

# Phase stratification of an electron liquid in the new superconductors

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Analysis of the experimental situation in lanthanum cuprate suggests the coexistence of two phases: one conducting and one insulating. This situation would explain certain features of the normal state.

Over the time which has elapsed since the discovery of so-called high-temperature superconductivity,<sup>1</sup> many important pieces of experimental evidence have been accumulated. Nevertheless, the question of whether the high values of  $T_c$  can be explained by an ordinary model remains open. We accordingly consider the problem from a different viewpoint in the present letter. Specifically, if the new superconductivity is caused by certain unusual properties of these materials, we would naturally expect to see manifestations of these properties even in the normal state. In other words, we concentrate exclusively on the properties of the normal phase, particularly those of lanthanum compounds. "Pure"  $\text{La}_2\text{CuO}_4$  is a special case in that it has a body-centered tetragonal lattice in its tetragonal phase. The primitive cell therefore contains precisely one structural unit of  $\text{La}_2\text{CuO}_4$ , corresponding to a half-filled Brillouin zone. [We assume below that since the structural transition from  $T_{OT} \approx 500$  K is not of an electronic nature (in contrast with Ref. 2, for example), it is a small effect against the background of a broad zone,  $\sim 1-2$  eV.] However, the resistance of "pure"  $\text{La}_2\text{CuO}_4$  is very large ( $\sim 0.1 \Omega \cdot \text{cm}$ ), depends weakly on the temperature above, say, 150 K, and exhibits a localization behavior at lower temperatures. On the other hand, doping with Sr to a level of a few percent increases the conductivity by two orders of magnitude, giving rise to a pronounced metallic behavior. A Mott-insulator state arising from strong Coulomb correlations would be the only presently known alternative to a Fermi-liquid state (Ref. 3, for example). It would then seem that the resistance of "pure"  $\text{La}_2\text{CuO}_4$  should obey an activation law with a large energy gap. Since this is

not what we see experimentally, the finite conductivity is linked with an uncontrollable doping as a result of oxygen vacancies or a deviation from stoichiometry. Even at a lower doping level, however, the conductivity should vary with the temperature in accordance with the temperature dependence of the mobility.

We will not gloss over these contradictions, but rather treat them as important facts. We will attempt to propose yet another alternative explanation, specifically, the coexistence of two phases, conducting and insulating, in  $\text{La}_2\text{CuO}_4$ .

The  $\text{La}_2\text{CuO}_4$  lattice is characterized by an octahedral coordination of  $\text{CuO}_6$ . With a cubic symmetry, the  $\text{Cu}^{2+}$  ion ( $d^9$  electron configuration) corresponds to a degenerate Jahn-Teller term  $E_g$ . The presence of La atoms lowers the symmetry to tetragonal and in principle lifts the degeneracy of the  $E$  term. Let us assume, however, that the Jahn-Teller Hamiltonian is still of the form

$$\begin{pmatrix} \lambda Q_3 + E'_3 & \lambda Q_2 \\ \lambda Q_2 & -\lambda Q_3 + E'_2 \end{pmatrix}, \quad (1)$$

where the matrix acts on the coordinates  $(\eta_3, \eta_2)$  in the electron wave function  $\psi = \eta_3\psi_{3x^2-r^2} + \eta_2\psi_{x^2-y^2}$  (the notation is that of Ref. 4). We are thereby assuming that the tetragonal splitting is smaller than the Jahn-Teller energy  $E_{JT}$ , so a strong polaron coupling is still characteristic of the copper ion in the  $d^9$  configuration.

We first assume that there are no divalent states of copper at all in the system [for definiteness, we assume that the copper ions are monovalent ( $d^{10}$ )]. We introduce a conduction band, constructed in a self-consistent way for this configuration, in terms of, say, oxygen  $p$  orbitals. Such a band will be half-filled. Now taking one electron (or, more precisely, one hole) and putting it in place of a copper, we form a local polaron level ( $d^9$ ) with an energy  $E_0$  (Fig. 1). If  $E_0$  is above the Fermi level ( $\mu_0$ ) in the conduction band, a polaron state is not preferable. At  $E_0$  below the bottom of the conduction band, all the carriers go into localized states (an analog of a Mott insulator<sup>4</sup>).

There is a third possibility, in which the polaron level occupies an intermediate position. In this case the chemical potential is pinned at  $E_0$  (Refs. 5 and 6), and the

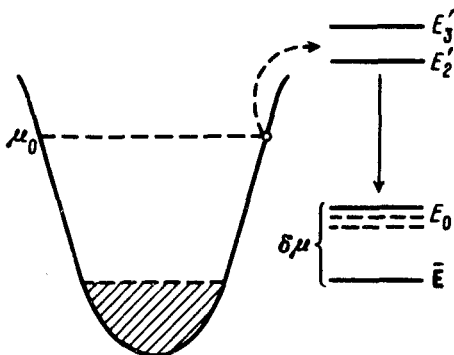


FIG. 1.

