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SPIN AND ELECTRON CORRELATIONS  
IN THE COPPER OXIDES AND THEIR ROLE  
FOR HIGH TEMPERATURE SUPERCONDUCTIVITY

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## I. Introduction

The recent discovery of superconductivity in ceramic copper oxides<sup>/1/</sup> has prompted the reexamination of possible mechanisms for superconductivity at relatively high temperatures. The most obvious structural features of the superconducting oxides is that they have planes of copper atoms linked by oxygen atoms in a roughly square arrangement. The electrons involved in chemical bonding between atoms of copper and oxygen play a crucial role; they appear to carry the electrical current<sup>/2/</sup>. The problem is to understand how electrons (or the equivalent holes) can couple together to form the Cooper pairs required for superconductivity.

The nature of the attractive interaction and the type of the Cooper pairing in these materials have led to various and controversial statements<sup>/2,3/</sup>. Some theories describe the way in which holes on neighbouring oxygen atoms might couple through the influence of electrons on an intervening copper atom, thus forming the Cooper pair required for superconductivity. Concerning the pairing interaction, Schrieffer<sup>/3/</sup> suggested the grouping of theoretical efforts in several broad classes, those based on 1) lattice vibrations, 2) charge fluctuations (excitons, plasmons) and 3) spin fluctuations and electron correlations (antiparamagnons, spin polarons, spin bags).

Recent investigations of the high- $T_c$  perovskite superconductors suggest that the nonphonon mechanism for their superconductivity can be more relevant. There are very important reasons to believe in the role of strong electron correlation effects and a need to go beyond the band theory<sup>/4,5/</sup>. A better picture is that of the Mott insulator<sup>/6/</sup>, in which the electrons are not in extended states. The presence of antiferromagnetism makes it clear that the electron system is highly correlated. However, in the model with a strong electron correlation, such as the Hubbard model, a crude mean-field-type argument could favour almost any kind of symmetry broken states. Therefore we need careful competition among the Mott insulating behaviour, superconductivity and antiferromagnetism. It is clear from the plenty of experimental results that the spins and carriers in the copper oxides are coupled in a very nontrivial way. Although the spin-mediated carrier pairing has not been confirmed, it is

obvious that any theory of superconductivity must account for the role of antiferromagnetic correlations.

Unfortunately, we have, at the present time, no complete formal theory of the high-temperature superconductors, but we do have a number of hints towards the theory, and the application of these hints to the copper oxides. Some of these procedures are adaptations of techniques that have proved useful in other areas of physics such as elementary particle physics, quantum field theory, the quantum Hall effect, heavy fermion systems, etc. There is much hope that these beautiful theories would clarify a very difficult problem of the microscopic description of the high- $T_c$  superconductivity. A more complete data set from a variety of experiments is required, however, before this phenomena can be understood.

In this paper, we shall be concerned with the problem of how the electron and spin correlation effects can be involved in the specific character of superconductivity in the copper oxides. Our primary interest here is directed to the question: Is the coupling between spin and electron variables vital for high- $T_c$  superconductivity?

## 2. Electronic Structure of High- $T_c$ Materials

Before starting a detailed discussion on the mechanism of superconductivity in the high- $T_c$  compounds, it is very important to know their electronic structure and furthermore the nature of the states induced on the Fermi level by a chemical substitution or stoichiometry changes. To obtain information of the above type one must carry out realistic band-structure calculations. Such calculations, which have been performed in numerous papers (see recent review articles<sup>/2,7/</sup>), give a very detailed description of the one-particle electronic states in these materials. Unfortunately, these calculations immediately show up a problem which is related to that encountered in other late 3d transition metal oxides (CuO, NiO). This difficulty is connected with the fact that the one-particle band theory predicts undoped copper oxides  $\text{La}_2\text{CuO}_4$  and  $\text{YBa}_2\text{Cu}_3\text{O}_6$  to be metallic whereas these are in fact to be antiferromagnetic insulators with a relatively big gap of 1.5 - 2 eV. For transition metal monooxides this problem has been known to be a result of the breakdown of the one-electron-band description due to the strong Coulomb interaction of the 3d tight-binding electrons<sup>/6/</sup>. The question concerning the copper oxides arises naturally: Do the high- $T_c$  compounds also belong to the class of strongly correlated systems?

