MEETINGS AND CONFERENCES

Scientific session of the Division of General Physics and Astronomy of the Academy of Sciences of the USSR (25 January 1989)

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A scientific session of the Division of General Physics and Astronomy of the USSR Academy of Sciences was held on 25 January 1989 at the S. I. Vavilov Institute of Physics Problems of the USSR Academy of Sciences. At this session the following report was presented:

G. M. Éliashberg. Current carriers and magnetism in high-temperature superconductors.

A brief summary of the report is published below.

G. M. Éliashberg. *Current carriers and magnetism in high-temperature superconductors.* From the moment of discovery of high-temperature superconductors[1] an experimental investigation of a broad spectrum of their properties that is without precedent with respect to intensiveness and the variety of the methods employed is being carried on. One of the most important results achieved up to now is the elucidation of the quantum mechanical nature of the current carriers and magnetism in these compounds. All the copper oxide materials known at present have a sharply expressed layer structure, and their magnetic and transport properties are determined primarily by the valence state of the copper and oxygen ions in the so-called cupratic plane (Fig. 1). This state can change depending on the composition of the other elements of the construction which thus play a regulating role. The two systems that were the first to have been discovered have been studied in greatest detail until now: $La_{2-x}M_xCuO_4$, M = Ca, Sr, Ba; $YBa_2Cu_3O_{6+y}$. For $T > 500$ K the copper ions in La_2CuO_4 form a body-centered tetragonal lattice and are situated in an octahedral oxygen surrounding. The neighboring CuO_2 planes are at a distance of ~ 6.65 Å from each other and are shifted by one half of the diagonal of the square of Fig. 1. Between these planes is situated a layer of 2LaO. In the temperature range $T < 500$ K a small orthorhombic distortion occurs which corresponds to a deviation of the octahedra from the c axis which is perpendicular to the planes. The details of the structure and the (T, x) phase diagram are given in the review article of Ref. 3. In $YBa_2Cu_3O_{6+y}$ pairs of closely situated cupratic planes (~ 3.2 Å with the Y layer squeezed between them are separated by a (BaO)CuO_y (BaO) sandwich. The oxygen coordination of the copper ions from the CuO_2 planes is shown for the cross-sections (a, c) and (b, c) in Fig. 2.

With a partial replacement of the trivalent La by a bivalent alkali-earth metal a sharp change takes place in the properties of $La_{2-x}M_xCuO_4$: from an antiferromagnetic dielectric with $T_N = 300$ K ($x = 0$) the system is converted into a conductor with conductivity of a metallic nature. For M = Sr the highest temperature of transition into the superconducting state $T_c = 40$ K in the case of ceramic samples is achieved for $x \sim 0.17$—0.20. A further increase in x leads to a decrease in T_c, and for $x > 0.3$ there is no superconductivity. In single crystals the attained values of T_c do not exceed 13 K. Thus, superconductivity in this system exists only in the range of a disordered solid solution.

$YBa_2Cu_3O_6$ is an antiferromagnetic dielectric with $T_N = 500$ K. The copper plane in the aforementioned sandwich does not contain any O ions, and the structure is tetragonal. The highest value of $T_c = 93$ K is attained for $y = 1$ when once again an ideal structure is realized which now turns out to be orthorhombic: the additional O ions are situated along chains of CuO along one of the directions a and b. We note that one of the new systems $Y_{1-y}Ca_yTlCu_2O_7$ has a structure similar to $YBa_2Cu_3O_{6+y}$, but the CuO_y plane is replaced by a TlO plane (Fig. 3). The properties of this system are determined by the composition of the (Y, Ca) layer, and from an antiferromagnetic dielectric ($y = 0$) the system goes over into a metallic state with $T_c \sim 80$ K ($y = 1$).[4] This emphasizes the regulating role of the layers with variable composition: they do not have a direct relevance to the mechanisms of superconductivity and magnetism.

1. *Valence states of the Cu and O ions in the preelectic and lightly doped phases of $La_{2-x}Sr_xCuO_4$ and $YBa_2Cu_3O_{6+y}$*. The structure of magnetic phases in these systems has by now been studied in some detail. Considerable information on the dynamics of spin fluctuations is also available.[3,5] We here note only some results. The magnetic moments of the sublattices are equal at $T = 0$ respectively to $0.5\ \mu_0$ and $0.66\ \mu_0$ for La_2CuO_4 and $YBa_2Cu_3O_6$ which is

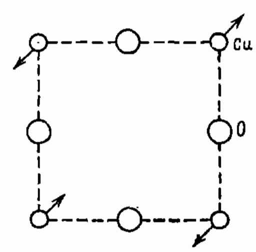

FIG. 1.

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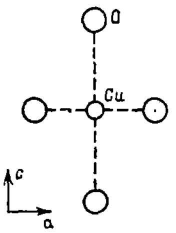

FIG. 2.

close to the theoretical value of $0.68\,\mu_0$ for (the quasi-two-dimensional) Heisenberg model with $s = 1/2$ and magnetic moment of $1.1\,\mu_0$ (as of a Cu^{2+} ion). This points to the high degree of localization of the magnetic states. The exchange interaction between nearest neighbors in a plane is $J_{\parallel} = 0.12$ MeV and between planes is $J_{\perp} \approx 0.002$ MeV. A small anisotropy of the interaction leads to the orientation of spins in a plane as shown in Fig. 1.

