ELECTRON ENERGY SPECTRUM AND MAGNETIC INTERACTIONS
IN HIGH-\(T_c\) SUPERCONDUCTORS

S.A. Turshevskii, A.I. Liechtenstein, V.P. Antropov, V.A. Gubanov

Institute of Chemistry and Institute of Metal Physics,
Ural Science Center, Academy of Sciences, Sverdlovsk, USSR

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 \(\text{La}_2\text{CuO}_4\) and \(\text{YBa}_2\text{Cu}_3\text{O}_6\) with the strongest antiferromagnetic superexchange being in the ab plane \([1,2]\). Non-superconducting "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 \([3]\)

\(T_{N1} \approx 450\ K\) for \(x=1\) and \(T_{N2} \approx 80\ K\), but \(T_{N1} = 230\ K\) and \(T_{N2} = 10\ K\) for \(x=0.375\).

We have tried to describe magnetic interactions in high-\(T\) superconductors basing on the LMTO band structure calculations. Exchange interaction parameters can be deduced from the effective Heisenberg Hamiltonian:

\[
H_{\text{ex}} = \frac{1}{2} \sum_{\mathbf{r}_{ij}} \mathbf{S}_i \cdot \mathbf{S}_j
\]

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 \([4,5]\):

\[
J_{ij} = \frac{1}{2} \frac{\mathbf{I}_i \cdot \mathbf{I}_j}{\mathbf{S}_i \cdot \mathbf{S}_j} \sum_{\mathbf{F}_r} \Psi_{\mathbf{F}_r}^{(l)} \Psi_{\mathbf{F}_r}^{(l)} \ \text{Im} \ G_{\mathbf{F}_r \mathbf{F}_r}^{(l)}(E) \ G_{\mathbf{F}_r \mathbf{F}_r}^{(l)}(E) \ dE
\]

where

\[
G_{\mathbf{F}_r \mathbf{F}_r}^{(l)} = \frac{1}{\Omega_{\text{av}}} \int \frac{d^3 \mathbf{k}}{2\pi^2} \sum_{\mathbf{F}_n} \frac{\Psi_{\mathbf{F}_n}^{(l)}(\mathbf{k}) \Psi_{\mathbf{F}_n}^{(l)}(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{r}}}{\mathbf{k} \cdot \mathbf{k}}
\]
- is the nondiagonal Green function which can be calculated through the energy spectrum $K_n(\vec{k})$ and $\gamma_{kl}(\vec{k})$ of the LMT0 hamiltonian. $I_{ni}$ in formulae (2) is interatomic exchange parameters of atom $i$. Due to the sharp dependence of nondiagonal Green function $G_{nl}(\vec{k})$ 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$_2$Cu$_3$O$_7$ systems are given in the Table.

Strong anisotropy of exchange interactions in the ab plane and along the c axis in La$_2$CuO$_4$ is obviously seen. The value of Neel temperature found agrees well with the experimental data available. In the YBa$_2$Cu$_3$O$_7$ system there is strong antiferromagnetic Cu-O Cu interaction in the CuO$_2$ plane, which results in antiferromagnetic ground state of YBa$_2$Cu$_3$O$_6$.

Superechange of Cu1-04 Cu2 type is antiferromagnetic also, in accordance with the experiment. Using the simplest mean field approximation $T_n = \frac{1}{3} |J| z S(S+1)$, 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 Cu1-04-Cu1 chains (which follows from NMR experiments [6] also) does not influence antiferromagnetic ordering, as when $c = 1$ all the chains are broken.

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

We have performed also a number of LMT0 spin-polarised calculations for GdBa$_2$Cu$_3$O$_6$ and GdBa$_2$Cu$_3$O$_7$ 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 $\mu_B$. The estimation of stability parameters [8] leads to the conclusion of more stable antiferromagnetic ordering: the difference of $J_o$ parameters is 230 K ($O_x$) and 180 K ($O_y$). The value of $\Sigma$ integral in antiferromagnetic phase of GdBa$_2$Cu$_3$O$_6$ 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 \( \text{YBa}_2\text{Cu}_3\text{O}_7 \) and \( \text{La}_2\text{CuO}_4 \) (for \( s=1/2 \) and \( t_{\text{Cu}}=0.07 \text{ Ry}, t_0=0.11 \text{ Ry} \))

<table>
<thead>
<tr>
<th>pair</th>
<th>( R_{ij} )</th>
<th>( t_{ij}^{\text{res}} ) (mRy(^{-1}))</th>
<th>( J_{ij} ) (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{YBa}_2\text{Cu}_3\text{O}_7 )</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cu2-02-Cu2</td>
<td>(0 1 0)</td>
<td>50.8</td>
<td>-157</td>
</tr>
<tr>
<td>Cu2-03-Cu2</td>
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<td>-42.8</td>
<td>-132</td>
</tr>
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<td>Cu1-04-Cu2</td>
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<td>-9.9</td>
<td>-31</td>
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<tr>
<td>Cu1-01-Cu1</td>
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<td>225</td>
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<tr>
<td>Cu2-02</td>
<td>(0.5 0 0)</td>
<td>112.3</td>
<td>545</td>
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<tr>
<td>02-02</td>
<td>(0.5 0.5 0)</td>
<td>35.5</td>
<td>270</td>
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<tr>
<td>( \text{La}_2\text{CuO}_4 )</td>
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</tr>
<tr>
<td>Cu 01-Cu</td>
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<tr>
<td>Cu 02-Cu</td>
<td>(0 0 1)</td>
<td>-0.45</td>
<td>1.4</td>
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REFERENCES