moduli, due to the SPT are calculated in the mean-field framework. The $La_{2-x}(Sr,Ba)_xCuO_{4-y}$ system is also adopted as a model system for performing scaling analysis in the hydrodynamic limit. It is shown that the observed experimental results in the literature could be understood in terms of Landau theory incorporating the scaling analysis near the SPT temperature.

(4) The Landau approach is extended to take the influence of the applied pressure, doping concentration, and oxygen deficiency on the high-temperature transition temperature T_0 into account quantitatively. Good agreement between theory and experimental results was obtained.

(5) Some results of ultrasonic measurements on a $La_{1.88}Sr_{0.12}CuO_4$ single crystal are also reported. Our experimental results together with the results obtained from other groups are used to extract the values of the coupling constants.

(6) The possible interplay between the structural instabilities and superconductivity is discussed. Analysis implies that the existence of a structural instability associated with the lattice deformation in the conduction planes in the low temperature region may have positive effect on superconductivity and the release of this instability in any form may reduce T_c in this material system.

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