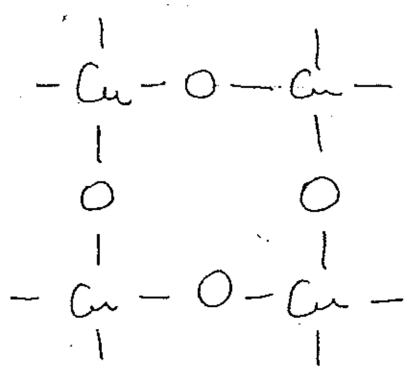
High-Tc Superconductors

Discovered in 1986.

Current record 133K (154k under pressure).

Widely believed that all the action is in the common factor i.e. in the CuO_2 planes.

The structure is two dimensional.

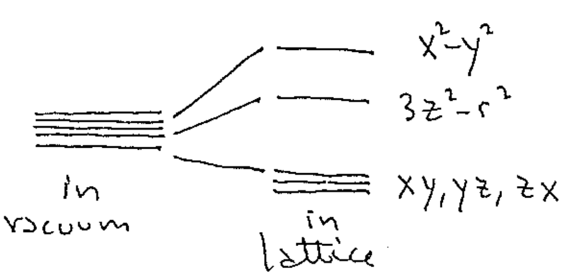


Square lattice of coppers, with oxygens in between.

Copper is in Cu^{++} and oxygen in O^{--}

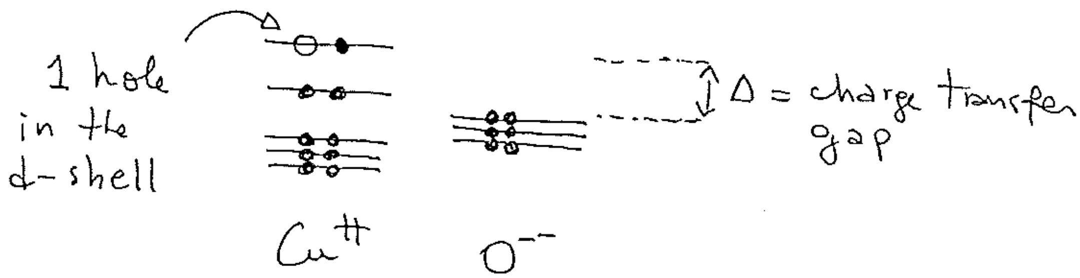
O^{--} means that the p-orbitals are full.

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 Cu^{++}, which is a cage of oxygens, rotational invariance is broken:

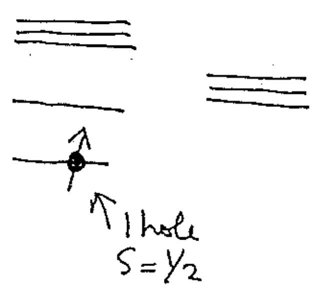


2.

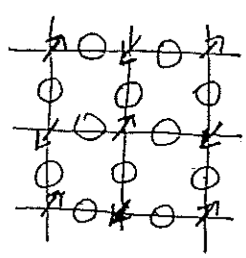
The number of electrons corresponds to the following situation:



This usually is inverted and the hole language is used.

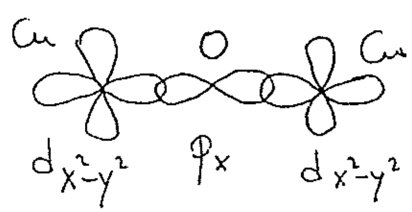


Then, the situation is:

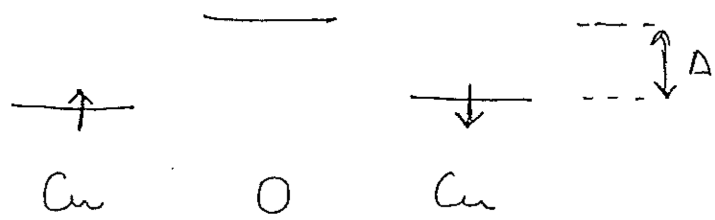


(we are assuming that there is one hole per Cu–O)

