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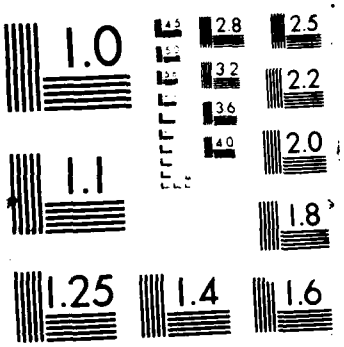
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Theory of the Tetragonal-to-Orthorhombic Structural Phase Transition in La_2CuO_4

by

D. Sahu and Thomas F. George

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Departments of Chemistry and Physics
State University of New York at Buffalo
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Abstract

A phenomenological free energy for the tetragonal-to-orthorhombic structural phase transition in La_2CuO_4 is derived from symmetry principles. The critical properties of the model free energy are studied by renormalization group methods and compared with experiment.

1. INTRODUCTION

The discovery of high-T_c superconductivity in doped La_2CuO_4[1] and related compounds[2] has raised the question as to which phonons are important in stabilizing or producing the superconducting state. It has been speculated[3,4] that the phonons associated with the breathing motion of the distorted oxygen octahedra in these compounds might be of interest in understanding the mechanism of superconductivity. However, a recent X-ray and neutron scattering experiment[5] on undoped and doped La_2CuO_4 single crystals has found no evidence for the breathing motion; instead, it is the optical phonon associated with rotation of the oxygen octahedra which goes soft at the tetragonal-to-orthorhombic transition. Since this structural transition involving rotation of oxygen octahedra is itself of interest, as in the case of the ideal perovskite $SrTiO_3$,[6,7] we have undertaken a theoretical study of the above transition. Our motivation in undertaking such a study is that the critical properties of the structural transition in La_2CuO_4 are expected to be different from that of $SrTiO_3$ because of symmetry considerations.

The high-temperature structure of La_2CuO_4 is body-centered tetragonal with space group I4/mmm. Each Cu atom sits at a site of 4/mmm symmetry and is surrounded by six O atoms in a distorted octahedral arrangement. The positions of the atoms in the unit cell is schematically given in Fig. 1 of Ref. 8. Upon a second-order phase transition to an orthorhombic structure with space group Cmca, the Cu-atom site symmetry is lowered to 2/m. The transition temperature in recent experiments[5] was found to be T_c = 423 K, although in an earlier experiment[9] T_c was as high as 533 K. The soft phonon responsible for the structural transition is an optic mode (called the Σ_4 mode in Ref. 5), which corresponds to local rotation of oxygen octahedra with Cu-atoms as centers. Since an oxygen atom in a plane normal to the tetragonal axis is shared by two

neighboring Cu atoms, the sense of rotations of the octahedra in two adjacent cells are opposite to each other; the basal plane unit cell of the ordered structure thus corresponds to an enlarged $\sqrt{2} \times \sqrt{2}$ structure associated with the high-temperature phase. The soft-phonon wave vector $\vec{q} = (\frac{1}{2},\frac{1}{2},0)$ corresponds to the X-point of the Brillouin zone (see Fig. 3 of Ref. 8). The orthorhombic strain e_{xy} and the integrated X-ray intensity of the superlattice spots have been found experimentally to grow in the ordered phase with the same exponent, namely, $2\beta_{exp} = 0.550$.

2. LANDAU THEORY AND COUPLING TO STRAINS

In order to construct a phenomenological theory for the structural transition, we concentrate on the particular normal modes associated with the rotation of the oxygen octahedra. These modes belong to the two-dimensional irreducible representation E of the little group of the wave vector whose point group symmetry is C_{4v}. Since the wave vectors $\vec{q} = (\frac{1}{2},\frac{1}{2},0)$ and $\vec{q}' = (\frac{1}{2},-\frac{1}{2},0)$ are equivalent to each other, the star of $\vec{q}$ has only a single arm. Since the normal modes for rotation of an oxygen octahedron are two-dimensional, there are two equivalent axes, namely $\vec{\xi} = [110]$ and $\vec{\eta} = [\bar{1}10]$ (the former being defined as the direction making an angle of $\pi/4$ to a nearest-neighbor Cu-O bond), of local rotation with the Cu atoms as centers. All the normal modes of vibration of the solid can be found using standard group theoretic techniques.[10] The displacements of all the octahedra for the two equivalent rotations above can be written as

$$\vec{u}_{\ell\xi} \equiv \psi_\xi p[a(\hat{e}_{1x},-\hat{e}_{1y},-\hat{e}_{2x},\hat{e}_{2y}) + b(-\hat{e}_{3z},\hat{e}_{4z},\hat{e}_{5z},-\hat{e}_{6z})]\exp(i\vec{q}\cdot\vec{\ell}) \quad , \qquad (1)$$