Trying to understand a very complex nature of the electronic

structure of copper oxides, Sawatzky /7/ has called attention to the fact that despite a broad density of states (6-7 eV) in the high temperature compounds the electrons at least in the CuO planes and chains should be considered in a highly correlated limit. If one investigates the full band-structure picture, one can immediately see that the broad density of states results, to a great extent, from splitting due to a different symmetry of subbands but not from true dispersion due to the translational symmetry. One important aspect here is that the metallic behaviour can occur even though the Coulomb correlation is very large. We can conclude that the high temperature compounds are strongly correlated systems showing various types of insulating and metallic states induced by the chemical substitution or stoichiometry changes. This gives the heuristics for the searching of an appropriate pairing mechanism.

To summarize, we formulate here, following Sawatzky /7/, main conclusions of this chapter:

1. The superconducting copper oxides are strongly correlated systems;
2. The additional holes are in the oxygen 2p states;
3. There is a very strong oxygen hole - copper ( $d^9$ ) anti-ferromagnetic exchange (if the oxygen hole is in  $(x^2-y^2)$  symmetry);
4. A large oxygen-oxygen transfer integral causing a large ( $O_{2p}$ ) band width; the copper-oxygen ( $x^2-y^2$ ) transfer integral is large;
5. The copper-copper antiferromagnetic superexchange is also large.

### 3. Model Hamiltonians

As far as the  $CuO_2$  planes in the high- $T_c$  compounds are concerned, the general consensus now is that a natural model with which one can start to discuss the electronic properties is the suitable extended Hubbard model or the Anderson-lattice-type model. Our main aim will be to find an appropriate model to describe the properties of high- $T_c$  materials, so we consider both of them.

The Anderson-lattice-type Hamiltonian models including the band-structure and correlation effects, connected with charge fluctuation processes /7,8,13/ have the form:

$$H = H_1 + H_2 + V_1 + V_2. \quad (I)$$

Here  $H_1$  is the Hubbard Hamiltonian of the tight-binding  $d$ -electrons in the Cu-O planes

$$H_1 = \sum_{i\zeta} \epsilon_{i\zeta} a_{i\zeta}^\dagger a_{i\zeta} + \sum_{ij\zeta} t_{ij} a_{i\zeta}^\dagger a_{j\zeta} + \frac{1}{2} U \sum_{i\zeta} n_{i\zeta} n_{i-\zeta}, \quad (2)$$

where  $i$  labels the copper atomic site,  $\zeta$  is the spin,  $a_{i\zeta}$  is the annihilation operator for an electron,  $\epsilon_{i\zeta}$  is the site energy measured from the chemical potential  $\mu$ ,  $t_{ij}$  is the transfer integral and  $U$  is the on-site Coulomb repulsion.  $H_2$  is the Hamiltonian for the oxygen 2p band electrons

$$H_2 = \sum_{k\zeta} E(k) C_{k\zeta}^\dagger C_{k\zeta} \quad (3)$$

$V_1$  is the hybridization term

$$V_1 = V_0 \sum_{i\zeta} (a_{i\zeta}^\dagger C_{i\zeta} + C_{i\zeta}^\dagger a_{i\zeta}). \quad (4)$$

The last term  $V_2$  describes the intersite Coulomb interaction

$$V_2 = \sum_{ij\zeta\zeta'} \left\{ V_{ij}^{cc} n_{i\zeta}^c n_{j\zeta'}^c + V_{ij}^{aa} n_{i\zeta}^a n_{j\zeta'}^a + V_{ij}^{ca} n_{i\zeta}^a n_{j\zeta'}^c \right\}. \quad (5)$$

The above Hamiltonian consists of those terms which are of importance in influencing qualitatively the physical properties of the studied systems.

