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ELECTRON ENERGY SPECTRUM AND MAGNETIC INTERACTIONS IN HIGH-T_c SUPERCONDUCTORS

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The character of magnetic interactions in La-Sr-Cu-O and Y-Ba-Cu-O systems is of primary importance for analysis of high-T_c superconductivity in these compounds. Neutron diffraction experiments showed the antiferromagnetic ground state for nonsuperconducting La_2CuO_4 and $YBa_2Cu_3O_6$ with the strongest antiferromagnetic superexchange being in the ab plane [1,2]. Nonsuperconducting "1-2 3" system has even two Neel temperatures T_{N1} and T_{N2}. The first one corresponds to the ordering of Cu atoms in the CuO_2 planes, T_{N2} reflects the antiferromagnetic ordering of magnetic moments in CuO chains relatively to the moments in the planes T_{N1} and T_{N2} depend strongly on the oxygen content [3] (T_{N1}=450 K for [illegible] and T_{N2} 80 K, but T_{N1}=230 K and T_{N2}=10 K for x=0.55).

We have tried to describe magnetic interactions in high-T_c superconductors basing on the LMTO band structure calculations. Exchange interaction parameters can be defined from the effective Heisenberg hamiltonian:

$$H_{eff} = -1/2 \sum_{ij} J_{ij} \vec{S}_i \vec{S}_j \qquad (1)$$

When the magnetic moments are not too large, as copper magnetic moments in superconducting oxides, J_{ij} parameters can be defined through the non-local magnetic susceptibility of spin-restricted solution for the crystal [4,5]:

$$J_{ij} = \frac{1}{2} \frac{I_i - I_j}{S_i - S_j} \sum_{LL'} \tau^{ij}_{LL'} \qquad (2)$$

where

$$\tau^{ij}_{LL'} = 1/\pi \int^{E_F} \mathrm{Im}\, G^{ij}_{LL'}(E) \cdot G^{ji}_{L'L}(E)\, dE \quad , \qquad (3)$$

$$G^{ij}_{LL'} = 1/\Omega_{BZ} \int_{BZ} d\vec{k} \sum_n \frac{\psi_{ni}(\vec{k}) \psi^*_{nj}(\vec{k})}{E - E_n(\vec{k})} e^{i\vec{k}\cdot\vec{R}_{ij}} \qquad (4)$$

– is the nondiagonal Green function which can be calculated through the energy spectrum $E_n(\vec{k})$ and $\psi_{nL}(\vec{k})$ of the LMTO-hamiltonian. J_i in formulae (2) is interatomic exchange parameters of atom i. Due to the sharp dependence of nondiagonal Green function $G^{ij}_{LL'}(E)$ on the E the integral (3) should be calculated as contour integral in complex plane.

The results of nonlocal magnetic susceptibility calculations and the values of exchange interaction parameters for La CuO and $YBa_2Cu_3O_7$ systems are given in the Table.

Strong anisotropy of exchange interactions in the ab plane and along the c axis in La_2CuO_4 is obviously seen. The value of Neel temperature found agrees well with the experimental data available. In the $YBa_2Cu_3O_7$ system there is strong antiferromagnetic Cu-O Cu interaction in the CuO_2 plane, which results in antiferromagnetic ground state of $YBa_2Cu_3O_6$. Superexchange of Cu1-O4-Cu2 type is antiferromagnetic also, in accordance with the experiment. Using the simplest mean field approximation $T_N = \frac{1}{3}|J|zS(S+1)$, where z is the number of the nearest magnetic neighbours, it is possible to estimate Neel temperature values. They are T_{N1} = 265-314 K, T_{N2} = 61 K agree well with the experimental data. Large ferromagnetic moment exchange in Cu1-O4-Cu1 chains (which follows from NMR experiments [6] also) does not influence antiferromagnetic ordering, as when δ = 1 all the chaines are broken.

In the planes of "1-2-3"system there are quite strong antiferromagnetic Cu-O and O-O interaction which appear due to holes in oxigen subbands. These results are in line with the magnetic model of oxigen holes pairing in high-T_c superconductors suggested in [7].

We have performed also a number of LMTO spin-polarised calculations for $GdBa_2Cu_3O_6$ and $GdBa_2Cu_3O_7$ both for ferromagnetic and antiferromagnetic ordering of magnetic moments. For antiferromagnetic state the energy gap of 0,04 ev is formed at the Fermi level. Spin splitting of Gd f-states equals to 5 ev, and magnetic moment of Gd atoms is 6.5 μ_B. The estimation of stability parameters [8] leads to the conclusion of more stable antiferromagnetic ordering: the difference of J_0 parameters is 230 K (O_6) and 180 K (O_7). The value of s-f integral in antiferromagnetic phase of $GdBa_2Cu_3O_7$ appears to be about 20 K, and correspond to small changes of T_c when Gd atoms enter the crystal lattice.

Table. Exchange interaction parameters for $YBa_2Cu_3O_7$ and La_2CuO_4 (for s=1/2 and I_{Cu}=0,07 Ry, I_O=0,11 Ry)

pair	$\hat{R}_{ij}$	$\gamma^{ij}_{dd(pp)}$ (mRy^{-1})	J^{ij} (K)
$YBa_2Cu_3O_7$			
Cu2-O2-Cu2	(0 1 0)	-50,8	-157
Cu2-O3-Cu2	(1 0 0)	-42,8	-132
Cu1-O4-Cu2	(0 0 1)	-9,9	-31
Cu1-O1-Cu1	(0 1 0)	72,5	225
Cu2-O2	(0,5 0 0)	112,3	545
O2-O2	(0,5 0,5 0)	35,5	270
La_2CuO_4			
Cu-O1-Cu	(1 0 0)	73,5	227
Cu-O2-Cu	(0 0 1)	-0,45	1,4

REFERENCES

[1] D.Vaknin, S.K.Sinha, D.E.Moncton et.al. Phys.Rev.Lett.58(1987)2301
[2] W.I.F.David, W.T.A.Harrison, J.M.F.Gunn. Nature 327(1987)310
[3] G.Shirane, ICM'88, Paris, Abstracts, p.295
[4] V.A.Gubanov, S.A.Turshevski et.al. Physica C, 153-155(1988)123
[5] K.Terakura, N.Hamada et.al.J.Phys.F.12(1982)1661
[6] B.A.Aleksashin, A.M.Bogdanovich et.al.Pisma v ZETF,48(1988)263
[7] G.Chen and W.A.Goddard, Science 239(1988)899
[8] Liechtenshtein A.I., Katsnelson M.I. et al. JMMM,65(1987)41