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MAGNETIC INTERACTIONS IN HIGH-T_c SUPERCONDUCTORS

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Abstract. – The failures of the band theory to stabilize the observed antiferromagnetic ground state in La_2CuO_4 are analyzed based on our understanding of the Mott insulators and of the heavy fermion superconductors. Assuming that the superconducting transition occurs through Bose condensation in the two-dimensional $Cu - O_2$ planes, we present physical arguments that the metallic nature of the planes between $Cu - O_2$ layers may enhance T_c significantly.

In view of the many proposals that high temperature superconductivity may be due to magnetic interactions, it is important to understand the nature of the antiferromagnetic (AFM) correlation which has been observed in both La_2CuO_4 and $YBa_2Cu_3O_6$. We have calculated the spin-polarized band structure of La_2CuO_4 using the LMTO method [1]. Both ferromagnetic (FM) and AFM band structures were found to be *unstable*. The conclusions are similar to an earlier calculation of Leung *et al.* [2] for Sc_2CuO_4. However, they have shown that the AFM state could be stabilized if degenerate bands at the Fermi energy were lifted by the AFM moment, and only the lower of these two bands were preferentially occupied. Applying this approach in a series of super cell calculations, we find AFM strongest in stoichiometric La_2CuO_4 where the antibonding pdσ band is exactly half-filled. Shifting the Fermi energy away from the half-filled limit, either by Ba or Sr doping or by oxygen vacancy, suppresses antiferromagnetism. These conclusions are consistent with our quantum Monte-Carlo simulations of a two-dimensional extended Hubbard model on a square lattice with one copper- and two oxygen-atoms per unit cell [3]. In the half-filled limit, we found strong AFM correlation with appreciable singlet pairing among Cu atoms, using parameters comparable to band structure calculations. Away from the half-filled limit, we found the long range AFM order gradually suppressed, which is in agreement with our band structure prediction. The failure of the band theory to stabilize the observed AFM ground state indicates an inadequacy of the local spin density approximation in describing the intra atomic Coulomb repulsion U.

The situation is somewhat similar to the Mott insulators which represents one of the most dramatic failures of the local density band theory. It has been shown by Terakura *et al.* [4] that the AFM ground states are obtained by the band theory; but in the case of FeO or CoO the observed insulating gaps were not obtained, and in the case of NiO they are an order of magnitude too small. The mechanism for the breakdown of the local-density band theory in the Mott insulators has recently been reviewed by Brandow [5]. Because of crystal field splitting of the 3d states, the different orbital exchange parameter J can be much smaller than the self-exchange parameter U. Orbital dependence of the exchange and correlation potential is neglected in the local-spin-density approximation, which amounts to averaging over these two very different quantities. It thereby missed the main point of the Mott picture, namely, that the unoccupied orbital lies above that of an occupied orbital by an amount of order U. The problem is greatly reduced in wide-band materials where U is strongly screened so that the mechanism for the Mott splitting is weakened. In the case of the monoxides, the O-p states lie significantly lower in energy than the transition metal 3d states so that the overall band width W is smaller than U. In the high T_c superconductors, $E_d \cong E_p$ which leads to a rather large band width ($W \geq 9$ eV) [6]. Nevertheless, the system is near a metal-insulator transition so that the screening is not very effective.

In the limit of strong electron-electron correlation (large U), there could be additional many-body corrections to the band structure due to charge or spin fluctuations. This is best illustrated in the case of heavy fermion superconductors, which are characterized by extremely large values of the linear coefficient of the specific heat and of the magnetic susceptibility, which is interpreted as implying fermionic quasiparticles bearing a very large effective mass m^* at low temperature. By contrast, values of m^* deduced from transport measurements are not significantly enhanced, which suggested that the energy dependence of the self-energy may dominate its momentum dependence [7]. In this case, it can be shown that the Fermi surface will not be affected by the mass enhancement, and indeed our theoretical Fermi surface [8] was confirmed by experiment [9]. As the temperature is raised, m^* rapidly decreases to normal values. This suggests that the self-energy corrections diminish rapidly away from the Fermi energy, and explains the good agreement between the band structure and angle resolved photo emission for UPt_3 even for f-states that lie within 0.1 eV from E_F (m^* is a factor of 21 larger than the band mass) [10]. The magnetic fluctuations

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responsible for the mass enhancement in the thermodynamic measurements may also be the pairing mechanism for its superconductivity. Our recent quantum Monte-Carlo simulations [11] of a two-dimensional Anderson lattice showed strong AFM correlation above the single-impurity Kondo temperature (T_K). Below T_K, both the local moments and the AFM correlations are suppressed, and in some cases FM correlations start to develop. While AFM correlations favor nearest neighbor anisotropic singlet pairing, the FM correlations could support p-wave triplet-pairing superconductivity. The transformation from AFM to FM correlations can be understood based on the temperature dependence of the mass enhancement. In the case of high T_c superconductors, the experimental measured values for m^* ranged from a factor of 1 to 4 when compared with the band masses [12]. Thus, the role of the magnetic fluctuations in these compounds remains unclear.

The recent discovery of high temperature superconductivity in bismuth and thallium based copper oxides has provided new insight into the mechanism of superconductivity. The superconducting transition temperatures depend strongly on the number of $Cu-O_2$ layers in the unit cell; for example, $Bi_2Sr_2CuO_6$ (2201) which has only one $Cu-O_2$ layer has a comparatively low T_c of about 6-22 K while the two-layer compound $Bi_2Sr_2CaCu_2O_8$ (2212) superconducts at 84 K. Comparing the band structures, we find that the high T_c compound has Bi-p bands crossing the Fermi energy so that the Bi-O planes which lie between the $Cu-O_2$ layers are metallic while in the low T_c compound the Bi-O layers are nearly insulating [13]. Since the chain layers between the $Cu-O_2$ planes in the 123 compound are also metallic, we propose that the presence of these metallic layers between the $Cu-O_2$ planes plays an important role in determining T_c. In this picture, we assume that the superconducting transition occurs through Bose condensation of quasi- particles in the two-dimensional $Cu-O_2$ layers. This transition cannot be entirely two-dimensional, since fluctuations prevent the transition from occurring at a finite temperature. Table I shows the experimentally measured coherence lengths normal to the $Cu-O_2$ planes, ξ_c, and the $Cu-O_2$ interlayer spacing, d_{Cu_Cu} for the 214, 123 and 2212 systems. In $La_{2-x}Sr_xCuO_4$, where there is no metallic layer between the $Cu-O_2$ planes, the coherence length is long enough to allow supercurrent to flow directly between the layers, but in $YBa_2Cu_3O_7$ and $Bi_2Sr_2CaCu_2O_8$, ξ_c is shorter than the distance between the two $Cu-O_2$ planes. In both cases, however, ξ_c is comparable to the distance d_{Cu_M} from the $Cu-O_2$ layer to the metallic chain layer or Bi-O plane, so the supercurrent could then flow between $Cu-O_2$ layers by taking advantage of the metallic states on the intervening layers, essentially hopping from copper-oxygen layer to copper-oxygen layer by resonant tunneling through the metallic interlayer.

Table I. – *Interlayer separations and coherence lengths (in Å) for a number of high temperature superconductors.*

	d_{Cu_Cu}	d_{Cu_M}	ξ_c
$La_{2-x}Sr_xCuO_4$	6.6	–	7 – 13
$YBa_2Cu_3O_7$	8.2	4.1	4.8 – 7.0
$Bi_2Sr_2CaCu_2O_8$	12.1	4.4	4.0
$Bi_2Sr_2CuO_6$	12.3	4.5	–

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