Lecture 30

Hubbard model

Heisenberg model is too oversimplified to be taken seriously as a theory of ferromagnetism in metals. Most importantly, it doesn't take into account the fact that d-electrons are itinerant, i.e. not localized.

The simplest model which takes the itinerant character of the d-electrons into account — Hubbard model.

Start from the second-quantized Hamiltonian for interacting electrons in periodic potential.

$$\mathcal{H} = \int d\vec{r}\, \psi_\sigma^+(\vec{r}) \left(-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r}) \right) \psi_\sigma(\vec{r}) +$$

$$+ \frac{1}{2} \int d\vec{r}\, d\vec{r}\,' V(\vec{r}-\vec{r}\,') \psi_\sigma^+(\vec{r}) \psi_{\sigma'}^+(\vec{r}\,') \psi_{\sigma'}(\vec{r}\,') \psi_\sigma(\vec{r})$$

Rewrite this in the Wannier representation, assuming only a single band (d-band) is relevant (Fermi surface is entirely within the d-band) — OK for transition metals: Fe, Ni, Co, Mn, Cr.

$$\psi_\sigma^+(\vec{r}) = \sum_i \varphi_i^*(\vec{r})\, c_{i\sigma}^+$$

Here $\varphi_i(\vec{r})$ is the d-band Wannier function, localized at site i.

The Hamiltonian becomes:

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

$$+ \frac{1}{2} \sum_{ijkl} \int d\vec{r}\, d\vec{r}\,' \; \varphi_i^{*}(\vec{r}) \varphi_j^{*}(\vec{r}\,') \varphi_k(\vec{r}\,') \varphi_l(\vec{r}) \cdot$$

$$\cdot V(\vec{r} - \vec{r}\,') \cdot c_{i\sigma}^{+} c_{j\sigma'}^{+} c_{k\sigma'} c_{l\sigma}$$

Simplest approximation for the interaction term: leave only the matrix element with $i=j=k=l$ — others are smaller since Wannier functions are localized.
Then we obtain:

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

Electrons are assumed to interact only when they [redacted] are on the same lattice site.
This model is much more complicated than the Heisenberg model.
Simplest thing to do is again mean-field theory.

$$n_{i\sigma} = \langle n_{i\sigma} \rangle + n_{i\sigma} - \langle n_{i\sigma} \rangle$$

leaving only terms linear in fluctuations, we obtain:

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

$$\left. + n_{i\downarrow} \langle n_{i\uparrow} \rangle \right]$$

Parametrize:

$$\langle n_{i\uparrow} \rangle = n\left(\frac{1+\xi}{2}\right)$$

$$\langle n_{i\downarrow} \rangle = n\left(\frac{1-\xi}{2}\right)$$

$n = \langle n_{i\uparrow} \rangle + \langle n_{i\downarrow} \rangle$ – average electron density per site.

$\xi = \frac{\langle n_{i\uparrow} \rangle - \langle n_{i\downarrow} \rangle}{n}$ – average degree of spin polarization.

Then we obtain:

$$H = -t \sum_{\langle ij \rangle} \left(c_{i\sigma}^{+} c_{j\sigma} + h.c. \right) - \frac{Un\xi}{2} \sum_{i} \left(n_{i\uparrow} - n_{i\downarrow} \right)$$

$$+ \frac{Un}{2} \sum_{i} \left(n_{i\uparrow} + n_{i\downarrow} \right)$$

The last term is unimportant – can be absorbed in the Fermi energy.

Diagonalize the Hamiltonian by Fourier transform:

$$H = \sum_{k} \varepsilon_k c_{k\sigma}^{+} c_{k\sigma} - \frac{Un\xi}{2} \sum_{k} \left(c_{k\uparrow}^{+} c_{k\uparrow} - c_{k\downarrow}^{+} c_{k\downarrow} \right)$$

$$\varepsilon_k = -t \sum_{\vec{\lambda}} \cos\left(\vec{k} \cdot \vec{\lambda} \right)$$

Calculate n and ξ using this Hamiltonian:

$$n = \langle n_{i\uparrow} \rangle + \langle n_{i\downarrow} \rangle =$$

$$= \frac{1}{N} \sum_k \left[\langle n_{k\uparrow} \rangle + \langle n_{k\downarrow} \rangle \right] =$$

$$= \frac{1}{N} \sum_k \left[n_F(\varepsilon_{k\uparrow} - \varepsilon_F) + n_F(\varepsilon_{k\downarrow} - \varepsilon_F) \right]$$

$$\varepsilon_{k\uparrow} = \varepsilon_k - \frac{Un\xi}{2}$$

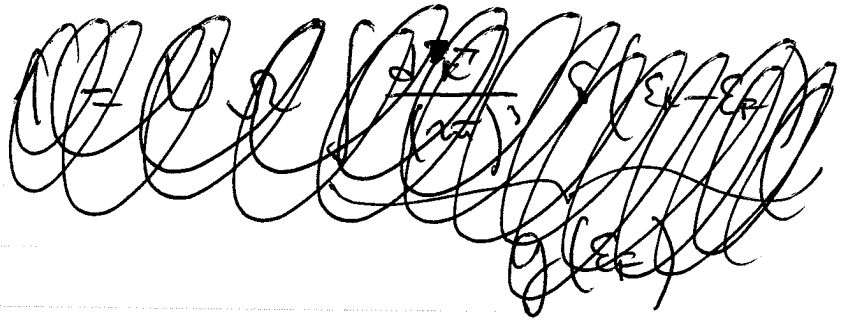
$$\varepsilon_{k\downarrow} = \varepsilon_k + \frac{Un\xi}{2}$$

$$n\xi = \frac{1}{N} \sum_k \left[n_F(\varepsilon_{k\uparrow} - \varepsilon_F) - n_F(\varepsilon_{k\downarrow} - \varepsilon_F) \right]$$

Find the condition for the appearance of a nonzero spin polarization ξ.

$$n\xi = \frac{1}{N} \sum_k \left[n_F(\varepsilon_k) - \frac{Un\xi}{2} \frac{dn_F}{d\varepsilon_k} - n_F(\varepsilon_k) - \right.$$

$$\left. - \frac{Un\xi}{2} \frac{dn_F}{d\varepsilon_k} \right] = -\frac{Un\xi}{N} \sum_k \frac{dn_F}{d\varepsilon_k}$$



$$\frac{dn_F}{d\varepsilon_k} \approx -\delta(\varepsilon_k - \varepsilon_F)$$

$$\frac{1}{N}\sum_k \delta(\varepsilon_k - \varepsilon_F) = g(\varepsilon_F) \text{ - density of states at Fermi energy (per site per spin).}$$

Thus we obtain:

$$g(\varepsilon_F)\, U = 1$$

Solution with nonzero spin polarization exists when:

$$g(\varepsilon_F)\, U > 1 \quad \text{- Stoner criterion.}$$

Physics: balance of the kinetic energy cost of spin polarization and the interaction energy gain.

Stoner criterion also sheds light on why only metals with unfilled d or f bands are ferromagnetic: bands have to be narrow to give high density of states at Fermi energy. Narrow bands ~~are~~ come from deeper atomic orbitals (such as d or f) where electrons are more localized (t is smaller).