Lecture 27

# The Mott transition

Consider a lattice of hydrogen atoms. According to the band structure for any distance between the atoms the electron wave functions will overlap, band will be formed and the solid will be conductor (we have 1 electron per unit cell, thus half filling). This cannot be true for large distance between the atoms. Indeed moving one electron from one atom to another creates two ions $H^+$ and $H^-$. It will cost too much of Coulomb energy to have such a state.

This inter-electron interaction which is neglected in the band structure analysis will make system insulating. Then the good description is the local picture of independent hydrogen atoms

Increasing density will lead to the Mott metal-insulator transition.

One can estimate the critical density for this transition in the following way. Assume that we are in the metallic state where conduction electrons screen the Coulomb potential of the ion.

$$V = -\frac{e^2}{r} e^{-\frac{r}{\lambda_{TF}}} \qquad \text{(Lecture 15)}$$

$$\lambda_{TF}^{-2} = 4\pi^2 e^2 N(\varepsilon_F) \simeq \frac{4}{r_0 a_0},$$

where $r_0 = n_0^{-1/3}$ – lattice constant for the simple cubic lattice and $a_0 = \frac{\hbar^2}{me^2}$ – Bohr radius.

For large $\lambda_{TF}$ the bound state (hydrogen atom) will be formed with typical wave function size $\simeq a_0$. For small $\lambda_{TF}$ the potential would be too weak to form a bound state.

We can estimate when the bound state will disappear comparing kinetic and potential energies

For small $\lambda_{TF}$ the radius of the wave function $r \sim \lambda_{TF}$. Then the kynetic energy is $\sim \frac{\hbar^2}{m \lambda_{TF}^2}$ and the potential is $\sim \frac{e^2}{\lambda_{TF}}$

If $E_{kin} >> E_{pot}$ then the well is too shallow to bind the particle. Then

$$\frac{\hbar^2}{m \lambda_{TF}^2} \sim \frac{e^2}{\lambda_{TF}} \Rightarrow \lambda_{TF} \sim \frac{\hbar^2}{m e^2} = a_0$$

Substituting $\lambda_{TF} = \frac{\sqrt{r_0 a_0}}{2} = a_0$ we that for $r_0 > 4 a_0 \approx 2 Å$ we have the insulating state and for $r_0 < 4 a_0$ - metallic. Such metal - insulator transition is indeed observed in certain transition metal oxides ($NiO$, $V_2O_3$, $VO$). For hydrogen it is possible that in Jupiter pressure is so high that leads to metallic hydrogen

# Hubbard model

The simple tight binding model that describes this phenomenon is the Hubbard model

$$H = -t \sum_{i,j,s} (c^{+}_{is} c_{js} + h.c) + U \sum \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

We consider nearest neighbor hopping between sites $i$ and $j$. $n_{is} = c^{+}_{is} c_{is}$ is the density operator. In this model the Coulomb interaction is replaced by the on site repulsion. We consider this model at half filling, $n = 1$, one electron per site. There are two limiting case

$t = 0 \iff$ Insulator. The ground state has exactly 1 electron on each site. This state is highly degenerate because each electron may have spin $s = \pm 1/2$

Degeneracy is $2^N$ ($N$ - number of sites)

The first exciting state consists of one empty site (hole) and one doubly occupied (doublon) It has energy $U$.