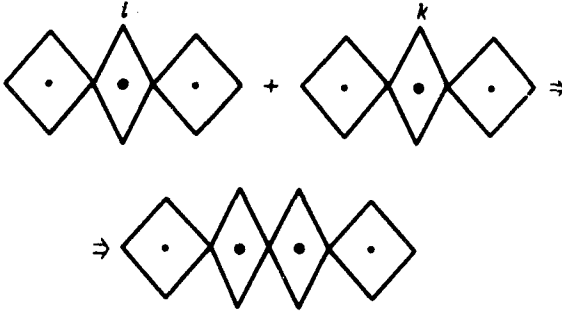


FIG. 2.

polaron levels are only partially filled. When we take the temperature into account, we conclude that upon hybridization each cell acquires an additional mean tetragonal distortion  $\langle Q_3 \rangle \neq 0$ . The hybridization of a local level with the conduction band is reduced by another factor because of the overlap of the lattice coordinates  $\exp(-E_{JT}/\omega)$ ; this effect again corresponds to a slow restructuring of the lattice (slow at the scale of the phonon frequencies). If hybridization is ignored, the population of the local levels is determined by the conditions for a thermodynamic equilibrium.

The structure of  $\text{La}_2\text{CuO}_4$  is such that an attraction between ordinary localized levels is essentially inescapable. As can be seen from Fig. 2, each of the two electrons ( $i$  and  $k$ ) in the cells causes an elastic shear strain near its own cell. Ignoring Coulomb interactions for the moment, we see that there is a possible advantage in terms of the elastic energy if the two electrons are in adjacent cells. Such a formation would correspond to a bipolaron. Even larger clusters could then appear. The position of the chemical potential would correspondingly decrease by an amount  $\delta\mu$ , which is equal to the energy required for one localized level to split off from a cluster. The electron density in the band and that in the clusters satisfy the following respective proportions:

$$n_c = \int_0^{E_0 - \delta\mu} \nu(E) dE, \quad n_i = \int_{E_0 - \delta\mu}^{\mu_0} \nu(E) dE.$$

Let us examine the structure of a cluster in  $\text{La}_2\text{CuO}_4$  in more detail. Oxygen atoms in the  $ab$  plane are collectivized between two neighboring cells. For simplicity, we assume that the bond between the oxygens (O-La-La-O) along the  $c$  axis is also rigid. A Jahn-Teller strain in certain neighboring cells is obviously equivalent to a local shear:

$$Q_3 \Rightarrow 6^{-1/2} (2u_{zz} - u_{xx} - u_{yy}), \quad Q_2 \Rightarrow 2^{-1/2} (u_{xx} - u_{yy}),$$

where  $u_{ik} = 1/2(\partial u_i / \partial x_k + \partial u_k / \partial x_i)$  is the strain tensor. The elastic energy per unit volume is now

$$\frac{1}{2} (c_{11} - c_{12})(Q_3^2 + Q_2^2). \quad (2)$$

This energy should be considered along with Jahn-Teller Hamiltonian (1). According to this interpretation, the clusters mentioned above would be manifested as local shear in the  $\text{La}_2\text{CuO}_4$  lattice.

What would the appearance of a cluster in real space imply? (If a cluster is large enough, it could be treated as a nucleating region of a new phase.) Since there must be one electron in each localized level (more precisely, one hole, for the  $d^9$  configuration with respect to  $d^{10}$ ), there are no carriers in the conduction band, because of electrical neutrality in this spatial region. In other words, a cluster corresponds to a "droplet" of an insulating phase. In the static picture of the coexistence of insulating and conducting phases, the conductivity would vanish if the ratio  $n_c/n_i$  were less than the percolation limit. In the three-dimensional case, this situation would correspond to  $n_c/n_i \sim 0.15$ , and in the two-dimensional case to  $\sim 0.5$ . We would like to link the sharp differences between the conductivity of "pure"  $\text{La}_2\text{CuO}_4$  and that of the doped compound to specifically a proximity to the percolation limit. The coexistence of carriers of two types in  $\text{La}_2\text{CuO}_4$  would be necessary in order to explain, for example, the presence of a normal Pauli contribution to the susceptibility in the case of a simultaneous localization nature of the resistance at low temperatures.

A thermodynamic analysis is capable of telling us only the relative concentrations of the insulating and conducting phases. It cannot tell us the extent to which the "droplets" are broken up. Coulomb effects must be taken into account in order to resolve this question. Since all the energies involved here are at the atomic order of magnitude, the dimensions of the droplets or clusters forming a "fog" in the  $\text{La}_2\text{CuO}_4$  lattice would probably be small. The percolation approach would thus be of a limited nature, and even below the percolation threshold the conductivity might be low but nonzero. These questions are presently being studied. We wish to stress once more that the clusters are not static; i.e., the overall state is dynamic, although the characteristic frequency is associated with the lattice dynamics.

Doping changes the total number of carriers in the band in Fig. 1, lowers the local symmetry (by virtue of the Coulomb charge), and creates inhomogeneities, which may pin the clusters or droplets.

We do not have space here to do more than mention that a structural transition would not be difficult to link with a third-order anharmonicity in the product of representations  $E_g \times F_{2g} \times F_{2g}$ , where the three-dimensional representation  $F_{2g}$  contains a strain corresponding to rotations of octahedra.

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