Phys 726 – Lecture 18

Kondo Lattice Model

* Last class, we motivated the model

$$\hat{H}_{KLM} = -t \sum_{\langle ij \rangle} (c_i^\dagger c_j + c_j^\dagger c_i) + J \sum_i \tfrac{1}{2} c_i^\dagger \vec{\sigma} c_i \cdot \vec{S}_i$$

which was meant to describe the interaction between itinerant outershell electrons and a localized f-orbital electronic moment

→ t sets the scale for the electronic conduction band width; the ~~[illegible]~~ exchange coupling $J>0$ (antiferromagnetic) encourages the electron on atomic site i to form a singlet with the spin there

→ at half-filling, and in the limit $J \gg t$, the system is a nonmagnetic ~~[illegible]~~ insulator made up of internal singlets at each site i

→ moving away from half-filling amounts to doping this strong coupling limit with (heavy) holes and electrons

→ Based on a mean field treatment with $\vec{S} = \frac{1}{2} f^\dagger \vec{\sigma} f$ and a bilinear decomposition in $V = \frac{3J}{8} \langle f^\dagger c \rangle$, we found a mean field dispersion

$$E^{n}_{k\alpha} = \frac{1}{2}\left[\varepsilon_k - \mu_c - \mu_f + n\sqrt{(\varepsilon_k - \mu_c + \mu_f)^2 + 4V^2} \right]$$

chemical potential to set the conduction electron filling

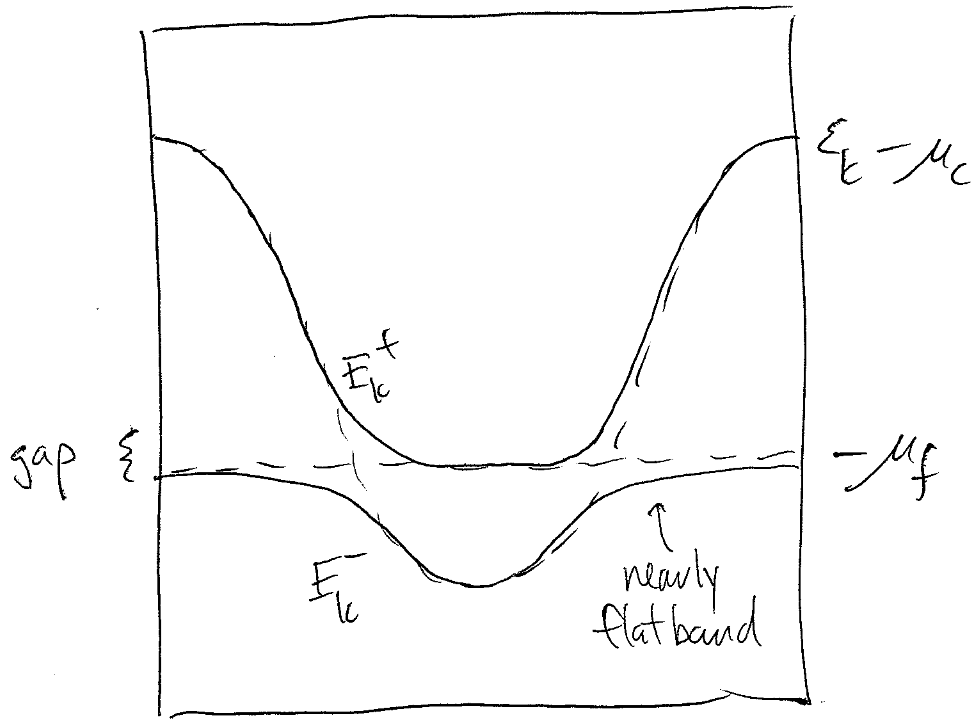
chemical potential to set $\langle f^\dagger f \rangle = 1$ so that $\frac{1}{2} f^\dagger \vec{\sigma} f \simeq \vec{S}$ (enforcing constraint on average)

order parameter of the mean field theory, determined self-consistently

→ a careful calculation shows that

$4V^2 \sim W^2 e^{-4W/3J}$, where $W \sim t$ is the conduction band width,

and $\frac{m^*}{m} = 1 + e^{+4W/3J}$



→ small gap and large effective mass controlled by factors $e^{-4W/3J}$ and $e^{+4W/3J}$

→ But if W/J is too large ($J \ll t$) then the Kondo energy scale is exponentially small, and it's in danger of losing out in competition with other kinds of magnetic order

Ruderman – Kittel – Kasuya – Yosida (RKKY) interaction

* Consider the limit in which $\sum_i \frac{1}{2} c_i^\dagger \vec{\sigma} c_i \cdot \hat{\vec{S}}_i$ is a weak perturbation of the free-electron Fermi sea that is the ground state of

$$\hat{H}_0 = -t \sum_{\langle ij \rangle} (c_i^\dagger c_j + c_j^\dagger c_i) = \sum_k \varepsilon_k c_k^\dagger c_k$$

