Phys 726 – Lecture 17

* We have seen how Coulomb repulsion between electrons in a solid can give rise to local magnetic moments and low-energy effective theories of Heisenberg form

→ but what happens when localized quantum spins and itinerant electrons coexist?

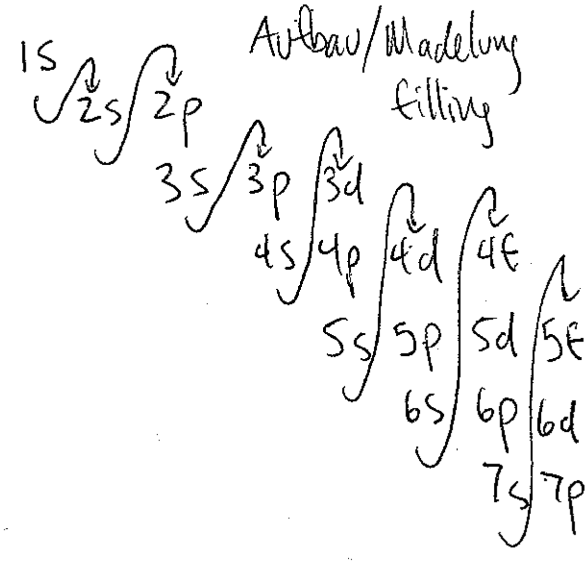
→ physical examples: Simple metals doped with magnetic ions (e.g. Fe impurities in Cu); bulk intermetallic compounds containing unpaired electrons in inner shells (e.g. UPt_3)

$$U: [Rn]\, 7s^2\, 5f^3\, 6d^1$$

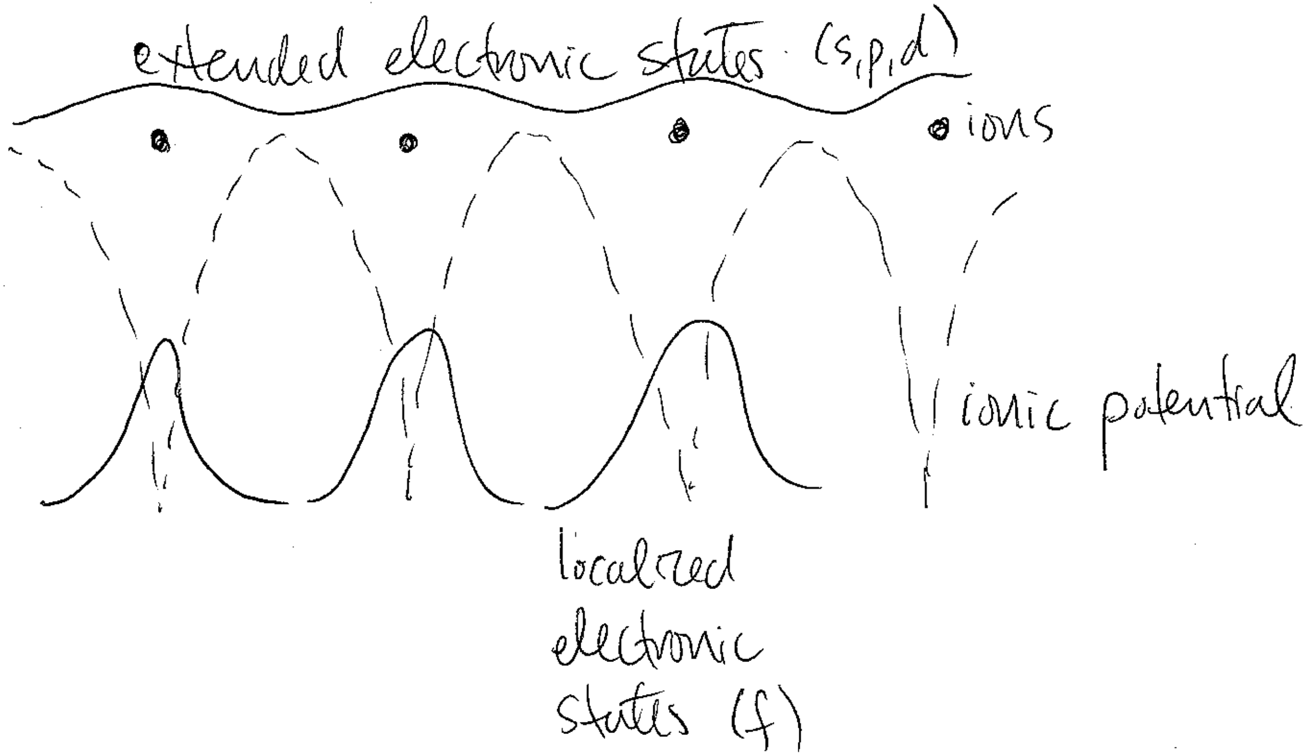
$7s^2$: big and inert

$5f^3$: compact and magnetic

Aufbau/Madelung filling



* Simplified picture



→ now have two species of fermion:

