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., UPt₃).

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

Extended electronic states (s,p,d) ions

Localized electronic states (f)

Now have two species of fermion:

$c^+_i$, $c_i$ for the conduction electrons

$f^+_i$, $f_i$ for the core electrons

Periodic Anderson Model

$$H_{PAM} = -t \sum_{i,j} \langle c^+_i c_j + c^+_j c^+_i \rangle + \sum_i \left[ \xi f^+_i f_i + U (f^+_i f_i - 1)^2 \right]$$

$$+ \sum_i (V^* f^+_i c_i + V c^+_i f_i)$$
Here, \( t \) is the hopping integral (which controls the width of the conduction band); \( E_f \) is the binding energy of an electron in a core level; \( V \) is the strength of the Coulomb interactions that favour unit occupancy.

\[ \rightarrow \text{In rare earth crystals known as "Kondo lattice materials", the appropriate parameters are} \]

\[ |V| \ll E \ll U \text{ and } E_f \ll U \]

\[ \uparrow \text{and f electrons hybridize only very weakly} \]

\[ \uparrow \text{Coulomb energy is the largest scale in the problem} \]

\[ \Rightarrow \langle f^+ f \rangle \approx 1 \text{ charge fluctuations are suppressed and} \]

\[ \hat{S} = \frac{1}{2} \hat{f}^\dagger \hat{f} = \hat{\tau} \text{ behaves as a spin-half moment} \]
\[ H_{\text{Kondo}} = -t \sum_{\langle ij \rangle} (c_i^+ c_j + c_j^+ c_i) + J \sum_i \frac{1}{2} c_i^+ i \sigma c_i \cdot S \]

Exchange interaction
Strength: \( J \approx \frac{W}{U} \)

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

→ two regimes possible:

\[ t \approx J \quad \text{or} \quad \frac{t}{J} \ll 1 \]

Strong tendency to form local singlets

Cartoon at half-filling and large \( J \):

One conduction electron per site bound on a local singlet

\[ \text{gap to spin and charge excitations} \]
away from half-filling, the large-$J$ KAM 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

\[ H = -t \sum_{\langle ij \rangle} (c_i^+ c_j + c_j^+ c_i) + J \sum_i \frac{1}{2} c_i^+ \sigma^z c_i - \frac{1}{2} \sum_i \cdot \cdot \cdot \]

where \( \vec{S} = \frac{1}{2} \epsilon_i^+ \vec{\sigma} \cdot \vec{\epsilon}_i \) is a spin-half operator

when \( \epsilon_i^+ \epsilon_i = 1 \)

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

\[ \frac{1}{4} c_{i \sigma}^+ c_{i \sigma} \cdot f^+ \delta f = -\frac{3}{4} \chi_0^+ \chi_0 + \frac{1}{4} \chi_+^2 - \chi_-^2 \]

where \( \chi^\mu = \frac{1}{\sqrt{2}} f^+ \sigma^\mu c \) and \( \sigma^\mu = (1, \vec{\sigma}) \)

for \( \mu = 0, 1, 2, 3 \)

We want to treat the hybridization operators at the mean field level.
What is a mean-field approximation? Suppose the operator $\hat{A}$ has an expectation value $\langle \hat{A} \rangle$. Then we can write

$$\hat{A} = \langle \hat{A} \rangle + (\hat{A} - \langle \hat{A} \rangle) = \langle \hat{A} \rangle + \delta \hat{A}$$

where $\langle \hat{A} \rangle$ is the average value and $\delta \hat{A}$ is the fluctuation about the average.