$$\vec{u}_{\ell\eta} \equiv \psi_\eta p[a(\hat{e}_{1x},\hat{e}_{1y},-\hat{e}_{2x},-\hat{e}_{2y}) + b(-\hat{e}_{3z},-\hat{e}_{4z},\hat{e}_{5z},\hat{e}_{6z})]\exp(i\vec{q}\cdot\vec{\ell}) \quad , \qquad (2)$$

where ℓ labels the unit cell, a and b are fixed constants, p is proportional to the rotation angle, $\hat{e}_{i\alpha}$ ($i = 1,\ldots,6$ and $\alpha = x,y,z$) label the Cartesian components α of the unit vectors associated with the i-th O atom of the octahedron ($i = 1,2$ refer to the O atoms along the tetragonal z-axis, and $i = 3,4,5,6$ to the basal plane O atoms labeled in a counterclockwise sense), and ψ_ξ, ψ_η are the order parameters.

The transformation properties of the order parameters under generators of the high-temperature space group I4/mmm allow us to construct an invariant-free energy associated with the interactions among the octahedra. These transformation properties are,

$$\Psi \rightarrow r\Psi \text{ under } (C_4|000) \tag{3}$$

$$\Psi \rightarrow -\Psi \text{ under } (C_{2x}|000) \text{ and } (I|000) \quad , \tag{4}$$

where $\Psi \equiv \begin{pmatrix} \psi_\xi \\ \psi_\eta \end{pmatrix}$ is a 2-component column vector, $r = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$, $(C_4|000)$ represents a 4-fold rotation about the z-axis, $(C_{2x}|000)$ is a 2-fold rotation about the x-axis, and $(I|000)$ is an inversion through the origin. Since the phase factors $\exp(i\vec{q}\cdot\vec{\ell})$ in Eqs. (1) and (2) are all real, the order parameters ψ_ξ and ψ_η are both real. The Landau free energy invariant under symmetry operation of the generators of the space group, to fourth order in the order parameters, is therefore

$$F - F_N = \tfrac{1}{2}r(\psi_\xi^2+\psi_\eta^2) + \tfrac{1}{2}g|\vec{\nabla}\Psi|^2 + u_1(\psi_\xi^4+\psi_\eta^4) + u_3\psi_\xi^2\psi_\eta^2 \quad , \tag{5}$$

where r, g, u_1 and u_3 refer to the material parameters of the system, and F_N is the free energy of the disordered phase. Equation (5) is in the same universality class as the three-dimensional (d = 3) xy-model with a cubic anisotropic field.

Writing, as usual, $r = \alpha(T - T_c)$, where α is a constant, we see that for $T < T_c$, the orthorhombic phase will be stable. The direction of the 2-fold rotation axis in the basal plane will depend on the relative values of the parameters u_1 and u_3. For $u_1 > 0$ and $(2u_1 - u_3) < 0$, the minimum energy states are either ($\psi_\xi \neq 0$, $\psi_\eta = 0$) or ($\psi_\xi = 0$, $\psi_\eta \neq 0$), and the 2-fold rotation axes are along the $\pm\hat{\xi}$- or $\pm\hat{\eta}$-directions. For $u_1 > 0$ and $(2u_1 \pm u_3) > 0$, the states of minimum energy are $\psi_\xi = \psi_\eta = \psi \neq 0$, and the 2-fold axes are along $\xi = \pm\hat{\eta}$-directions. The space group symmetry of the ordered phase is found to be Cmca in agreement with experiment.

We now discuss the coupling of the order parameters to the orthorhombic strain $e_6 = 2e_{xy} = \left[\frac{\partial u_x(\vec{r})}{\partial y} + \frac{\partial u_y(\vec{r})}{\partial r}\right]$, where $u_\alpha(\vec{r})$ ($\alpha = x,y$) is the α-component of the local displacement field of the center of mass. The transformation properties of the second rank tensor e_6 are the same as that of the product $\psi_\xi\psi_\eta$. Thus the symmetry-restricted form of strain-order parameter coupling energy, to second order in e_6, is found to be $F_c = ce_6\psi_\xi\psi_\eta + \frac{1}{2}C_{66}e_6^2$, where c is a coupling constant and C_{66} is the usual elastic constant. Hence for a given order parameter $\psi = \psi_\xi = \psi_\eta$ discussed above, the minimum value of strain is proportional to the square of the order parameter. This is precisely the experimental situation.

3. CRITICAL PROPERTIES

We have examined the critical properties of the model free energy, Eq. (5), by using renormalization group techniques following Refs. 11 and 12 to order ϵ =

4 - d, where d is the spatial dimension. The flow properties of the free energy in the parameter space (u_3, u_1) on the critical surface are shown in Fig. 1. There are four fixed points of which H, the Heisenberg fixed point, is stable. Since the observed transition is second order, we conclude that the critical exponents of the structural transition in La_2CuO_4 should be that of the three-dimensional Heisenberg model with a two-component order parameter. We find the standard critical exponents to be $\eta = 0$ and $1/\nu = 1.60$, so that $\beta = 0.3125$. The experimental value of β is[5] $\beta_{exp} = 0.275$. As pointed out by Birgeneau et al,[5] the experiments could not be performed very close to T_c, thus indicating that β_{exp} may not be very precise. Hence the agreement between the theoretical value of β above and the experimentally determined value seems reasonable.