→ In the crystal momentum language, the perturbation is

$$\hat{H}_1 = J \sum_j \frac{1}{2} \left(\frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{-i\vec{k}\cdot\vec{R}_j} c_{\vec{k}}^\dagger \right) \vec{\sigma} \left(\frac{1}{\sqrt{N}} \sum_{\vec{k}'} e^{i\vec{k}'\cdot\vec{R}_j} c_{\vec{k}'} \right) \cdot \hat{\vec{S}}_j$$

$$= \frac{J}{2} \sum_{\vec{k}\vec{k}'} c_{\vec{k}}^\dagger \vec{\sigma} c_{\vec{k}'} \cdot \frac{1}{N} \sum_j e^{i(\vec{k}'-\vec{k})\cdot R_j} \hat{\vec{S}}_j$$

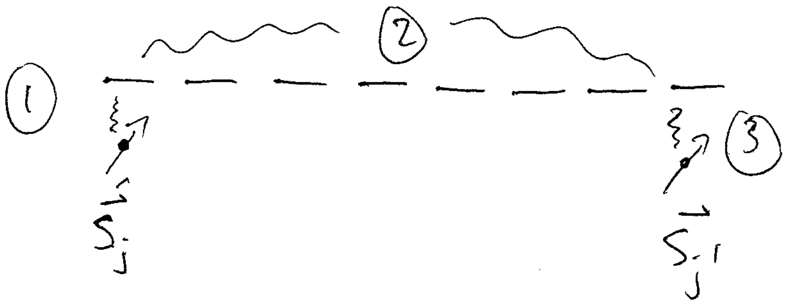
$$= \frac{J}{2} \sum_{\vec{k}\vec{k}'} c_{\vec{k}}^\dagger \vec{\sigma} c_{\vec{k}'} \cdot \hat{\vec{S}}_{\vec{k}'-\vec{k}}$$

→ Since the unperturbed Fermi sea is nonmagnetic and $\vec{\sigma}$ is ~~traceless~~ traceless

$$\langle F|\hat{H}_1|F\rangle = \frac{J}{2}\sum_{\vec{k}\vec{k}'}\sum_{\alpha\beta} \langle F|\underbrace{c^\dagger_{\vec{k}\alpha} c_{\vec{k}'\beta}}_{\delta_{\vec{k}\vec{k}'}\delta_{\alpha\beta}}|F\rangle\, \vec{\sigma}_{\alpha\beta}\cdot\hat{\vec{S}}_{\vec{k}'-\vec{k}}$$

$$= \frac{J}{2}\sum_{k}\langle \hat{n}_k\rangle\,(\mathrm{tr}\,\vec{\sigma})\cdot\hat{\vec{S}}_{\vec{k}'-\vec{k}} = 0$$

→ leading order contribution at second order



① Spin j interacts with electron at site j via $\hat{\vec{S}}_j\cdot\frac{1}{2}c^\dagger_j\vec{\sigma}c_j$

② Disturbance propagates in space and time

③ Disturbance interacts with spin at site j' via $\hat{\vec{S}}_{j'}\cdot\frac{1}{2}c^\dagger_{j'}\vec{\sigma}c_{j'}$

$$\hat{H}_1 = \frac{J}{2}\sum_{kk'} c_k^\dagger \vec{\sigma} c_{k'} \cdot \hat{\vec{S}}_{k'-k} = \frac{J}{2}\sum_{kq} c_k^\dagger \vec{\sigma} c_{k+q} \cdot \hat{\vec{S}}_q$$

→ Need overlap between states

$$|\psi_1\rangle = e^{-i\hat{H}_0 t}\,\hat{H}_1\,|F\rangle \quad \text{(perturb then evolve to time } t\text{)}$$

$$|\psi_2\rangle = \hat{H}_1\, e^{-iH_0 t}\,|F\rangle \quad \text{(evolve to time } t \text{ then perturb)}$$

$$\langle\psi_2|\psi_1\rangle = \langle F|\, e^{+iH_0 t}\,\hat{H}_1\, e^{-iH_0 t}\, H_1\,|F\rangle$$

$$= \frac{J^2}{4}\sum_{\substack{kk'\\qq'}}\sum_{\substack{\alpha\beta\\\mu\nu}} \langle F|\, e^{+iH_0 t}\, c_{k\alpha}^\dagger \vec{\sigma}_{\alpha\beta} c_{k+q,\beta}\cdot \hat{\vec{S}}_q$$

$$e^{-iH_0 t}\, c_{k'\mu}^\dagger \vec{\sigma}_{\mu\nu} c_{k'+q',\nu}\cdot \vec{S}_{q'}\, \cancel{}\,|F\rangle$$

$$= \frac{J^2}{4}\sum_{\substack{kk'\\qq'}}\sum_{\substack{\alpha\beta\\\mu\nu}} \langle F|\, e^{+iH_0 t}\, c_{k\alpha}^\dagger\, e^{-iH_0 t}\cdot e^{+iH_0 t}\, c_{k+q,\beta}$$