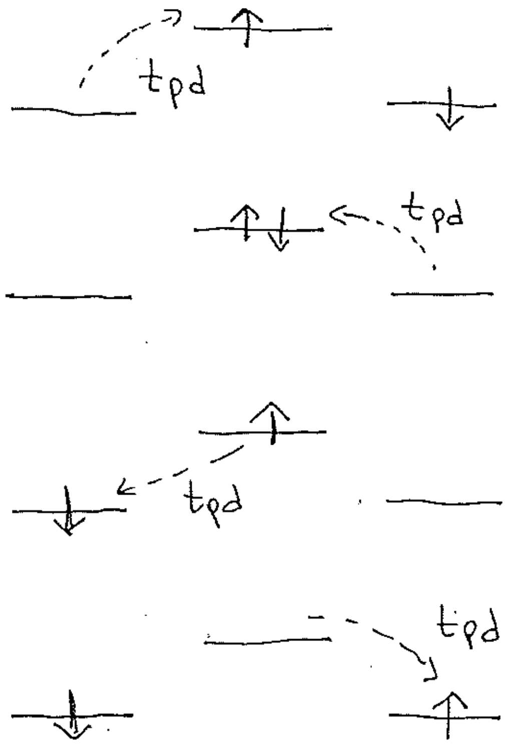
Now, how do these spins interact?



There is an overlap between orbitals that allows for the movement of holes from Cu to O and viceversa.



Those spins can be interchanged in four steps



E paid = Δ

E paid = 2Δ + U_p

E paid = Δ

Effective coupling $J \propto \dfrac{t_{pd}^4}{\Delta^2 (2\Delta + U_p)}$ (superexchange)

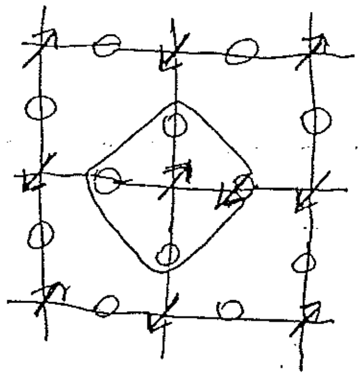
$J \sim 0.1\,eV$, $t_{pd} \sim 1\,eV$
$\Delta \sim 2\text{-}3\,eV$
$U_p \sim 4\,eV$
$U_d \sim 10\,eV$

4.

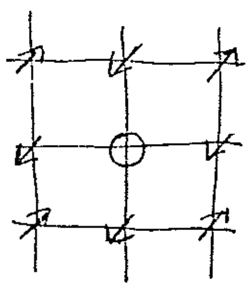
$$H = J\sum_{\langle ij\rangle} \vec{S}_i \cdot \vec{S}_j \quad \text{(Heisenberg)}$$

$\langle ij\rangle$: Cu-Cu links

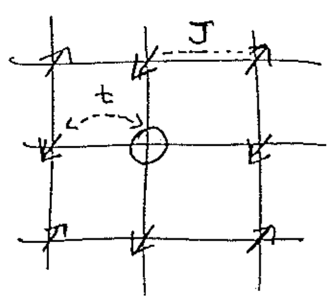
What happens with more holes?



The new hole goes to an oxygen (on Cu a large U_d 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.

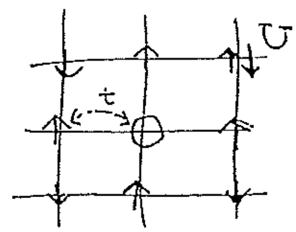


Oxygens are gone. Per site there are 3 possibilities: ↗, ↙ or O. These holes can move into what we call the "t-J model"



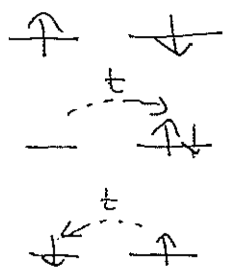
An equivalent model is the one band Hubbard model:

$$H = -t \sum_{\substack{\langle ij \rangle \\ \sigma = \uparrow,\downarrow}} \left(c^{+}_{i\sigma} c_{j\sigma} + h.c. \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$



← difference with t-J model. At $U \gg t$ they become equivalent.

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:



$E = U$

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

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

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