Mott insulators and Hubbard Model

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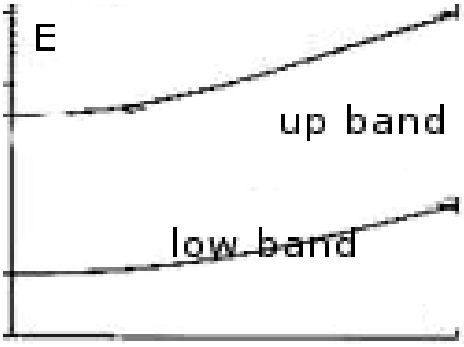
Hubbard Model

Band theory is very successful at describing 'small interaction', 'low temperature' and 'ordered' systems. However, it can not explain why some metal oxides that were predicted to be conductors by band theory were in fact insulators. Mott found out the answer. It is the effect of 'Column interaction'. When all sites are half filled and the electron-electron interaction is much larger than the hoping term (the overlap of two neighbor electrons wave function), two electron cannot be in one site, so they can not move anymore. In other words, we can say: because band theory assume electrons are delocalized and solve the total system in a "one electron" wave function. This is the difference.
In order to show the repulsion of two electron, Hubbard introduced a 'U*n1*n2' term into the Hamiltonian.

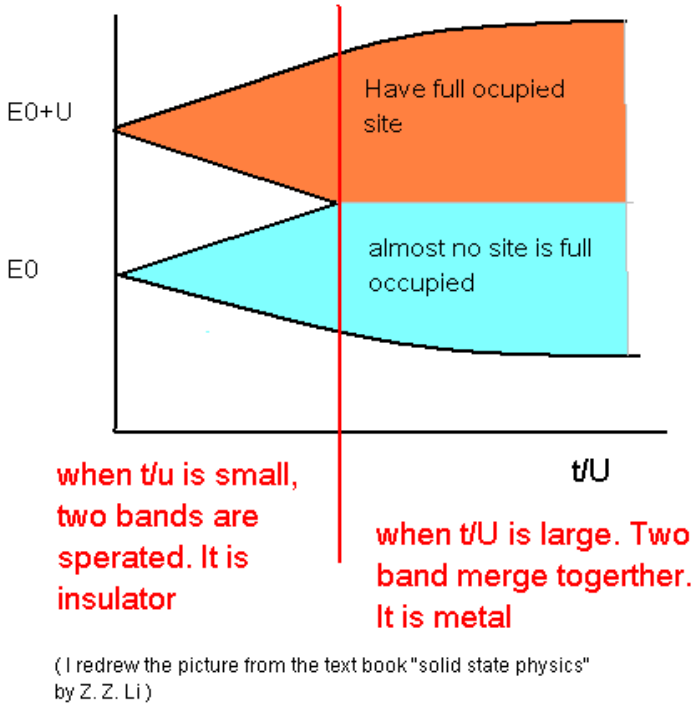
$$H = t\sum_{\substack{i\neq j\\ \sigma}} c_{i\sigma}^{+}c_{j\sigma} + \mu\sum_{i,\sigma} c_{i\sigma}^{+}c_{i\sigma} + u\sum_{i} c_{i\uparrow}^{+}c_{i\downarrow}c_{i\uparrow}^{+}c_{i\downarrow}$$

So, the total energy will be very high if there are two electrons on one site causing the system to prefer to choose a lower energy state.



(this picture shows the column repulsion U term opens a gap with a width U between the full occupied site and non-full occupied site)

After introducing the Hubbard Model, the strong interaction will open a gap between the previous 'continuous' band in 'band theory when U is sufficiently large. This resembles a competition between the kinetic energy and the potential energy. If 't/U' is larger enough, the two separated bands are going to merge together!!



(I redrew the picture from the text book "solid state physics" by Z. Z. Li)

The time when the two bands merge together is the point this material changes from Mott insulator into conductor. It is called 'insulator -metal' transition.

Hubbard model successfully explained why some oxide is insulator why some is not. It is all dependent upon the fraction of (t/U). So , to some material where "t" is sensitive to pressure, we can change it from insulator to metal just by adding more pressure. Then, the atoms distance will decrease, and there will be more overlap "t" of the neighbor electrons' wave function. Since the hopping constant "t" increases, it is possible for electrons to move. This is only one way of "MIT"

Hubbard Model's disadvantage and t-J Model

How ever, it is too difficult to solve the Hubbard Model completely, because the degree of freedom is proportional to 4^N (N is the number of sites). Today even computers cannot solve system with more than 100 electron using Hubbard model.
So what we can do is find out the best approximation of the Hubbard model in each particular restriction.
When U>>t, two electrons do not want to share one site any more. So, people introduced the t-J model for average electron number per site smaller than 1 situation. This means that when we choose t-J model, the maxim dimension is 3^N instead of 4^N. This greatly simplified the problem.