## $U = 0$ – Metallic state

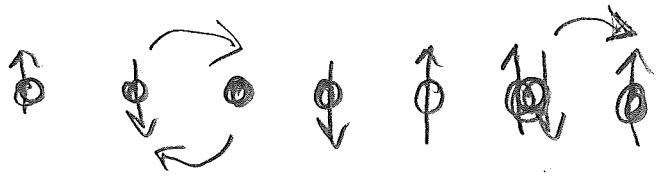
Here we have band

$$\varepsilon_k = -2t\,(\cos k_x a + \cos k_y a + \cos k_z a)$$

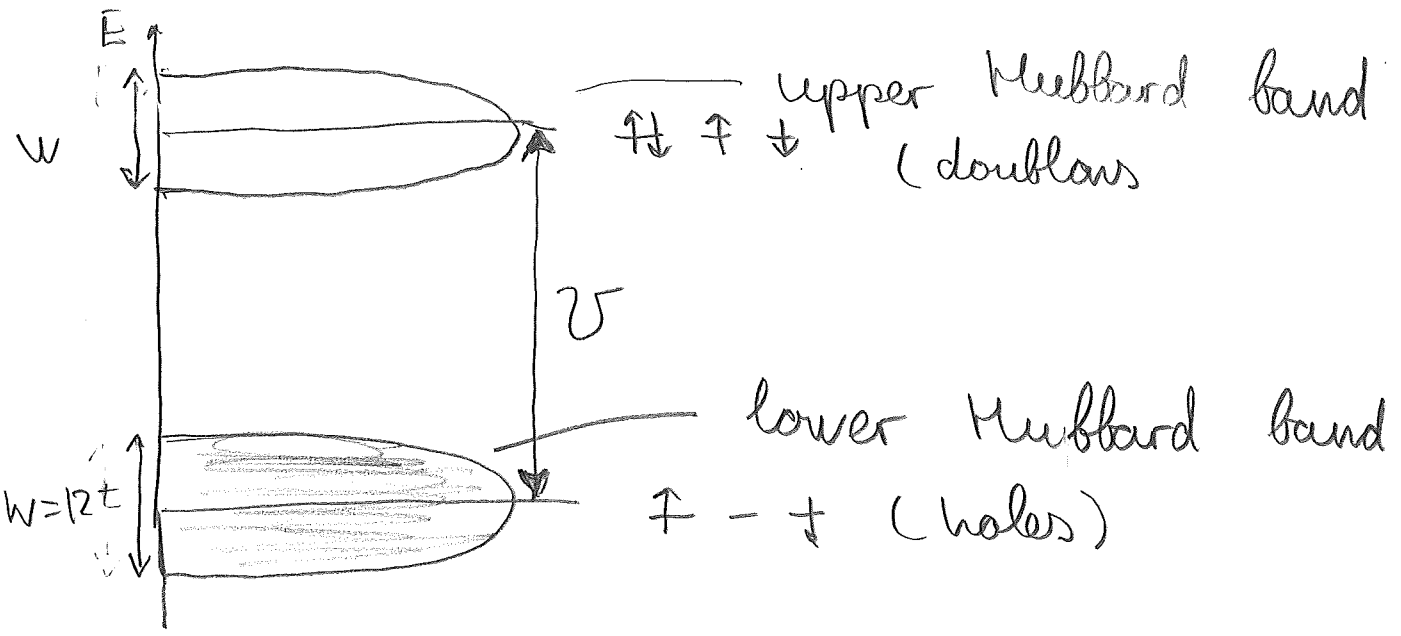
with the band width $W = 2zt = 12t$

Let us start from the insulating state and include hopping perturbatively, $t \ll U$

With the finite hopping present holon and doublon became mobile



Since motion of holon and doublon doesn't lead to interaction they form bands with the band width $W = 12t$

