Lecture 31

Mott insulators and antiferromagnetism

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

Consider half-filled band – one electron per site.

If $U = 0$, this Hamiltonian describes a metal at any t, only the effective mass increases as t decreases ($m^* \sim \frac{1}{t}$).

This continues to be true at nonzero U as long as $\frac{U}{t}$ is not too large.

At some point, roughly when $\frac{U}{zt} \sim 1$, it becomes energetically favorable for electrons to localize, each in its own site to minimize the interaction energy. Such a state is an insulator and is called Mott insulator. It is distinct from band insulator: at half-filling the material should be a metal ~~[illegible]~~ according to band theory, but can be insulating due to electron-electron interactions.

An important question in a Mott insulator is what happens with the spin of the localized electrons.

If we take $t \to 0$, i.e. $H = U \sum_{i} n_{i\uparrow} n_{i\downarrow}$,

The GS of this Hamiltonian is 2^N-fold degenerate - spin at every site can be either up or down.

This degeneracy is lifted when $t \neq 0$.
To see how this happens, consider a 2-site problem.

$$H = -t\left(c_{1\sigma}^{+} c_{2\sigma} + c_{2\sigma}^{+} c_{1\sigma}\right) + U \sum_{i=1,2} n_{i\uparrow} n_{i\downarrow}$$

Assume $\frac{t}{U} \ll 1$ and do perturbation theory in $\frac{t}{U}$.

At zeroth order, we have $2^2 = 4$-fold degenerate ground state of $H^U = \sum_{i=1,2} n_{i\uparrow} n_{i\downarrow}$:

$$|\uparrow,\uparrow\rangle, \quad |\uparrow,\downarrow\rangle, \quad |\downarrow,\uparrow\rangle, \quad |\downarrow,\downarrow\rangle.$$

$$\text{let } H^t = -t\left(c_{1\sigma}^{+} c_{2\sigma} + c_{2\sigma}^{+} c_{1\sigma}\right)$$

Second order perturbation theory correction to H^U is given by:

$$\langle a | \delta H | b \rangle = -\sum_{n}{}' \frac{\langle a | H^t | n \rangle \langle n | H^t | b \rangle}{\langle n | H^U | n \rangle}$$

Here a, b = one of the 4 degenerate ground states of H^U and n are all the excited states.

$$H^t |\uparrow,\downarrow\rangle = -t\left(c_{1\uparrow}^{+} c_{2\uparrow} + c_{1\downarrow}^{+} c_{2\downarrow} + c_{2\uparrow}^{+} c_{1\uparrow} + c_{2\downarrow}^{+} c_{1\downarrow}\right) c_{1\uparrow}^{+} c_{2\downarrow}^{+} |0\rangle =$$

$$= -t\left(c^+_{1\downarrow} c_{2\downarrow} c^+_{1\uparrow} c^+_{2\downarrow} + c^+_{2\uparrow} c_{1\uparrow} c^+_{1\uparrow} c^+_{2\downarrow} \right)|0\rangle =$$

$$= -t\left(-c^+_{1\downarrow} c^+_{1\uparrow} c_{2\downarrow} c^+_{2\downarrow} + c^+_{2\uparrow} c^+_{2\downarrow} c_{1\uparrow} c^+_{1\uparrow} \right)|0\rangle =$$

$$= -t\left(c^+_{1\uparrow} c^+_{1\downarrow} + c^+_{2\uparrow} c^+_{2\downarrow} \right)|0\rangle =$$

$$= -t\left(|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle \right).$$

Analogously, we get:

$$H^+ |\downarrow, \uparrow\rangle = t\left(|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle \right)$$

Thus we have:

$$\langle \uparrow\downarrow, 0 | H^+ | \uparrow, \downarrow \rangle = -t$$

$$\langle \uparrow\downarrow, 0 | H^+ | \downarrow, \uparrow \rangle = t$$

$$\langle \uparrow\downarrow, 0 | H^+ | \uparrow, \uparrow \rangle = \langle \uparrow\downarrow, 0 | H^+ | \downarrow, \downarrow \rangle = 0$$

since $H^+ |\uparrow, \uparrow\rangle = H^+ |\downarrow, \downarrow\rangle = 0$ due to Pauli principle.