Moreover, as the first step, a large part of the current theoretical activity dealing with high-temperature superconductors focuses on the properties of the Hubbard one-band Hamiltonian or a suitably extended Hubbard Hamiltonian. In the past two years it has become widely accepted that the copper oxides must almost certainly be best described as strongly correlated systems. A strong coupling point of view involving charge and spin fluctuations within a two-band extended Hubbard model has been recently proposed by many authors /5-7,12-23/.

Here we consider a radical but hopefully compelling physical picture introduced by Emery /16/. Emery has proposed that an appropriate description of this system is provided by a suitably extended Hubbard model that allows for motion of holes in both copper 3d and

oxygen 2p states. It was shown that, for one hole per unit cell, the holes are largely at the copper sites and the system is an antiferromagnetic insulator. Added holes go onto oxygen sites and are superconducting in virtue of the magnetic coupling mediated by copper spins. Originally, the properties of the model were worked out for intermediate coupling<sup>/16/</sup>. In the following paper<sup>/17/</sup> the model and the mechanism for superconductivity have been elaborated in the strong-coupling limit.

The Emery Hamiltonian is given by<sup>/17/</sup>

$$H = \sum_{ij\delta} \epsilon_{ij} a_{i\delta}^{\dagger} a_{j\delta} + \frac{1}{2} \sum_{ij\delta\delta'} U_{ij} a_{i\delta}^{\dagger} a_{i\delta} a_{j\delta'}^{\dagger} a_{j\delta'} \quad (6)$$

where  $i$  is  $(m,n)$  for a copper site and  $(m+1/2,n)$  or  $(m,n+1/2)$  for an oxygen site. The vacuum consists of  $\text{Cu}^+$  (all 3d states occupied) and  $\text{O}^{2-}$  (all 2p states occupied), and the  $a_{i\delta}^{\dagger}$  creates holes of spin  $\delta$  in copper 3d ( $x^2-y^2$ ) orbitals or oxygen 2p<sub>x</sub> or 2p<sub>y</sub> orbitals. It is assumed that a factor  $(-1)^{m+n}$  is absorbed into the  $a_{i\delta}^{\dagger}$  for copper and oxygen creation operators in a cell  $m = (m,n)$  to take account of signs in hopping integrals. The site-diagonal terms  $(\epsilon_{ii}, U_{ii})$  are  $(\epsilon_p, U_p)$  and  $(\epsilon_d, U_d)$  for O 2p and Cu 3d states, respectively. There is an interaction  $U_{ij} = V$  between holes at neighbouring Cu, O sites. It is assumed that there is a hopping integral  $\epsilon_{ij} = t$  between Cu-O neighbours. In principle, there is also a direct oxygen-oxygen hopping  $t_p$  but, for the sake of simplicity, it has been ignored, since a reasonable tight-binding fit to the band structure may be obtained with a negligible value of  $t_p$ .

The type of question which becomes particularly interesting now is: How strongly are electrons correlated in the high- $T_c$  superconducting materials? Estimations have been performed in a few papers<sup>/12, 18-20/</sup>. Emery<sup>/17/</sup> has assumed  $t \approx 1$  eV,  $U_p \approx 5-7$  eV and  $U_d \approx 8-10$  eV, which together imply  $\Delta = \epsilon_p - \epsilon_d = 1-2$  eV. The magnitude of  $V$  is taken as a fit parameter. It is worth noticing that Hamiltonian (6) must also include a direct ferromagnetic exchange  $J \approx 0.2-0.5$  eV between holes at neighbouring Cu and O sites. This term will be considered later.

#### 4. Effective Hamiltonians

In this section, we discuss how the initial model Hamiltonians of the one-band Hubbard model, periodic Anderson model or the Emery model must be transformed to new effective Hamiltonians in order to

clearly bring out the possible superconducting mechanism which is intrinsic of the models.