The magnetic state is based on the Cu^{2+} ion which is in the $3d^9_{x^2-y^2}$ state. This is indicated by x-ray methods (photoemission, absorption near the edge of the K band and others) combined with theoretical analysis (see Refs. 6, 7, which contain references to experiment, and Ref. 8). The large value of $J_{\parallel}$ is associated with the strong hybridization of $3d^9_{x^2-y^2}$ with $02p_{x,y}$ which leads to superexchange. The effective filling of the d-shell accompanying this turns out to be equal to ~ 9.4.[8] Hybridization, in the first instance, is also connected with the large value of splitting of 3d states: the one nearest to the ground state, $3z^2 - r^2$ lies higher by ~ 1.4 eV.[7] The charge of the cupratic plane in the dielectric phase corresponds to $(CuO_2)^{2-}$ in $YBa_2Cu_3O_6$ the copper ions in the governing layer, the so-called Cu1 are in the monovalent state.[3] Therefore this plane is a dielectric of the Mott type. The gap according to different estimates amounts to 2–4 eV.

As a result of the replacement of La^{3+} with Sr^{2+} the lacking electron is taken from the cupratic plane. Due to the high energy of detachment of the third electron from Cu^{2+} this leads to the formation of a hole in the initially full 2p shell of O. Experiment convincingly supports such a picture (cf. references in the papers of the present author[9]). In the case of $YBa_2Cu_3O_{6+y}$ for $y < 0.4$–0.5 basically a transition of the Cu1 ions into the bivalent state occurs, and the charge of the cupratic planes remains almost unchanged. With a further increase of y here also holes appear in the 2p shell of O. A number of observations shows that at low concentration the holes are localized. Without dwelling on a discussion of the different models of localization we note only that the appearance of even a low concentration of holes destroys the weak interplane exchange and destroys the long-range

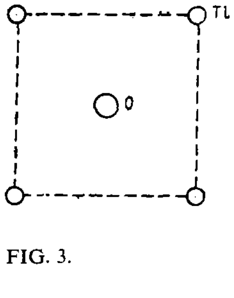

FIG. 3.

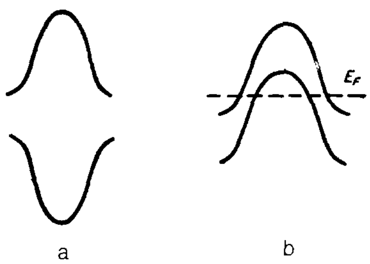

FIG. 4.

magnetic order. In $La_{2-x}Sr_xCuO_4$ this occurs already at $x \sim 0.02$; in $YBa_2Cu_3O_{6+y}$ the picture is more complicated for the reason indicated above.

2. *Metallic state.* For $x \gtrsim 0.05$ in $La_{2-x}Sr_xCuO_4$ a delocalization of holes occurs. The situation near the threshold concentration is quite complicated: in contrast to a usual doped semiconductor here a significant role is played by the exchange coupling of localized holes with a system of copper spins.[7] But at a concentration considerably higher than the threshold one, the holes are in a band state. As is now becoming ever more clear the structure of the valence band near its upper edge is determined primarily by a direct hybridization of the oxygen p-orbitals.[6,7] If the plane lattice consisted only of oxygens, then in the strong-coupling approximation we would have the spectrum (reduced to the Brillouin zone corresponding to Fig. 1):

$$\varepsilon(p) = \varepsilon_0 \pm 4t \cos\left(\frac{1}{2} p_x a\right) \cdot \cos\left(\frac{1}{2} p_y a\right),$$
$$-\frac{\pi}{a} \leqslant p_x, \quad p_y \leqslant \frac{\pi}{a}. \tag{1}$$

Both branches are degenerate along the entire band boundary. Taking into account the Cu^{2+} potential and the jumps over the oxygen outside the plane leads to lifting of the degeneracy (Fig. 4a). The magnitude of t, apparently, lies within the range 0.5–0.7 eV and this leads near the top of the band to an effective mass $m^* \lesssim m$ and a Fermi energy of $E_F = 1.6\,(m^*/m)x^*$ eV, x^* is the number of holes per cell of CuO_2. Apparently in $La_{2-x}Sr_xCuO_4$ $x^* = x$. In $Ba_2Cu_3O_7$ $x^* = 0.5$, if the CuO chains are neutral. Since here the cupratic planes are doubled, then taking into account the jumping of holes between the planes the qualitative picture of the spectrum should have the form shown in Fig. 4b. If one interprets on the basis of this model the results of the experimental determination of the Fermi surface[10], then the Fermi level must lie as shown in Fig. 4b. A more detailed analysis enables one to explain also the small "pockets" of electronic type.