Thus we obtain:

$$\langle \uparrow, \downarrow | \delta H | \uparrow, \downarrow \rangle = -\frac{2t^2}{U}$$

$$\langle \uparrow, \downarrow | \delta H | \downarrow, \uparrow \rangle = \frac{2t^2}{U}$$

From the above, it can be easily shown that δH can be written in terms of electron spin operators.

$$S_i^a = \frac{1}{2} C_{i\sigma}^+ \tau^a_{\sigma\sigma'} C_{i\sigma'}$$

τ^a – Pauli matrices.

$$\tau^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \tau^+ = \begin{pmatrix} 0 & 2 \\ 0 & 0 \end{pmatrix}, \tau^- = \begin{pmatrix} 0 & 0 \\ 2 & 0 \end{pmatrix}.$$

Consider the matrix elements of:

$$S_1^z S_2^z = \frac{1}{4} n_1 n_2 =$$

$$= \frac{1}{4} \left(C_{1\uparrow}^+ C_{1\uparrow} - C_{1\downarrow}^+ C_{1\downarrow} \right) \left(C_{2\uparrow}^+ C_{2\uparrow} - C_{2\downarrow}^+ C_{2\downarrow} \right) =$$

$$= \frac{1}{4} \left(C_{1\uparrow}^+ C_{1\uparrow} + C_{1\downarrow}^+ C_{1\downarrow} \right) \left(C_{2\uparrow}^+ C_{2\uparrow} + C_{2\downarrow}^+ C_{2\downarrow} \right) =$$

$$= -\frac{1}{2} \left(C_{1\uparrow}^+ C_{1\uparrow} C_{2\downarrow}^+ C_{2\downarrow} + C_{1\downarrow}^+ C_{1\downarrow} C_{2\uparrow}^+ C_{2\uparrow} \right)$$

$$\langle \uparrow, \downarrow | S_1^z S_2^z - \frac{1}{4} n_1 n_2 | \uparrow, \downarrow \rangle = -\frac{1}{2}$$

$$\langle \uparrow, \downarrow | S_1^z S_2^z - \frac{1}{4} n_1 n_2 | \downarrow, \uparrow \rangle = 0.$$

$$\langle \uparrow, \downarrow | \frac{1}{2} S_1^+ S_2^- | \downarrow, \uparrow \rangle =$$

$$= \frac{1}{2} \langle \uparrow, \downarrow | C_{1\uparrow}^+ C_{1\downarrow} C_{2\downarrow}^+ C_{2\uparrow} | \downarrow, \uparrow \rangle =$$

$$= \tfrac{1}{2} \langle \uparrow,\downarrow | c^+_{1\uparrow} c_{1\downarrow} c^+_{2\downarrow} c_{2\uparrow} c^+_{1\downarrow} c^+_{2\uparrow} |0\rangle =$$

$$= \tfrac{1}{2} \langle \uparrow,\downarrow | c^+_{1\uparrow} c^+_{2\downarrow} |0\rangle = \tfrac{1}{2}$$

Thus it is clear that δH can be written as:

$$\delta H = \frac{4t^2}{U}\left[S_1^z S_2^z - \underbrace{\tfrac{1}{4} n_1 n_2}_{-\frac{1}{4}} + \tfrac{1}{2}\left(S_1^+ S_2^- + \text{h.c.}\right)\right] =$$

$$= \frac{4t^2}{U} \vec{S}_1 \cdot \vec{S}_2 + \text{const.}$$

Generalizing to many sites, the spin Hamiltonian in the large $\frac{U}{t}$ limit is given by:

$$H = \tfrac{1}{2} J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$

$$J = \frac{4t^2}{U}$$

Thus neighboring spins in a Mott insulator want to antialign:

↑ ↓ ↑ ↓ ↑

↓ ↑ ↓ ↑ ↓

Such spin ordering is called antiferromagnetic. It does not lead to macroscopic magnetization $\Rightarrow$ much more difficult to detect than ferromagnetic ordering. It was only seen experimentally in the 1950's, when neutron scattering techniques were developed.

Physics behind $J \sim \frac{t^2}{U}$: electrons on neighboring sites in a Mott insulator want their spins antialigned because this allows them to lower their energy by hopping to a neighboring site and back. If the spins were aligned, this would be impossible by Pauli principle.

Most known antiferromagnets are Mott insulators (or nearly Mott insulators).

Thus we can summarize the physical origins of magnetism as:

1. Ferromagnetism occurs mostly in metals. Physics — lowering of electron-electron interaction energy due to spin alignment.

2. Antiferromagnetism occurs mostly in Mott insulators. Physics — lowering of electron kinetic energy due to antialignment of neighboring spins.

Examples of AF: La_2CuO_4, MnO.