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Electronic Models of High-T_c Superconductors

I. Sega
J.Stefan Institute, E.Kardelj University of Ljubljana
61111 Ljubljana, Yugoslavia

A brief rewiev is given of some current proposals to explain the newly discovered high temperature superconductivity in copper oxides.

Since the discovery of superconductivity (SC) in Ba-doped La_2CuO_4 by Bednorz and Müller announced in January 1986 /1/, the scientific community has witnessed an unprecedented boom in the activity on any subject so far. The follow-up experiments performed in other centres soon confirmed their results. Moreover, the T_c was even pushed up by substituting Sr for Ba and by subjecting the material to high pressure /2/. The excitement culminated in the discovery of the ("second generation") SC material $YBa_2Cu_3O_7$ /3/ with T_c as high as 92 K. Furthermore, recently a whole new class (the "third generation") of high-T_c superconducting oxides were discovered with the record-breaking $Tl_2Ba_2Ca_{n-1}Cu_nO_y$ compound reaching the critical temperature of 125 K /4/. It goes without saying that in these three years an enormous body of experimental work has been published /5/ from which some common features in the physical properties of these materials emerge: all materials have strong two-dimensional anisotropy in crystal structure as well as in physical properties, the carrier concentration is much lower than in ordinary SC and can be controlled by changing the component elements. Morover in the limit of low carrier concentration the semiconductor phase exists and by now it is well established that it is antiferromagnetically (AF) ordered /6/.

From the theoretical point of view it appears that we are still rather far from understanding the underlying mechanism of high-T_c SC in these materials. The theories which have been proposed /5, 7/, can be devided mainly into two groups: a) the weak coupling models and b) the theories based either on strong electron-phonon coupling or

The common feature of many of the theories is that they assume the validity of the classical, BCS scenario for SC, and seek for a mechanism that would raise the SC transition temperature T_c according to the well known formula of this theory:

$$k_B T_c = \Theta exp(-1/\lambda_{eff}), \tag{1}$$

where Θ is the characteristic energy scale for the attraction between electrons near the Fermi surface and $\lambda_{eff} = VN(0) \ll 1$. $N(0)$ is the density of electron states at the Fermi level and V measures the interaction strength. As is well known, the conventional phonon mechanism gives rise to $T_c \leq 20 - 30$, which had been considered the highest attainable T_c before the advent of new SC copper oxides, especially in view of years of failure in search for SC materials with T_c exceeding this limit. But in principle there are no restrictions imposed on the value of T_c /8/, especially if one consideres mechanisms other then the (normal) phonon mechanism. Thus an increase in the density of states at the Fermi surface, induced for example by the proximity to some structural (or other) instability /10/, can, according to the BCS formula, result in higher SC transition temperature. Other mechanisms to raise T_c are also possible, based, e.g., on excitonic mechanism /8, 11/ or on formation of bipolarons /12/, or still other mechanism resulting from an exchange of excitations other then phonons (e.g. magnons). [Note that in some cases the coupling need not be weak.]

A different approach , first emphasized by Anderson /13/, views the superconductivity in layered cuprates as a new, i.e., non BCS-type electronic system, where strong correlation among electrons plays a particular role.

To better understand this issue one should look at the electron structure of the layered copper oxides, the symplest of them being $La_{2-x}Sr_xCuO_4$. The CuO-octahedron in pure La_2CuO_4 (see figure) is stretched along the c-axis due to cooperative Jahn-Teller effect, with both appex oxygens having little (or no) effect on the distribution of charge in the CuO planes. In the plane there is strong hybridization between the Cu $3d_{x^2-y^2}$ and O $2p_{x,y}$ orbitals of adjacent oxygens, resulting in the two bands, the bonding (lower) and the antibonding (upper) band with

a number of nonbonding, almost dispersionless bands in between, which are believed to be unimportant. Since in the ground state there is one hole/Cu (relative to a filled shell $(3d^{10}, 2p^6)$ configuration) the antibonding band of pure La_2CuO_4 is exactly half-filled, which should give a metal. It is instead a semiconducting AF with the bulk $T_N \approx 230K$.

The symplest model to describe the underlying physics is the 1-band Hubbard

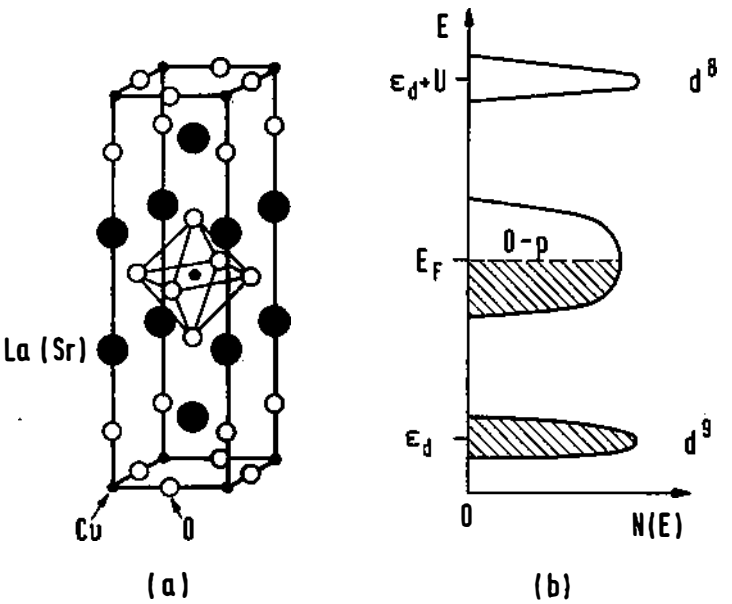

Fig. 1. a) Structure of the $La_{2-x}Sr_xCuO_4$ compound; b) structure of electronic bands in hole representation (schematically). d^9 and d^8 bands pertain to copper and U is the on-site Coulomb repulsion.