3. *Interaction between carriers and superconductivity.* Little doubt remains now that the superconductivity in the oxide superconductors in its basic features corresponds to the BCS theory, whose main element is the formation at $T < T_c$ of Cooper pairs. To the line of reasoning introduced earlier (cf., for example, Ref. 11) one can add that new data show that the pairs are singlets: observation of a jump in the temperature dependence of the relaxation time of the spin of the ^{17}O nucleus, the gap nature of the temperature dependence of the depth of penetration of the magnetic field, and a direct observation of the gap on the volt-ampere characteristic by the method of tunnel microscopy.[12] The most ade-

quate apparatus is a formalism based on an explicit taking into account of the delayed nature of interactions and enabling one to extend the BCS theory to the strong-coupling region. A discussion of various contributions to the interaction function $\lambda(\omega)$ ($\int\lambda(\omega)d\omega = \lambda$ — a dimensionless coupling constant) is contained in the author's paper of Ref. 9. The central problem that remains is the elucidation of the role played by the relatively soft (0.1–0.2 eV) modes of electronic origin. In the first instance these are fluctuations of the spin system both of the triplet and of the singlet nature, and also the d—d transitions — fluctuations of the orbital state of the copper ion which were first discussed by Weber. In connection with these transitions we note the following. An increase in the concentration of holes on the 02p shells in the cupratic plane should lead to a diminishing of their hybridization with Cu3d.[6,9] At the same time the energy interval between the orbital 3d states $x^2 - y^2$ and $3z^2 - r^2$ will diminish and this will lead to an increase of their contribution to $\lambda(\omega)$. This effect must be considerably more strongly pronounced in $YBa_2Cu_3O_7$ than in $La_{1.85}Sr_{0.15}CuO_4$ since the concentration of carriers in the latter is significantly smaller. This is in agreement also with the greater value of the oxygen isotopic effect in the second of the compounds mentioned above. On the other hand the existence of a large number of modes in the phonon spectra of these materials allows also a different interpretation of data on the isotopic effect.[13] The magnitude of the contribution of spin fluctuations to $\lambda(\omega)$ is also awaiting to be made more precise. One can hope that an improvement in the technique of tunnel spectroscopy will make information on $\lambda(\omega)$ more precise. In conclusion we note that the study of copper oxide superconductors has made more urgent the problem of describing a multielectron system in a crystal in the presence of a subsystem localized as a result of the Mott effect. We do not have for such a case an approach equivalent in its generality and effectiveness to the Landau theory of a Fermi liquid. Martin's argument[14] in favor of the applicability to such a system of general relations obtained by Luttinger and Ward in 1961 appears to be unconvincing. In this author's opinion in the presence of a Mott subsystem the Green's function for the electrons must have a surface of zeros in the Brillouin zone.[15] This surface corresponds to Anderson's pseudo-Fermi-surface similarly to the manner in which the surface of the poles of this function is the ordinary Fermi surface.

[1] J. G. Bednorz and K.-A. Müller, Z. Phys. **B64**, 189 (1986).
[2] C. W. Chu, P. H. Hor, R. L. Meng, L. Gao, Z. J. Huang, and Y. Q. Wang, Phys. Rev. Lett. **58**, 405 (1987).
[3] R. J. Birgenau and G. Shirane in *Physical Properties of High Temperature Superconductors* (Ed.) D. M. Ginsberg, 1989.
[4] J. Mizuki, Y. Kubo, *et al.*, Physica **C156**, 781 (1988).
[5] A. S. Borovik-Romanov, A. I. Buzdin, N. M. Kreĭnes, and S. S. Krotov, Pis'ma Zh. Eksp. Teor. Fiz. **47**, 600 (1988) [JETP Lett. **47**, 697 (1988)].
[6] E. B. Stechel and D. R. Jennison, Phys. Rev. **B38**, 4632 (1988).
[7] H. K. McMahan, R. M. Martin, and S. Sathpaty, Phys. Rev. **B38**, 6650 (1988).
[8] K. B. Garg, A. Bianconi, et al., Phys. Rev. **B38**, 244 (1988).
[9] G. M. Éliashberg, Pis'ma Zh. Eksp. Teor. Fiz. **48**, 275 (1988). [JETP Lett. **48**, 305 (1988)]; *High T_c from Russia*, World Scientific, Singapore, 1989.
[10] L. C. Smedskjaer, Y. Z. Liu, *et al.*, Physica **C156**, 269 (1988).
[11] L. P. Gor'kov and N. B. Kopnin, Usp. Fiz. Nauk **156**, 117 (1988). [Sov. Phys. Usp. **31**, 850 (1988)].
[12] S. L. Pryadkin and V. S. Tsoĭ, Pis'ma Zh. Eksp. Teor. Fiz. **49**, 268 (1989) [JETP Lett. **49**, (1989)].
[13] A. A. Golubov, Physica **C156**, 286 (1988).
[14] R. M. Martin, Phys. Rev. Lett. **48**, 362 (1982).
[15] S. A. Gordyunin and L. P. Gor'kov, Zh. Eksp. Teor. Fiz. **63**, 1922 (1972) [Sov. Phys. JETP **36**, 1017 (1972)]; J. Low Temp. Phys. **11**, 147 (1973).

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