$c^\dagger, c$ for the conduction electrons

$f^\dagger, f$ for the core electrons

→ periodic Anderson model

$$\hat{H}_{PAM} = -t \sum_{\langle ij \rangle} (c_i^\dagger c_j + c_j^\dagger c_i) + \sum_i \left[\epsilon_f f_i^\dagger f_i + U (f_i^\dagger f_i - 1)^2 \right]$$

$$+ \sum_i (V^* f_i^\dagger c_i + V c_i^\dagger f_i)$$

Here, t is the hopping integral (which controls the width of the conduction band; ϵ_f is the binding energy of an electron in a core level; U is the strength of the Coulomb interacts that favour unit occupancy.

→ In rare earth crystals known as "Kondo lattice materials", the appropriate parameters are

$$|V| \ll t \ll U \quad \text{and} \quad |\epsilon_f| \ll U$$

c and f electrons hybridize only very weakly

Coulomb energy is the largest scale in the problem

$\Rightarrow \langle f_i^\dagger f_i \rangle \hat{=} 1$

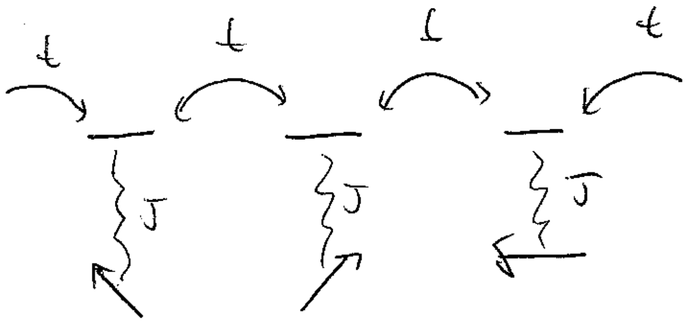
charge fluctuations are suppressed and $\hat{\vec{S}} = \frac{1}{2} f_i^\dagger \vec{\sigma} f_i$ behaves as a spin-half moment

$U \to \infty$ gives the Kondo Lattice model

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

exchange interaction strength $J \sim \frac{|V|^2}{U}$

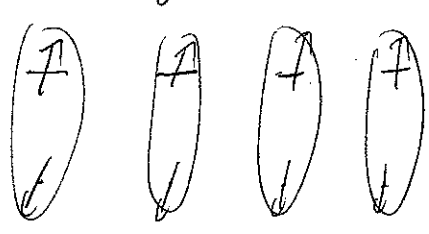
→ describes a periodic arrangement of quantum spins immersed in a conduction sea.