It is known<sup>/6,12/</sup> that the effective Hamiltonian for the one-band Hubbard system in the large  $U/t$  limit is given by

$$H^{\text{eff}} = -\frac{t^2}{2U} \sum_{ij} (1 - \vec{\delta}_i \cdot \vec{\delta}_j). \quad (7)$$

For a two-dimensional case, the Neel-type state which corresponds to orientations of the magnetic moment, such that number of antiparallel pairs is maximum, has the energy for this configuration per atom

$$E_N = -\frac{4t^2}{U}. \quad (8)$$

For the triangular structure where the spins on each sublattice form  $120^\circ$  angles with the spins on the other two sublattices the corresponding energy per atom is<sup>/6,12/</sup>

$$E_T = -\frac{9t^2}{2U}. \quad (9)$$

So the Neel state is not the correct ground state for system (7). At any finite temperature the system described by (7) exhibits no long-range order and the phase transition to an ordered state is then only truly possible at  $T = 0$ . Anderson<sup>/6/</sup> has suggested that the behaviour of this system can be well described within a resonance-valence-bond concept.

Cyrot<sup>/21/</sup> has put forward a similar approach starting from a degenerate Hubbard model. In the strong correlation limit he derived an effective Hamiltonian quite similar to (7). In the case of orbital degeneracy, however, the corresponding energy resulting from the virtual transition of the  $d$ -electrons to neighbouring sites, depends not only on the magnetic structure, but also on the particular orbitals that are occupied at the neighbouring sites.

Two models of interacting fermions, the Hubbard and Anderson models, have much in common<sup>/12,14,22/</sup>. For the Anderson lattice Hamiltonian<sup>/14,23/</sup> with the aid of a canonical perturbation expansion it is possible to construct an effective Hamiltonian which replaces interconfigurational hopping processes by effective interactions. In the second order this method gives<sup>/23/</sup>

$$H^{\text{eff}} = J_1 \sum_{ijj'} V_{ji} V_{ij'} [S_i^z (a_{j\uparrow}^+ a_{j'\uparrow} - a_{j\downarrow}^+ a_{j'\downarrow}) + S_i^z (a_{j\downarrow}^+ a_{j'\downarrow} - a_{j\uparrow}^+ a_{j'\uparrow}) + S_i^- a_{j\uparrow}^+ a_{j'\downarrow} + S_i^+ a_{j\downarrow}^+ a_{j'\uparrow}] + J_2 \sum_{ijj'_2} V_{ji} V_{ij'_2} a_{j_2}^+ a_{j'_2} \quad (10)$$

In the charge transfer regime, spins are localized at copper atoms and doping creates holes in oxygen 2p orbitals. There are two transitions which change the configuration of a single copper atom. The first transition is from a copper site to one of the surrounding oxygen atoms. The second transition is from an oxygen atom to a copper atom. These transitions are characterized by the energy difference  $\Delta$  and  $U - \Delta$ , respectively. Thus we have

$$J_1 = \left( \frac{1}{\Delta} + \frac{1}{U - \Delta} \right); \quad J_2 = \frac{1}{2} \left( \frac{1}{\Delta} - \frac{1}{U - \Delta} \right). \quad (11)$$

The operator  $a_{i_2}^+$  creates a hole in the p (x or y) orbital at an oxygen site;  $V_{ij}$  describes the d-p hybridization; the energy scale is defined by two parameters, the charge transfer energy  $\Delta = \epsilon_p - \epsilon_d$  and the Coulomb integral  $U$  for the copper 3d( $x^2 - y^2$ ) orbital. Depending on their values, various physical regimes can be described. At the present time the experimental data give evidence that in high  $T_c$  copper oxides  $U > \Delta$ . Zhang and Rice<sup>/24/</sup> in detail examined the case that  $U > \Delta$ . In the atomic limit, additional holes sit either at copper sites if  $\epsilon_p > U$  or at oxygen sites if  $\epsilon_p < U$ . In the first case, the hybridization may be included by eliminating oxygen sites to give an effective Hamiltonian for motion on copper sites alone. In the second case, it is not so apparent that one can eliminate the oxygen sites. In paper<sup>/24/</sup> it has been shown that the physics of the  $\text{CuO}_2$  layer in the second case is also described by the single-band effective Hamiltonian.