$$\cdot\, c_{k'\mu}^\dagger\, c_{k'+q',\nu}\,|F\rangle\,(\vec{\sigma}_{\alpha\beta}\cdot\hat{\vec{S}}_q)(\vec{\sigma}_{\mu\nu}\cdot\hat{\vec{S}}_{q'})$$

$$= \frac{J^2}{4}\sum_{\substack{kk'\\qq'}}\sum_{\substack{\alpha\beta\\\mu\nu}} \langle F|\, c_{k\alpha}^\dagger(t)\, c_{k+q,\beta}(t)\, c_{k'\mu}^\dagger(0)\, c_{k'+q',\nu}(0)\,|F\rangle$$

$$\times(\vec{\sigma}_{\alpha\beta}\cdot\hat{\vec{S}}_{\vec{q}})(\vec{\sigma}_{\mu\nu}\cdot\hat{\vec{S}}_{\vec{q}'})$$

$$= -\frac{J^2}{4} \sum_{\substack{kk' \\ qq'}} \sum_{\alpha\beta} \left(\vec{\sigma}_{\alpha\beta} \cdot \hat{\vec{S}}_{\vec{q}}\right)\left(\vec{\sigma}_{\mu\nu} \cdot \hat{\vec{S}}_{\vec{q}'}\right)$$

$$\times \langle F | c^\dagger_{k\alpha}(t)\, c^\dagger_{k'\mu}(0)\, c_{k+q,\beta}(t)\, c_{k'+q',\nu}(0) | F \rangle$$

$$\sim \langle F | c^\dagger_{k\alpha}(t)\, c_{k'+q',\nu}(0) | F \rangle \langle F | c^\dagger_{k'\mu}(0)\, c_{k+q\,\beta}(t) | F \rangle$$

$$- \langle F | c^\dagger_{k\alpha}(t)\, c_{k+q,\beta}(t) | F \rangle \langle F | c^\dagger_{k'\mu}(0)\, c_{k'+q'\nu}(0) | F \rangle$$

$$= \delta_{k,k'+q'}\, \delta_{\alpha\nu}\, G_k(t) \cdot \delta_{k',k+q}\, \delta_{\mu\beta}\, G_{k+q}(-t)$$

$$- \delta_{q,0}\, \delta_{\alpha\beta}\, G_k(0)\, \delta_{q',0}\, \delta_{\mu\nu}\, G_{k'}(0)$$

traces out $\vec{\sigma}_{\alpha\beta}$ traces out $\vec{\sigma}_{\mu\nu}$

NB $\delta_{k,k'+q'}\delta_{k',k+q} \Rightarrow q' = k - k' = -q$

$$= -\frac{J^2}{4} \sum_{kq} \sum_{\alpha\beta} \left(\vec{\sigma}_{\alpha\beta} \cdot \hat{\vec{S}}_{\vec{q}}\right)\left(\vec{\sigma}_{\beta\alpha} \cdot \hat{\vec{S}}_{-\vec{q}}\right) G_k(t)\, G_{k+q}(-t)$$

$$\sum_{\alpha\beta} \sigma^a_{\alpha\beta}\, \sigma^b_{\beta\alpha} = \mathrm{tr}\, \sigma^a \sigma^b = 2\delta^{ab}$$

$$= -\frac{J^2}{4} \sum_{kq} 2 G_k(t)\, G_{k+q}(-t)\, \hat{\vec{S}}_{\vec{q}} \cdot \hat{\vec{S}}_{-\vec{q}}$$

$$= -\frac{J^2}{4} \sum_{q} \left(2 \sum_{k} G_k(t)\, G_{k+q}(-t) \right) \vec{S}_{\vec{q}} \cdot \vec{S}_{-\vec{q}}$$

↑

nonlocal magnetic susceptibility

time averaged, $\chi(q) = 2 \sum_{k} \dfrac{n_{\vec{k}} - n_{\vec{k}+\vec{q}}}{\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}}}$

"Lindhard function"

and

$$\delta H = -\frac{J^2}{4} \sum_{q} \chi(q)\, \vec{S}_{\vec{q}} \cdot \vec{S}_{-\vec{q}}$$

$$= -\frac{J^2}{4} \sum_{jj'} \left(\frac{1}{N} \sum_{q} e^{i(\vec{R}_j - \vec{R}_{j'}) \cdot \vec{q}} \chi(q) \right) \vec{S}_j \cdot \vec{S}_{j'}$$

$$\equiv \sum_{jj'} J^{RKKY}_{jj'}\, \vec{S}_j \cdot \vec{S}_{j'}$$

* In the free-electron case,

$$\varepsilon_k = \frac{\hbar^2 k^2}{2m}$$

and $J^{RKKY}(r) \sim -J^2 D(\varepsilon_F) \frac{\cos 2k_F r}{(k_F r)^3}$ oscillations set by the length scale $2\pi/2k_F = \pi/k_F$

$\left(\text{or} \sim \frac{\sin(2k_F r + \pi d/2)}{r^d} \text{ in } d \text{ dimensions}\right)$

EXERCISE: What happens on a lattice?

e.g. square lattice with tight-binding dispersion $\varepsilon_k = -2t(\cos k_x a + \cos k_y a)$?