Charge distribution in high-T_c superconductors

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In a superconductor which has two groups of electrons (e.g., holes in CuO_2 planes and in a "reservoir" in a high-T_c superconductor), a charge redistribution occurs upon the transition of one of the subsystems to a superconducting state: The density of "active" carriers increases at $T < T_c$. This effect can explain several structural anomalies in the high-T_c superconductors. It changes the temperature dependence of the properties of the superconductor. It may lead to several effects at a contact of a high-T_c superconductor with a normal metal or a semiconductor.

Most of the high-T_c superconductors contain two distinct groups of electrons: the carriers in the CuO_2 "active" planes and the "reservoir"—the chains in the 1-2-3 high-T_c superconductors, or the BiO and TlO planes in the bismuth and thallium high-T_c superconductors. The relative distribution of charge between these subsystems is determined by many factors (Ref. 1, for example) and affects both the normal and superconducting properties. We would like to point out that this distribution may also depend on the temperature for a given specific compound. In particular, not only do the charge distribution and the density of holes in CuO_2 planes, n_h, affect T_c (Ref. 2); it is also true that the transition to a superconducting state causes a redistribution of charge, leading in particular to an increase in n_h at $T < T_c$. This effect can explain many structural and other anomalies observed in the high-T_c superconductors. It may have some important consequences.

We will explain this effect in the particular example of a model in which the superconductivity in the high-T_c superconductor is described as a Bose condensation of local pairs in CuO_2 planes. Although this picture may not be very realistic, there are several arguments in its favor:[3,4] the small values of ξ, the anomalously large values of $2\Delta_0/T_c$, and the large jump in the specific heat. The model of local pairs (bosons or a mixture of bosons and fermions) is being discussed widely in the literature,[5] sometimes being referred to as the "s-channel theory of superconductivity."[6] (The effect of a charge redistribution in a more conventional description of the high-T_c superconductivity, on the basis of the BCS model, was discussed in Ref. 7.)

In its simplest form, the situation of interest here can be modeled by a system of ideal bosons with a spectrum $\epsilon_b = \delta + (p/2m_b)$ (pairs in CuO_2 planes) and a system of free fermions, $\epsilon_f = p/2m_f$ (holes in a reservoir).[1)] We will be ignoring the interaction of fermions and bosons here, taking account of only a statistical effect: the possibility that holes will undergo a transition from the reservoir to CuO_2 planes, where these holes form pairs. (Incorporating an interaction does not alter the qualitative conclusions.)

The conservation law for the number of particles,

$$n_f + 2n_b = n = \text{const} \tag{1}$$

determines the common chemical potential of the system. Here n_f and n_b are the densities of fermions and bosons, which are given by integrals of corresponding Fermi and Bose distribution functions with respective chemical potentials μ and $\mu_b = 2\mu$ (so the chemical potential per hole is μ). If $n_b \neq 0$, a Bose condensation occurs at a temperature T_c. At $T \leqslant T_c$, the chemical potential is fixed at the bottom of the boson band: $\mu_b = \delta$. This fixing of the chemical potential leads to the basic effect mentioned above: an increase in $n_h = 2n_b$ with decreasing temperature below T_c. That this is true can be seen directly from the change in the number of fermions, n_f, at $T < T_c$, with $\mu = \delta/2$. Under this condition we find

$$n_f(T) = TC_0 \ln[\exp(\delta/2T) + 1], \tag{2}$$

where $C_0 = m_b/2\pi$. It can be seen from (2) that n_f increases with increasing T, and $n_h = 2n_b = n - n_f$ correspondingly decreases (see also Ref. 6). At a qualitative level, the effect in this model is associated with the following circumstance: In a single-component Fermi system, $\mu(T)$ falls off with increasing temperature: $\mu(T) = \mu_0 - T\exp(-\mu_0/T)$. This change guarantees conservation of the total number of fermions. In the case at hand, in contrast, $\mu(T)$ is fixed at $T < T_c$ as a result of Bose condensation. As a result, n_f increases with increasing T, and n_b correspondingly decreases. (This effect becomes even stronger in the BCS model, in which μ is not merely constant below T_c: it in fact decreases.[7)])

The value of T_c is given by the standard formula

$$T_c = \frac{3,31h^2 n_b^{2/3}}{m_b}, \tag{3}$$

but in our case n_b depends on the temperature through relations (1) and (2). Relation (3) is thus actually a self-consistent equation for T_c.

In the superconducting phase, on the other hand, the charge redistribution is always of one sign: The density of the active component (in the case at hand, bosons, or holes in CuO_2 planes) increases at $T < T_c$. In the normal phase, at $T > T_0$, there may again be a redistribution of a charge, in this case either sign, depending on which particles are present in greater number at low temperatures (the filling of the various states will clearly equalize at a sufficiently high temperature). Figure 1 shows examples of various possible types of behavior; the case of bands of finite width has been examined numerically here.