For the case  $2\Delta = U$  one can obtain from the two-band d-p model (2-4)<sup>/25/</sup>

$$H^{\text{eff}} = \sum_{ij_2} T_i^{\uparrow} A_{i_2}^+ A_{j_2} + I \sum_i \vec{\delta}_i^{\uparrow} \cdot \vec{S}_i^d + J \sum_{ij} \vec{S}_i^d \cdot \vec{S}_j^d \quad (12)$$

Hamiltonian (12) is the same as used for describing the kondo lattice systems and magnetic semiconductors<sup>/26/</sup>, however the physics involved is somewhat different.



An effective Hamiltonian for the Emery model (6) can be obtained by eliminating the available copper 3d states<sup>/17/</sup>. Then the effective Hamiltonian for a single added hole is

$$\begin{aligned}
 H_{\text{eff}}^E = & (t_1 + t_2) \sum_{\substack{m \neq \delta' \\ f \neq f'}} a_{m\delta'}^+ a_{m\delta} a_{m+f,\delta}^+ a_{m+f,\delta'} + \\
 & + t_2 \sum_{\substack{f \neq f' \\ m\delta}} a_{m+f,\delta}^+ a_{m+f,\delta'} + \\
 & + J \sum_{fm} (\vec{S}_m \cdot \vec{S}_{m+f} - 1/4) n_{m+f} - 2 \Delta E_c.
 \end{aligned}
 \tag{13}$$

Here the position index  $i$  defined in (6) equals  $m$  for a copper site at the corner of a cell and  $m+f$  for an oxygen site displaced by a distance  $f$   $(\pm 1/2, 0)$ ,  $(0, \pm 1/2)$  in one of the four directions;  $n_{m+f}$  is the occupation number at the site  $m+f$  and  $\Delta E_c$  is the change in the self-energy of a single copper hole in the presence of the oxygen hole. The following notation has been introduced:

$$t_1 = \frac{t^2}{\Delta} \quad ; \quad t_2 = \frac{t^2}{(u_d - 2V - \Delta)} \quad ; \tag{14}$$

$$J = \frac{2t^2}{\Delta + u_p - V} + \frac{2t^2}{u_d - 2V - \Delta} - J_D \quad ; \tag{15}$$

The results presented in this chapter are related to many other papers, where effective Hamiltonians have been derived. It is worth noticing that one can obtain more rich effective Hamiltonians. For example, in paper<sup>/27/</sup> a fourth-order Hamiltonian has been obtained which contains spins, charge and excitonic correlations.

### 5. Coexistence of Spin and Carrier Systems

Since an honest theoretical treatment of the obtained effective Hamiltonians is very complicated, perhaps it is instructive to look again at the physics involved. Recently, a very detailed analysis of

the questions of valency, correlation, magnetism and the nature of the charge carriers in the high- $T_c$  superconductors has been given in paper<sup>/28/</sup>. It has been argued that intra-atomic Coulomb interactions for a  $\text{CuO}_2$  sheet are large, but interatomic Coulomb terms and direct oxygen-oxygen transfer integrals are also very important. Itinerant carriers exist on the oxygen sublattice because of the large copper  $U_d$  energy. A spin  $-1/2$  Heisenberg system exists independent of the presence of carriers due to a poor screening in these materials. The copper-copper superexchange energy  $J$  is relatively large. The coexisting spin and carrier systems interact strongly, the most important cause being a virtual process involving the  $\text{Cu}(d^{10})$  configuration, which is lowered in the relative energy by Coulomb interactions with the carrier. Stechel and Jennison<sup>/28/</sup> believe that this process can produce a carrier transport with and without creating spin deviations and stabilizes holes in the oxygen  $p\delta$  orbitals. They claimed that the carriers are neither weakly coupled free particles nor spin polarons, but are something new: "spin hybrids", consisting of a coherent and nonperturbative mixture of local spin-orbital electronic configurations, some of which represent deviations in the local antiferromagnetic order.