→ two regimes possible: $t \gg J$ or $\underline{t \ll J}$

strong tendency to form local singlets

cartoon at half-filling and large J

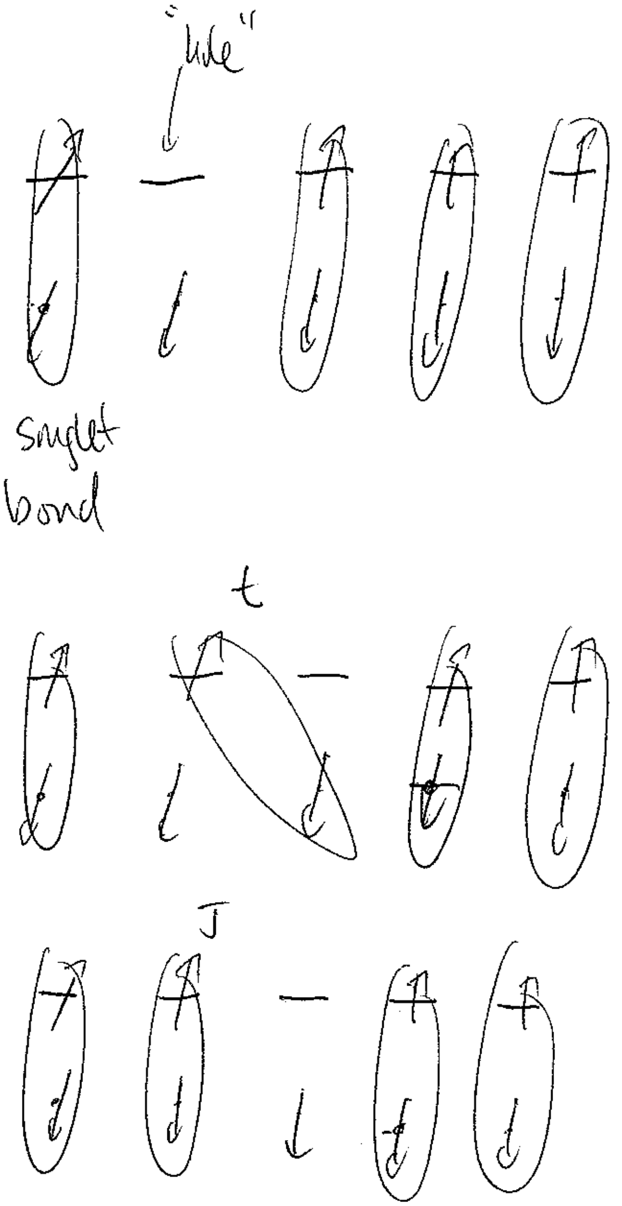


← one conduction electron per site bound in a local singlet

⇒ gap to spin and charge excitations

→ away from half-filling, the large-J KLM describes a "heavy metal"

→ addition holes ($n<1$) or electrons ($n>1$) propagate freely but their motion is sluggish because they have to move through the background of singlets



motion entails a disruption to the local environment through repeated breaking and reforming of singlets

Hybridization Mean Field

* KLM

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

where $\hat{\vec{S}} = \frac{1}{2} f_i^\dagger \vec{\sigma} f_i$ is a spin-half operator when $f_i^\dagger f_i = 1$

our approach will be to relax this constraint, enforcing it on average rather than exactly

→ identity

$$\frac{1}{4} c^\dagger \vec{\sigma} c \cdot f^\dagger \vec{\sigma} f = -\frac{3}{4} \hat{\chi}^{0\dagger} \chi^0 + \frac{1}{4} \hat{\vec{\chi}}^\dagger \cdot \hat{\vec{\chi}}$$

where $\hat{\chi}^\mu = \frac{1}{\sqrt{2}} f^\dagger \sigma^\mu c$ and $\sigma^\mu = (\mathbb{1}, \vec{\sigma})$ for $\mu = 0,1,2,3$

→ we want to treat the hybridization operators at the mean field level

* What is a mean-field approximation?

→ Sp. the operator $\hat{A}$ has an expectation value $\langle \hat{A} \rangle$. Then we can write

$$\hat{A} = \underset{\substack{\uparrow \\ \text{average} \\ \text{value}}}{\langle \hat{A} \rangle} + \underbrace{\left(\hat{A} - \langle \hat{A} \rangle \right)}_{\substack{\text{fluctuation} \\ \text{about the} \\ \text{average}}} \equiv \langle \hat{A} \rangle + \delta \hat{A}$$

$$\rightarrow \quad \hat{A}^\dagger \hat{A} = \left(\langle \hat{A} \rangle^* + \delta \hat{A}^\dagger \right) \left(\langle \hat{A} \rangle + \delta \hat{A} \right)$$

$$= |\langle \hat{A} \rangle|^2 + \langle \hat{A} \rangle \delta \hat{A}^\dagger + \langle \hat{A} \rangle^* \delta \hat{A} + \underbrace{\delta \hat{A}^\dagger \delta \hat{A}}_{\substack{\text{neglect if the} \\ \text{fluctuations are} \\ \text{small}}}$$

$$= |\langle \hat{A} \rangle|^2 + \langle \hat{A} \rangle \left(\hat{A}^\dagger - \langle \hat{A} \rangle^* \right) + \langle \hat{A} \rangle^* \left(\hat{A} - \langle \hat{A} \rangle \right) + O(\delta^2)$$

$$\cong \langle \hat{A} \rangle \hat{A}^\dagger + \langle \hat{A} \rangle^* \hat{A} - |\langle \hat{A} \rangle|^2$$

* In our case, we have a four-fermion operator

$$\frac{1}{4} c^\dagger \vec{\sigma} c \cdot f^\dagger \vec{\sigma} f = \underbrace{-\frac{3}{4} \hat{\chi}^{0\dagger} \hat{\chi}^{0}}_{\text{singlet channel}} + \underbrace{\frac{1}{4} \hat{\vec{\chi}}^{\dagger} \cdot \hat{\vec{\chi}}}_{\text{triplet channel}}$$