The charge redistribution with the temperature which was found above and which we have shown is sensitive to a transition of the system into a superconducting

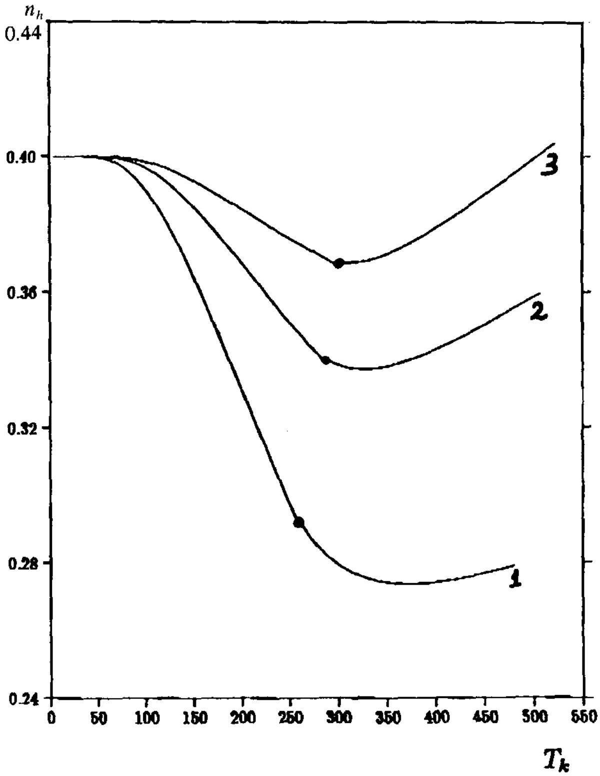

FIG. 1. Change in the density of holes, $n_h = 2n_b$, in a CuO_2 plane for the following parameter values. The width of the fermion band is $D = 1000$ K; the width of the boson band is $d = 2000$ K. Lines *1–3*—Values $\delta = 600$ K, 800 K, and 900 K, respectively, for the band shift. The points are the values of T_c at these parameter values.

state may have a number of consequences. In the first place, an increase in n_h (an increase in the positive charge in a CuO_2 plane at the expense of the reservoir) should be reflected in structural properties. For example, we might expect a decrease in the distance from Cu(2) to the "apex" oxygen lying on the c axis. A corresponding effect has been observed in Bi-2212 and Bi-2223 (Ref. 8); it has also been observed, but less reliably, in the 1-2-3 high-T_c superconductors (Refs. 9 and 10, but there is also a contradictory result[11]). The effect discussed above might furnish a natural explanation for the shift of the apex oxygen, although another mechanism for this shift is also possible: a redistribution of the "native" d hole at the Cu(2) from a $d_{x^2-y^2}$ state to a d_{z^2} state.[12]

Other anomalies observed in the high-T_c superconductors may also be related to a charge redistribution below T_c: an increase in the distortion of the CuO_2 plane itself,[13] structural features in the thermal expansion,[14] and structural features in the shift of the NQR frequencies.[15] An increase in the carrier density in a CuO_2 plane below T_c might modify the temperature dependence of various thermodynamic properties. In particular, it might steepen the $\Delta(T)$ curve near T_c and raise the value of $2\Delta_0/T_c$ (Ref. 7). These conclusions are in qualitative agreement with experimental results.[16]

Several interesting and important effects may arise from a redistribution of the charge and from a change in the behavior of the chemical potential below T_c in contacts of high-T_c superconductors with normal metals or semiconductors. This effect may be important in tunneling (in particular, it may cause an asymmetry of I–V characteristics), in thermoelectric effects, etc. The corresponding modification of the properties of the surface layer of a semiconductor in contact with a high-T_c superconductor could serve as a sensitive method for studying this effect. It may prove important in attempts to develop hybrid electronic devices based on film contacts of high-T_c superconductors with semiconductors.

We note in conclusion that similar effects, at least at contacts, may be accompanied by other phase transitions involving the formation of a band gap in the electron spectrum, e.g., insulator–metal transitions. The lowering of the energy of the occupied electronic states in systems of this sort and the corresponding decrease in the chemical potential may lead to a flow of the charge in them away from a contact with an ordinary metal. If there are two electronic subsystems in these systems, as in the high-T_c superconductors, there may be an internal redistribution of charge.

[1)] The boson system is assumed to be three-dimensional in order to avoid some complications which stem from Bose condensation in the two-dimensional case: A rather slight dispersion along the c axis is actually sufficient here. For simplicity, we assume that the system of fermions is two-dimensional.

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