$(0,0)$	$\|0\rangle$
$(\uparrow,0)$	$c_{1\uparrow}^{+}\|0\rangle$
$(0,\uparrow)$	$c_{2\uparrow}^{+}\|0\rangle$
$(\downarrow,0)$	$c_{1\downarrow}^{+}\|0\rangle$
$(0,\downarrow)$	$c_{2\downarrow}^{+}\|0\rangle$
$(\uparrow,\uparrow)$	$c_{1\uparrow}^{+}c_{2\uparrow}^{+}\|0\rangle$
$(\downarrow,\downarrow)$	$c_{1\downarrow}^{+}c_{2\downarrow}^{+}\|0\rangle$
$(\uparrow,\downarrow)$	$c_{1\uparrow}^{+}c_{2\downarrow}^{+}\|0\rangle$
$(\downarrow,\uparrow)$	$c_{1\downarrow}^{+}c_{2\uparrow}^{+}\|0\rangle$

The bases, using in the t-J model, is a sub space of Hubbard model bases. Each site only contains:(empty, up, down) three configurations.
In simplest two sites model, they are:

Totally 9=3^2 in the low band

However, the they cannot be constructed into the set of "2 electron" eigenstates of Hubbard model Hamiltonian which containing full occupied site state. We neglect the up band 7 configurations.

$$
\begin{array}{ll}
(\uparrow\downarrow,0) & c^{+}_{1\uparrow}c^{+}_{1\downarrow}|0\rangle \\
(0,\uparrow\downarrow) & c^{+}_{2\uparrow}c^{+}_{2\downarrow}|0\rangle \\
(\uparrow\downarrow,\uparrow) & c^{+}_{1\uparrow}c^{+}_{1\downarrow}c^{+}_{2\uparrow}|0\rangle \\
(\uparrow,\uparrow\downarrow) & c^{+}_{1\uparrow}c^{+}_{2\uparrow}c^{+}_{2\downarrow}|0\rangle \\
(\uparrow\downarrow,\downarrow) & c^{+}_{1\uparrow}c^{+}_{1\downarrow}c^{+}_{2\downarrow}|0\rangle \\
(\downarrow,\uparrow\downarrow) & c^{+}_{1\downarrow}c^{+}_{2\uparrow}c^{+}_{2\downarrow}|0\rangle \\
(\uparrow\downarrow,\uparrow\downarrow) & c^{+}_{1\uparrow}c^{+}_{1\downarrow}c^{+}_{2\uparrow}c^{+}_{2\downarrow}|0\rangle
\end{array}
$$

Project from whole space into sub-band space

The official way to derive the t-J model by using a projector to separate the total Hamiltonian into 3 parts. The first (1) and the final (3) term represent the previous two sub band separated by strong Column repulsion.

$$P_1HP_1 = t\sum_{ij\sigma}{}'(1-n_{i-\sigma})a^{\dagger}_{i\sigma}a_{j\sigma}(1-n_{j-\sigma}), \quad (1)$$

$$P_1HP_2 = t\sum_{ij\sigma}{}'(1-n_{i-\sigma})a^{\dagger}_{i\sigma}a_{j\sigma}n_{j-\sigma}, \quad (2)$$

$$P_2HP_1 = t\sum_{ij\sigma}{}'n_{i-\sigma}a^{\dagger}_{i\sigma}a_{j\sigma}(1-n_{j-\sigma}), \quad (2)$$

$$P_2HP_2 = t\sum_{ij\sigma}{}'n_{i-\sigma}a^{\dagger}_{i\sigma}a_{j\sigma}n_{j-\sigma} + U\sum_{i}n_{i\uparrow}n_{i\downarrow}. \quad (3)$$

In (1), no site is full occupied.
In (3) no site is empty and at least one site is fully occupied.

In (3) the hopping term represent the electron moving from one full occupied site to a half occupied site, making it into a fully occupied site.

The second term (2) represents the interaction of the two sub band. In the “large U” approximation(see picture in page 1). The up and low bands are not connected, so they should not have any hopping between them, as that electron jump from full occupied site to empty site. However, it is a very important part with an complex value and many orders added together which will infect the final result. It is similar to valcum energy in high energy

physics.

Actually, the mixed term is equivalent to the spin interaction term. Under low temperature and high U/t, the up band will be empty, so the (3) term in the Hamiltonian is neglectable.

Finally, we get the effective Hamiltonian:

$$H = \frac{1}{2} t \sum_{\langle i,j \rangle, \sigma} (1 - n_{i,\sigma}) C_{i\sigma}^{+} C_{j\sigma} (1 - n_{j,\sigma}) + J \sum_{\langle i,j \rangle} (\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j)$$

$$J = 4t^2 / U$$

in the Kinetic energy term. Only half filled site can donate a non zero term to total energy. It means, the electron can only jump from a half filled site to an empty site.