The Hamiltonian suggested on the basis of the above consideration is a two-band (for the copper and oxygen sublattices) extended Hubbard model<sup>/28/</sup>

$$\begin{aligned}
 H = & \sum_{i\delta} \epsilon_i n_{i\delta} + \frac{1}{2} \sum_{i\delta} U_i n_{i\delta} n_{i-2} + \sum_{ij\delta\delta'} V_{ij} n_{i\delta} n_{j\delta'} + \\
 & + \sum_{ij\delta} t_{ij} (a_{i\delta}^\dagger a_{j\delta} + \text{h.c.}) + \sum_{ij\delta\delta'} I_{ij} a_{j\delta'}^\dagger a_{i\delta} a_{i\delta}^\dagger a_{j\delta} ,
 \end{aligned}
 \tag{16}$$

where  $a_{i\delta}^\dagger$  creates a hole of spin  $\delta$  at a site  $i$  in the otherwise filled Cu ( $x^2-y^2$ ) and O ( $x$  or  $y$ ) level.

Charge carriers are introduced when the number of holes increases beyond one per unit cell. To describe superconductivity, it is necessary to derive the Hamiltonian for carrier holes coexisting and strongly interacting with the copper spin system. A formal definition of the spin-hybrid carrier Hamiltonian leads to the following expression<sup>/28/</sup>

$$H_{\text{eff}} = H_{\text{eff}}^1 + H_{\text{eff}}^2 ,
 \tag{17}$$

where  $H_1$  is a modified Heisenberg Hamiltonian to allow blocking of superexchange due to the presence of carriers

$$H_{\text{eff}}^1 = 2J \sum_{lh} (1 - N_{eh\uparrow})(1 - N_{eh\downarrow}) \vec{S}_{eA} \cdot \vec{S}_{e+h, B}, \quad (18)$$

where  $N_{eh\uparrow} = a_{eh\uparrow}^\dagger a_{eh\uparrow}$  is the number operator for holes at the oxygen site  $lh$  which sits between a copper at  $lA$  and at  $l+h B$ .

The carrier spin-coupling Hamiltonian is

$$H_{\text{eff}}^2 = 2I_{\text{eff}} \sum_{lh} \vec{S}_{eh} \cdot (\vec{S}_{eA} + \vec{S}_{e+h B}), \quad (19)$$

where  $S_{eh}$  is the spin operator for a hole at the oxygen site  $lh$ . The physical meaning of the "spin hybrid" is not very clear. The author's view of this spin hybrid is that if a spin-up hole is added to the system, the resulting quasiparticle is a linear combination of a spin-up hole and a spin-down hole on the oxygen sublattice. This is the origin of a specific interest of the model. Unfortunately, the main question whether the correlated or superconducting state will be the lowest in energy at any given density has not been solved for the model. However, a central result of the above investigation /28/ that a poor screening exists on a  $\text{CuO}_2$  sheet due to the nearly-filled-shell nature of the copper and oxygen ions and that this leads to significant intra-atomic and interatomic screened Coulomb interactions between quasiparticles is very interesting and important.

## 6. Magnetic Polarons and High-Temperature Superconductivity

An important practical consequence of the above results is that the spins and carriers in the copper oxides are coupled in a very nontrivial way. However, we lack a rigorous foundation of the problem. Here we attempt to give a flavor of the arguments which seem to support the spin-polaron pairing mechanism in the copper oxides.

Let us consider the Emery model (6). As the first step, one can consider only the second-order processes and neglect the fourth-order terms that lead to the copper-copper exchange. The parameters /17/ of Hamiltonian (13) have been chosen so that the background of copper holes is stable when an additional hole is added, which will reside primarily on the oxygen sites. This hole will hop from site to site; it does not hop as a bare carrier, however, but as a dressed object, polarizing the surrounding spins. This situation resembles the case of the magnetic semiconductors where under various regimes the bare carriers can be greatly renormalized and the relevant true

carriers must be considered. Investigations of the magnetic polarons /26/ permit us to clarify the nature of the true carriers at low temperatures. The physics may be clarified by dividing the Hamiltonian into two parts, a site diagonal term and a hopping term as in Eq. (13). The site diagonal term, for a single hole located in either the x or y bonds of the unit cell is /17/