Then

$$\hat{A}^\dagger \hat{A} = (\langle \hat{A} \rangle + \delta \hat{A} \dagger)(\langle \hat{A} \rangle + \delta \hat{A})$$

$$= \langle \hat{A} \rangle^2 + \langle \hat{A} \rangle \delta \hat{A} \dagger + \langle \hat{A} \rangle \delta \hat{A}^\dagger + \delta \hat{A} \dagger \delta \hat{A}$$

Neglect if the fluctuations are small,

$$= \langle \hat{A} \rangle^2 + \langle \hat{A} \rangle \delta \hat{A} \dagger + \langle \hat{A} \rangle \delta \hat{A}^\dagger + \delta \hat{A} \dagger \delta \hat{A} = O(\delta^2)$$

$$\approx \langle \hat{A} \rangle^2 + \langle \hat{A} \rangle \delta \hat{A} \dagger + \langle \hat{A} \rangle \delta \hat{A}^\dagger$$

$$= \langle \hat{A} \rangle \hat{A}^\dagger + \langle \hat{A} \rangle^\dagger \hat{A} \approx \langle \hat{A} \rangle^2 + \langle \hat{A} \rangle \delta \hat{A} \dagger + \langle \hat{A} \rangle \delta \hat{A}^\dagger$$
In our case, we have a four-fermion operator

\[
\frac{1}{4} \mathbf{c}^\dagger \mathbf{c} \cdot \mathbf{\xi}^\dagger \mathbf{\xi} = -\frac{3}{4} \chi^{0 \dagger} \chi^{0} + \frac{1}{4} \chi^{+ \dagger} \chi^{-} \chi^{0}
\]

- singlet channel
- triplet channel

\[\rightarrow \text{we'll assume } \langle \chi^{0} \rangle = 0 \text{ and treat the singlet channel at the mean-field level}\]

\[\chi^{0 \dagger} \chi^{0} = \langle \chi^{0} \rangle^{*} \chi^{0} + \chi^{+ \dagger} \chi^{-} \langle \chi^{0} \rangle - 1 \langle \chi^{0} \rangle^{2}\]

\[\rightarrow \text{Hamiltonian is}\]

\[\hat{H}_{\text{MF}} = - \epsilon \sum_{i,j} (c_i^\dagger c_j + c_j^\dagger c_i) - \sum_{i} (V_i \xi_i^+ c_i + V^*_i \xi_i^+ c_i^\dagger)\]

\[+ \frac{\alpha}{3J} \sum_{i,j} |V_i|^2 - \mu_c \sum_{i} c_i^\dagger c_i - \mu_f \sum_{i} \xi_i^+ \xi_i \]

where \[V = \frac{3J}{4J^{1/2}} \langle \chi^{0} \rangle = \frac{3J}{8} \langle \xi^\dagger \xi \rangle \quad \text{(self-consistency condition)}\]
\[ \text{assume hybridization field is uniform in the ground state: } V_i = V = (V/1) e^{i \theta} \]

\[ \text{assume } V \text{ is real and positive; although } <f^+c> \text{ is complex, use the U(1) gauge freedom associated with the invariance of } S = \frac{1}{2} f^+ e^{-i} f \text{ under } f \rightarrow e^{i \lambda} f \]

\[ \text{Hamiltonian becomes} \]

\[ H = \sum_{\mathbf{k}, \alpha} \left( C_{\mathbf{k} \alpha}^T f_{\mathbf{k} \alpha} \right) \begin{pmatrix} \varepsilon_{\mathbf{k}} - m_c & -V \\ -V & -m_c \end{pmatrix} \left( C_{\mathbf{k} \alpha} \right) + \frac{3N V^2}{2J} \]

\[ \text{BZ spin projection} \]

\[ \begin{array}{c}
\text{hybridization} \\
\text{wide band} \\
-\mu_c \text{ flat band}
\end{array} \]
Diagonalize to get eigenenergies

\[ E_{k}\alpha = \frac{1}{2} \left[ \varepsilon_k - z \mu + \sqrt{(\varepsilon_k - b)^2 + 4\mu^2} \right] \]

where

\[ 2\mu = \mu_c + \mu_f \]

\[ b = \mu_c - \mu_f \]

\[ E_{k}^c \]

\[ E_{k}^f \]

\[ \varepsilon_k - \mu_c \]

\[ -\mu_f \]

but we have to simultaneously adjust \( \mu \) and \( b \) (\( \mu_c \) and \( \mu_f \)) to achieve \( (E_{k}^c + E_{k}^f) = 1 \) and the desired conduction band filling