→ we'll assume $\langle \vec{\chi} \rangle = 0$ and treat the singlet channel at the mean-field level

$$\hat{\chi}^{0\dagger} \hat{\chi}^{0} = \langle \hat{\chi}^{0} \rangle^* \hat{\chi}^{0} + \hat{\chi}^{0\dagger} \langle \hat{\chi}^{0} \rangle - |\langle \chi^0 \rangle|^2$$

→ Hamiltonian is

$$\hat{H}_{MF} = -t \sum_{\langle ij \rangle} (c_i^\dagger c_j + c_j^\dagger c_i) - \sum_i (V_i^* f_i^\dagger c_i + V_i c_i^\dagger f_i)$$

$$+ \frac{8}{3J} \sum_i |V_i|^2 - \mu_c \sum_i c_i^\dagger c_i - \mu_f \sum_i f_i^\dagger f_i$$

where $V = \frac{3J}{4\sqrt{2}} \langle \hat{\chi}^0 \rangle = \frac{3J}{8} \langle f^\dagger c \rangle$ (self-consistency condition)

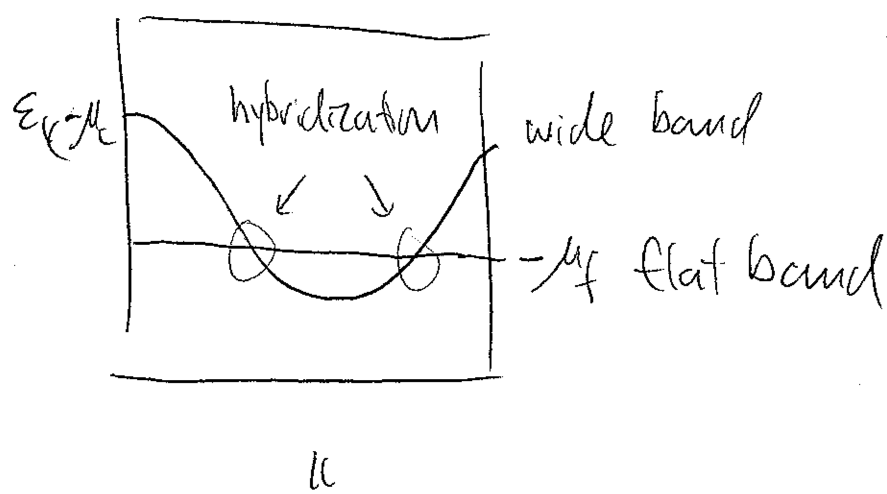
→ assume hybridization field is uniform in the ground state: $V_i = V = |V| e^{i\theta}$

→ assume V is real and positive; although $\langle f^\dagger c \rangle$ is complex, use the $U(1)$ gauge freedom associated with the invariance of $\hat{S} = \frac{1}{2} f^\dagger \vec{\sigma} f$ under $f \to e^{i\phi} f$

→ Hamiltonian becomes

$$\hat{H} = \sum_{k,\alpha} \left(c^\dagger_{k\alpha} \ f^\dagger_{k\alpha} \right) \begin{pmatrix} \varepsilon_k - \mu_c & -V \\ -V & -\mu_f \end{pmatrix} \begin{pmatrix} c_{k\alpha} \\ f_{k\alpha} \end{pmatrix} + \frac{8NV^2}{3J}$$

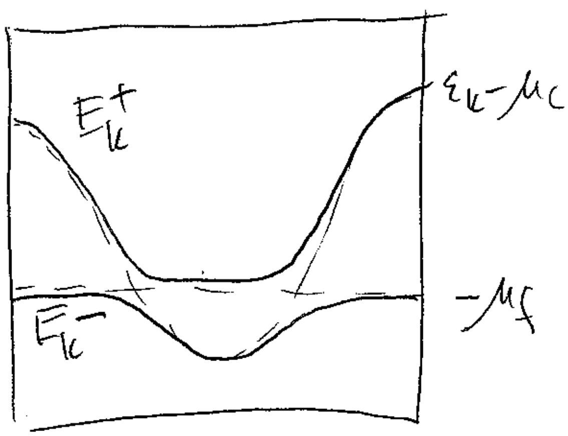
k: BZ; α: spin projection



* Diagonalize to get eigenenergies

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

where $2\mu = \mu_c + \mu_f$
$b = \mu_c - \mu_f$



→ but we have to simultaneously adjust μ and b (μ_c and μ_f) to achieve $\langle f^\dagger f \rangle = 1$ and the desired conduction band filling