High-Tc Superconductors

Discovered in 1986.
Current record 133K (154K under pressure).
Widely believed that all the action is in the common factor, i.e. in the CuO₂ planes.
The structure is two dimensional.

\[
\begin{align*}
\text{Cu} - \text{O} - \text{Cu} & \quad \text{Square lattice of} \\
\text{O} & \quad \text{Cu}^+ \\
\text{Cu} - \text{O} - \text{Cu} & \quad \text{oxygen in O}^{--}
\end{align*}
\]

O^{--} means that the p-orbitals are full.
\text{Cu}^+ is a bit more complicated. The shell that matters is the "d". If we would have rotational invariance this orbital would have a degeneracy 5. However, in the standard "environment" of the transition metal \text{Cu}^+, which is a cage of oxygens, rotational invariance is broken:

\[
\begin{align*}
\text{in vacuum} & \quad x^2-y^2, 3z^2-r^2 \\
\text{in lattice} & \quad xy, yz, zx
\end{align*}
\]
2. The number of electrons corresponds to the following situation:

\[ \text{1 hole in the d-shell} \]

\[ \text{Cu}^{2+} \quad \text{O}^{2-} \]

This usually is inverted and the hole language is used.

Then, the situation is:

\[ \begin{array}{cc}
\text{Cu}^{2+} & \text{O}^{2-} \\
\text{Cu}^{2+} & \text{O}^{2-} \\
\text{O}^{2-} & \text{Cu}^{2+} \\
\text{O}^{2-} & \text{Cu}^{2+} \\
\end{array} \]

(we are assuming that there is one hole per Cu-O)

Now, how do these spins interact?

\[ \text{Cu} \quad \text{O} \quad \text{Cu} \]

\[ d_{x^2-y^2}, p_x, d_{x^2-y^2} \]

There is an overlap between orbitals that allows for the movement of holes from Cu to O and vice versa.
These spins can be interchanged in four steps:

- $\uparrow \rightarrow \uparrow$ 
- $\downarrow \rightarrow \downarrow$ 
- $\uparrow \downarrow \leftrightarrow \downarrow \uparrow$ 
- $\uparrow \downarrow \leftrightarrow \downarrow \uparrow$

Effective coupling $J \propto \frac{t_{pd}}{\Delta^2 (\Delta + U_p)}$ (superexchange)

$J \approx 0.1\text{eV}$, $t_{pd} \approx 1\text{eV}$
$\Delta \approx 2-3\text{eV}$
$U_p \approx 4\text{eV}$
$U_d \approx 10\text{eV}$
\[ H = J \sum_i \sum_j \langle \vec{S}_i \cdot \vec{S}_j \rangle \] (Heisenberg)

Cu-Cu links

What happens with more holes?

The new hole goes to an oxygen (on Cu a large U is paid) and it tends to form a singlet state with a copper. This is called Zhang-Rice singlet. The effect is a state \( S=0 \) centered at the copper.

Oxygens are gone. Per site there are 3 possibilities: \( \uparrow, \downarrow \) or \( 0 \). These holes can move into what we call the "t-J model".

\[ J \]
An equivalent model is the one-band Hubbard model:

$$
H = -t \sum_{\langle ij \rangle} (C_i^\dagger C_j + h.c.) + U \sum_x N_{x\uparrow} N_{x\downarrow}
$$

At very large $U/t$ and half-filling the situation is that only one particle per site exists. Through a 2 steps process, the effective model at large $U/t$ is the Heisenberg model:

$$
J \propto \frac{t^2}{U}
$$

Then it is worth studying the one-band Hubbard model at $\langle n \rangle = 1$ to see the appearance of AF.