2 sites Hubbard model and T-J model

Since the T-J model is an approximation of Hubbard model. I tried to use the half filled sites as the ground state to calculate the total energy with the perturbation theory.

here are two sites two electrons Hamiltonian(total spin zero):

of the Hubbard model

0	0	-t	-t
0	0	t	t
-t	t	U	0
-t	t	0	U

and form T-J model (2X2) matrix. (I enlarge the matrix to compare with Hubbard model)

-J/2	J/2	0	0
J/2	-J/2	0	0
0	0	0	0
0	0	0	0

They both use the same basis

$(\uparrow,\downarrow)\ (\downarrow,\uparrow)\ (\uparrow\downarrow,0)\ \ (0,\uparrow\downarrow)$

From the T-J model, the two eigenstates are 0 and -J

The accurate solution of Hubbard Model 4 eigen-energy and eigenstates are

$$0 \qquad \frac{1}{\sqrt{2}}\left[(\uparrow,\downarrow)+(\downarrow,\uparrow)\right]$$

$$u \qquad \frac{1}{\sqrt{2}}\left[(\uparrow\downarrow,0)-(0,\uparrow\downarrow)\right]$$

$$\frac{1}{2}u-\frac{1}{2}\sqrt{16t^2+u^2} \qquad \frac{4t}{-u+\sqrt{16t^2+u^2}}\left[(\uparrow,\downarrow)-(\downarrow,\uparrow)\right]+\left[(\uparrow\downarrow,0)+(0,\uparrow\downarrow)\right]$$

$$\frac{1}{2}u+\frac{1}{2}\sqrt{16t^2+u^2} \qquad \frac{4t}{u+\sqrt{16t^2+u^2}}\left[(\uparrow,\downarrow)-(\downarrow,\uparrow)\right]-\left[(\uparrow\downarrow,0)+(0,\uparrow\downarrow)\right]$$

Compared with the second order perturbation result of the same Hamiltonian

the energy levels are 0 , U, 4t^2/U, 2U+4t^2/U

now, we are only interested in the fist and the third eigenstates' energy: (0 and 4t^2/U) which are the same as the result from T-J model's two eigenstates, it also show J value does equal to 4t^2/U. Another interesting thing is, the first order perturbation correction turn out to be zero.

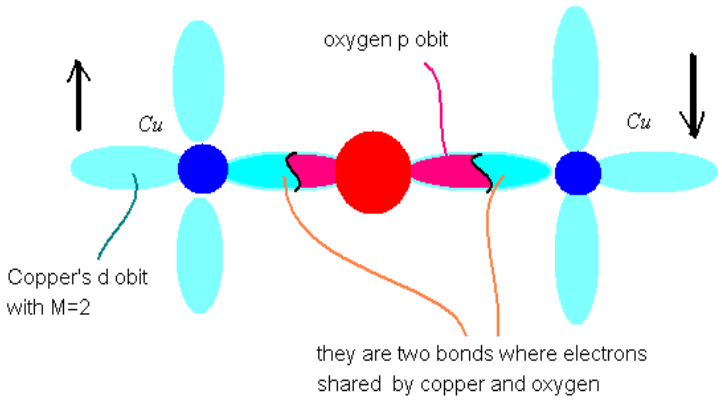
The solution also shows that the ground state for t-J model is anti-ferromagnetic. Its total spin is zero and it is antisymmetric.

T-J model in Copper Oxide

In High Tc Superconductor, T-J model successfully explained why pure Copper oxide is insulator and its ground state is anti-ferromagnetic.

The Copper plane without doping is a pure half filling sites system

because copper have one d electron site is half filed. It is kind of Mott insulator (I guess) because electron can not move free any more. We can see it in T-J Hamiltonian Kinetic energy term is zero in the nearly completely half filling situation. And the spin interaction J term decide the system ground state must be anti-ferromagnetic.



the Oxygen like a brige connect two copper. and they can exchange the electron.
This exchage strength donate a spin coupling constant "J"
It is also called "super exchange"
Since Oxigen already have two electons on p site. No aditional electron can pass it. So it is insulator.

Different from normal t-J model, in copper oxide, the J coupling strength is decided by the "super exchange" . When oxide's two neighbor copper has different spin, Oxide can build TWO bonds with them at the same time and share two electron with them. Since they have different spin, they can stay in oxide p site at the same time
Another point is, in High Tc SC Copper oxide, very small amount of doping can destroy the anti-ferromagnetic configuration. One more electron added into the Oxygen atom between two Copper atoms will make Oxygen iron site half full. The strong spin coupling between Oxygen and Copper which is stronger than Copper-Copper spin interaction will change Oxygen's both neighbor Copper d electrons into the same spin. Since the oxygen's d electron has a smaller orbital angular momentum than copper's d electron, the total system will be ferromagnetic.

[1] Hubbard J. Proc Roy Soc (London), 1963, A276: 238

[2] Hubbard J. Proc Roy Soc (London), 1964, A281: 401

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[4] Spalek *et al* Phys. Rev. B 18, 3748 (1978)

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[6] Hal Tasaki 1998 *J. Phys.: Condens. Matter* **10** 4353-4378