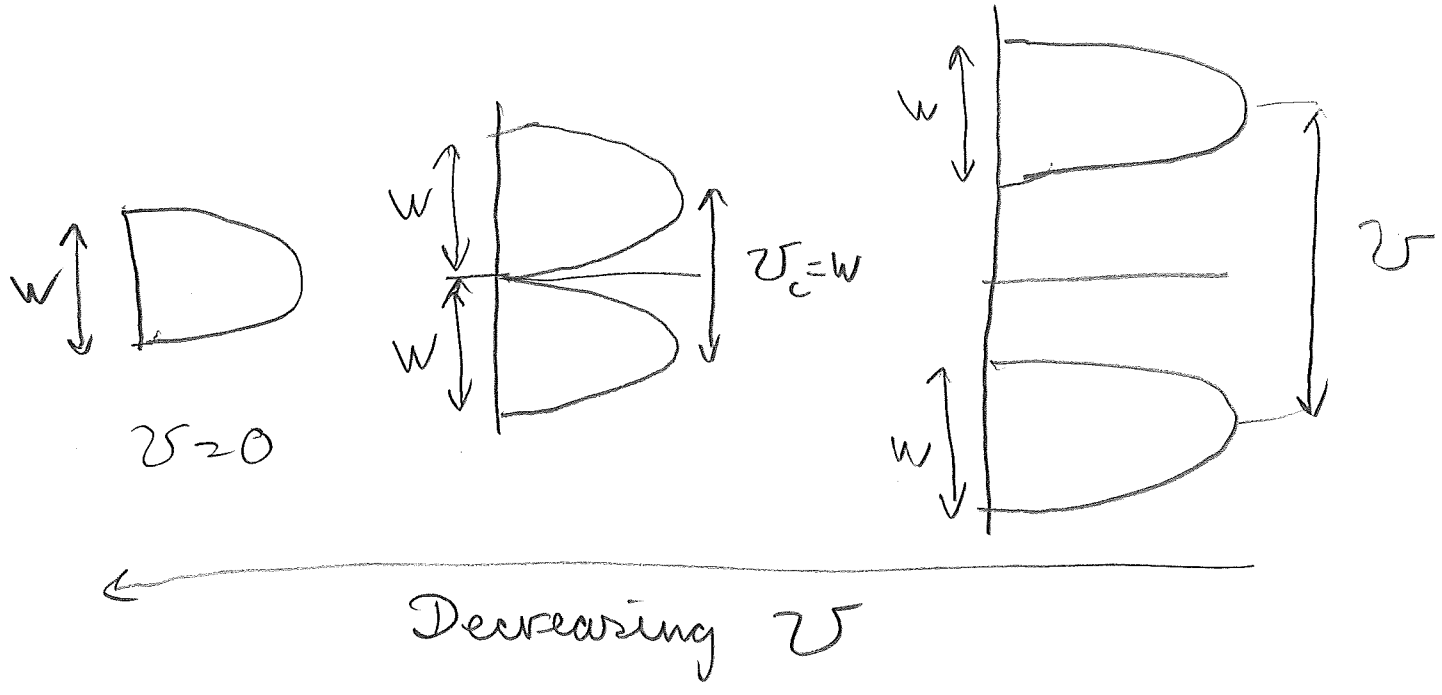



At half filling lower Hubbard band is fully occupied and one has insulator with the Hubbard gap $\Delta = U - 12t$.

Decreasing $U$ bands are coming closer.

at $U_c = 12t$ the gap disappears.

transition to metal — Mott-Hubbard transition



# Ground state of the Mott insulator

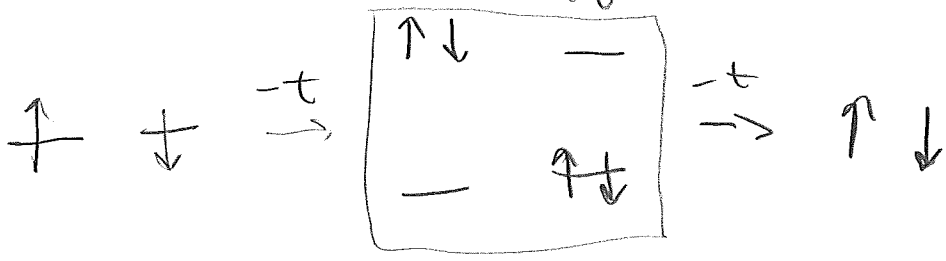
Consider two-site Hubbard model at half filling (2 electrons) for $t \ll U$.

For $t = 0$ there are 4 degenerate configurations

$$|\uparrow\uparrow, 0\rangle, |\downarrow\downarrow, 0\rangle, |\uparrow\downarrow, 0\rangle, |0, \uparrow\downarrow\rangle$$

Increasing hopping $t$ spin polarised states $|\uparrow\uparrow, 0\rangle, |\downarrow\downarrow, 0\rangle$ will not profit from hopping because of the Pauli principle

The states with the opposite spins can reduce their energy via virtual process

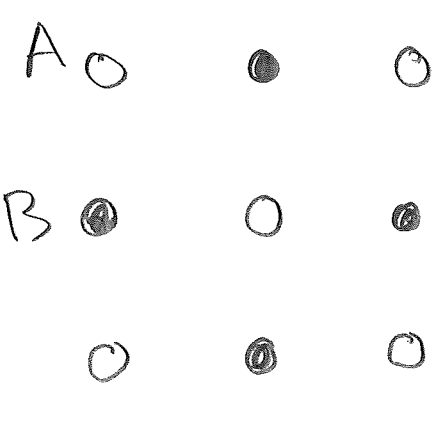



This superexchange produce the antiferromagnetic interaction between spins

$$H = J \vec{S}_i \cdot \vec{S}_j \quad \text{with} \quad J = \frac{4t^2}{U}$$

# Classical antiferromagnet

If the lattice is <u>bipartite</u> (can be split into two sublattices A and B) then the nearest neighbor interaction can be presented as the interaction between the different sublattices