In summary, using symmetry arguments we have developed a phonomenological free energy for the tetragonal-to-orthorhombic phase transition in La_2CuO_4. We have shown that the square of the order parameter and the orthorhombic strain scale with the same exponent 2β.

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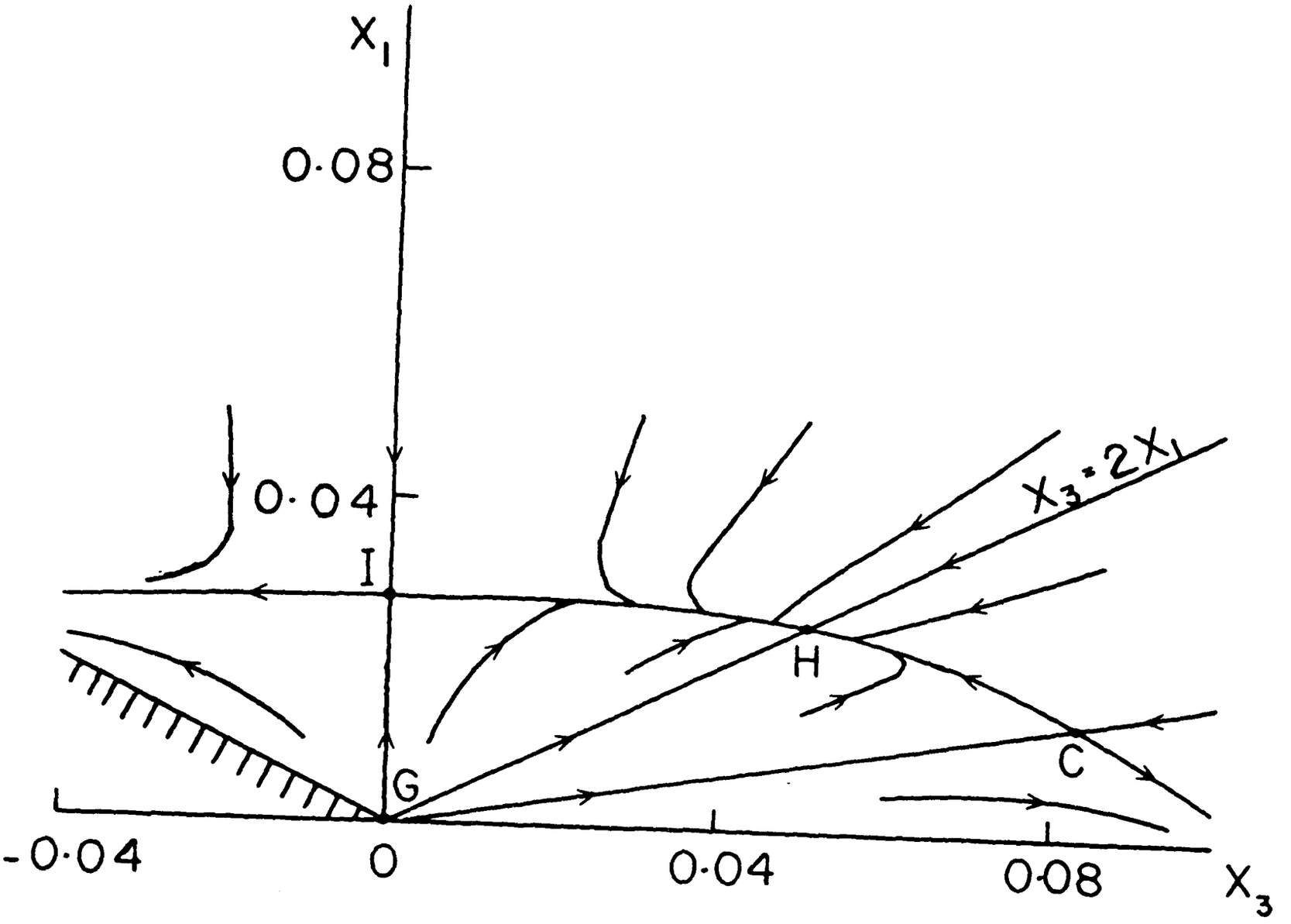

Figure 1

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FIGURE CAPTION

Fig. 1. Renormalization group flow diagram in the parameter space (x_3, x_1) of the model free energy, Eq. (5), where $x_i = u_i/(8\pi^2)$ $(i = 1,3)$. The four fixed points are labeled as G, I, H and C, which stand for Gaussian, Ising, Heisenberg and cubic, respectively. The hatched region as well as the region with $x_1 < 0$ are unstable regimes of the free energy.

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