model

$$H_{\mathrm{Hubb}} = -t \sum_{<ij>,s} c^{\dagger}_{is} c_{js} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \tag{2}$$

where the kinetic energy of the antibonding band is represented by the first sum and the second part of H in (2) takes care of the strong Coulomb on-site repulsion between holes. In spite of its apparent simplicity it is a nontrivial model, depending on t/U and the concentration of holes. From experimental evidence it is known that $t \ll U$, so that charge fluctuations must be strongly suppresed. Indeed, in this limit the double occupancy occurs only as a virtual fluctuation and can be eliminated to leading order in t/U to result in the effective 1-band Hubbard model (the so-called $t-J$ model):

$$H_{tJ} = -t \sum_{<ij>,s} d^{\dagger}_{is} d_{js} + \frac{4t^2}{J} \sum_{<ij>} \left(\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j \right), \tag{3}$$

where the Heisenberg-like spin-exchange interaction $J = 4t^2/U$ is responsible for the AF ordering already mentioned above. Here the operators d_{is}, $d^{\dagger}_{is}$ act on a subspace

with no doubly occupied sites. A more realistic model first introduced by Emery /14/ allows for a more complete treatment of distribution of charge among the Cu– and O–sites and was proposed to take account of the experimental fact that on doping the additional holes go onto the $2p$-orbitals of the oxygen atoms. However the 5-dimensional parameter space represents a tremendous obstacle to even the simplest analysis of the model. Moreover it is not at all clear wheather this model brings any new physics in comparison to the effective 1-band model (3). In fact, some recent results on the latter model /15/ are quite encouraging with respect to our understanding of SC and magnetism in these materials. It is also to be noted that under certain assumptions the more complicated model can be reduced to the $t-J$ model/16/, but other effective 1-band Hamiltonians, e.g. the Kondo-lattice model /17/, can also be obtained . Quite recently a comparison between the more general model and several effective 1-band models has been given /18/. The recent dicovery of the SC compound $Nd_{2-x}Ce_xCuO_4$ with electrons as charge carriers /19/ sheds some doubt on the validity of the 2-band model, which does not show the electron-hole symmetry implied by this latest discovery. Thus in the rest of our discussion we shall limit ourselves to the $t-J$ model only.

The $t-J$ model has been extensively studied in two dimensions. Due to exclusion of doubly occupied sites it is a 3-states/site problem and is therefore also suitable for numerical calculations. As the model correctly describes the appearance of AF ordering at half filling, the next question to ask is: what happens if we add holes, i.e. dope the system? One immediate difficulty emerges. The AF ordering of copper spins in the CuO planes is according to the theorem of Mermin and Wagner /20/ not possible at any finite temperature, so that the observed ordering in the La-compound must be a trully three-dimensional phenomenon. This does not mean that there can be no short rang AF order within the planes. Indeed, such ordering has been found to exist even well beyond the bulk transition temperature T_N . Even as doping reduces T_N to zero they do not vanish. On the other hand there is still no proof that there is long range order at $T=0$ either, although numerical results on finite systems, extrapolated to the thermodynamic limit, give a nonzero value for the staggered magnetization $m_{stag} \approx 0.3$ /21/. This subtle nature of the spin $S=\frac{1}{2}$ AF ordering within CuO planes has led Anderson /13/ to propose that it is a resonating valence bond (RVB) state in which pairs of spins are coupled into singlets with all posible spin pairings allowed. Upon doping two types of low lying elementary excitations appear: holons (bosons) of charge $+e$ and charge zero spinons with $S=\frac{1}{2}$ /22/. In this theory SC appears through condensation of holon-pairs whereas the spinon degrees of freedom give rise to some of

the experimentally observed features /23/. The bulk SC is realized through hopping of holon-pairs between copper plains, which makes it sensitive to interlayer distance, contrary to experiment.

In a number of alternative approaches to the possible SC in the $t - J$ model, the question of binding of holes has been addressed. In particular Bonča et al. /24/ have numerically studied one and two holes in a cluster of sixteen cells. Combining results from pair-binding energy and hole-density correlations they present evidence that two holes bind already for moderate exchange energy J even in the anisotropic limit. For one hole analytical results within a semiclassical mean field theory /25/ show that a long range dipolar distortion arround a hole forms, which enables the hole to delocalize. It also appears that in this model the pairing tendency has a *d*-wave symmetry /24, 26/. Although the experimental results are not yet conclusive, recent experiments on magnetic-flux quantization in a composite ring add evidence in favour of *s*-wave symmetry. Further progress may clarify this and other problems and hopefully add to the credibility of the $t - J$ model as the key to high-T_c superconductivity.

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