$$V_1 \sim \int \vec{b} \cdot (\vec{S}_1 + \vec{S}_2). \quad (20)$$

where  $\vec{b}$  is the spin of the oxygen hole and  $\vec{S}_1$  and  $\vec{S}_2$  are the spins on the neighbouring copper holes. When the hopping terms are included, the oxygen hole is free to move through the lattice. An accurate calculation of the hopping of the quasiparticle on the antiferromagnetic background has not been done. A number of theoretical models /29-34/ have been proposed recently to include the spin-polaron pairing for describing the high-temperature superconductivity. Emery's scenario /17,35/ claims that the dominant magnetic attraction comes from the enhanced superexchange when the oxygen holes are separated by an intervening oxygen site. The S-state pairing with  $T_c$  proportional to the Fermi temperature /17/

$$T_c \sim 4.52 \bar{t} k_F^2 a^2 \exp \left[ \frac{4\pi \bar{t}}{\lambda e(k_F)} \right]$$

is produced not only by an enhancement of superexchange interactions but also by zero-point kinetic energy and is characterized by a time scale which is short compared to that of the electronic motion. The enhancement of the interactions is a consequence of the inclusion of extended range interactions into a Hubbard model.

An interesting proposal has been made by Kamimura /34/, who has first pointed out that the inclusion of two bands of  $d(x^2-y^2)$  and  $dZ$  types interacting by the Hund's coupling as well as the electron correlation could play an important role for high-temperature superconductivity. He has shown that the interplay of Hund's coupling and superexchange interactions between holes in the  $d(x^2-y^2)$  band gives rise to an effective attractive interaction between spin-polarons created in the  $dZ$  band by doping. When a certain number of spin-polarons are created, they form spin-singlet pairs. These spin-polaron pairs are boson-like particles constructed from fermions, and the Bose-Einstein condensation occurs below a condensation temperature.

## 7. Conclusions

To summarize the results reported here, we illustrate the fact that it is possible to construct realistic models which are suitable for describing, at least partly, the properties of the superconducting copper oxides. The central question is whether this physical picture survives a rigorous quantitative analysis. It is highly desirable to get an exact formulation of the spin-polaron mechanism of the high temperature superconductivity. However, actual explicit calculations that have been performed up to now have with necessity mostly been made for oversimplified models and, of course, give only sketchy ideas about relevance of the spin-polaron mechanism. From a theoretical point of view, one must incorporate into this picture the phonon subsystem. Such an attempt has been made in recent paper<sup>/36/</sup>, where a new theoretical model trying to explain the high-temperature superconductivity in oxides has been proposed. It has been shown that when holes are introduced into the  $\text{CuO}_2$  planes, immobile ferromagnetic clusters are formed. There is a certain analogy of the ferromagnetic holeclusters considered in article<sup>/36/</sup> with ferron states of electrons in three-dimensional antiferromagnetic semiconductors. So, the question about the true nature of carriers in the copper oxides arises again. We hope that our analysis may be useful in further studies of the role of antiferromagnetic correlations. Much remains to be done before one may claim to have a fully settled theory of the high-temperature superconductivity.

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Спиновые и электронные корреляции в окислах меди и их значение для высокотемпературной сверхпроводимости

Рассмотрен вопрос о том, какую роль играют спиновые и электронные корреляционные эффекты в специфическом характере сверхпроводимости в окислах меди. Показано, что спиновые степени свободы и носители тока взаимодействуют друг с другом весьма нетривиальным образом. Приведены аргументы в пользу того, что в окислах меди может осуществляться магнитополяронный механизм сверхпроводимости.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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Kuzemsky A.L.

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Spin and Electron Correlations in the Copper Oxides and Their Role for High Temperature Superconductivity

The problem has been discussed of how the electron and spin correlation effects can be involved in the specific character of superconductivity in the copper oxides. It is shown that the spins and carriers in the copper oxides are coupled in a very nontrivial way. The arguments which seem to support the spin-polaron pairing mechanism in the copper oxides have been presented.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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