$$H = J \sum_{i,j} S_i^A S_j^B$$

Introducing new spin variables

$$\tilde{S}_i^A = S_i^A$$

$$\tilde{S}_i^B = -S_i^B$$ – changing sign of the spins for one sublattice

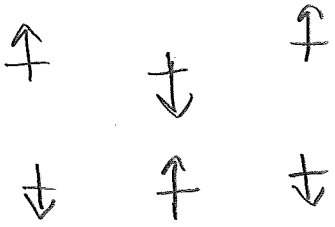
we transform our Hamiltonian to

$$H = -J \sum_{i,j} \tilde{S}_i^A \tilde{S}_j^B = -J \sum_{i,j} \tilde{S}_i \tilde{S}_j$$

which is the ferromagnetic Heisenberg model

Thus transition temperatures (as well as all thermodynamic properties in the absence of field) are the same for ferro- and antiferro-magnets (on bypartite lattice!)!!

The response to magnetic field would be different because in the ground state of the antiferromagnet two sublattices have opposite spin $S^A_i = S^+$, $S^B_i = S^-$



$\langle S \rangle = \langle S^+ + S^- \rangle = 0$ for $B=0$

In the mean field approximation we can write

$$\langle S^+ \rangle = \frac{1}{2} \tanh\left( \frac{-J\langle S^- \rangle + \mu_B B}{T} \right)$$

$$\langle S^- \rangle = \frac{1}{2} \tanh\left( \frac{-J\langle S^+ \rangle + \mu_B B}{T} \right)$$

Here we also see that replacing $S^- \to -S^-$ we obtain the mean field equation from the last lecture

For high temperatures $T >> J$ we can expand $\tanh x \approx x$ and add

$$\langle S \rangle = \langle S^+ \rangle + \langle S^- \rangle = -\frac{T_N}{T}\left(\langle S^- \rangle + \langle S^+ \rangle\right) + \frac{\mu_B B}{T}$$

Solving for $\langle S^+ \rangle + \langle S^- \rangle = \langle S \rangle$ we obtain

$$\langle S \rangle = \frac{\mu_B B}{T + T_N} \quad \text{with Néel temperature}$$

$$T_N = \frac{J}{2}$$

Note that the magnetic susceptibility stays constant at $T_N$.

Landau theory of antiferromagnet

$$F_L = \alpha\left(M_1^2 + M_2^2\right) + \beta\, \vec{M}_1 \cdot \vec{M}_2 + \gamma\left(M_1^4 + M_2^4\right) - \vec{B}\left(\vec{M}_1 + \vec{M}_2\right)$$

↑ interaction between sublattices

we can diagonalize quadratic form by going to $M_+ = M_1 + M_2$ and $M_- = M_1 - M_2$

Then the second order terms are

$$\left(\frac{\alpha}{2}+\frac{\beta}{4}\right)(M_1+M_2)^2+\left(\frac{\alpha}{2}-\frac{\beta}{4}\right)(M_1-M_2)^2$$

For $\beta > 2\alpha$ the coefficient in front of $M_1-M_2$ changes sign $\Rightarrow$ it is favorable to have $M_1 = -M_2 \neq 0$.

Denoting $\frac{\alpha}{2}-\frac{\beta}{4} = at$, $\frac{\alpha}{2}+\frac{\beta}{4} = b$

$$F_L = b M_+^2 + at M_-^2 + \frac{\gamma}{2}(M_+^4+M_-^4)+3\gamma M_+^2 M_-^2 - \vec{B}\vec{M}_+$$

Above transition point $M_- = 0$, $\vec{M}_+ = \frac{\vec{B}}{2b}$

$$\chi = \frac{\partial M_+}{\partial B} = \frac{1}{2b} = \text{const}$$

Below $T_N$ $M_-^2 = -\frac{at}{\gamma}$ and

$$M_+ = \frac{B}{2b+6\gamma M_-^2} = \frac{B}{2b-\frac{6at}{\gamma}}$$

Thus we have cusp in the susceptibility