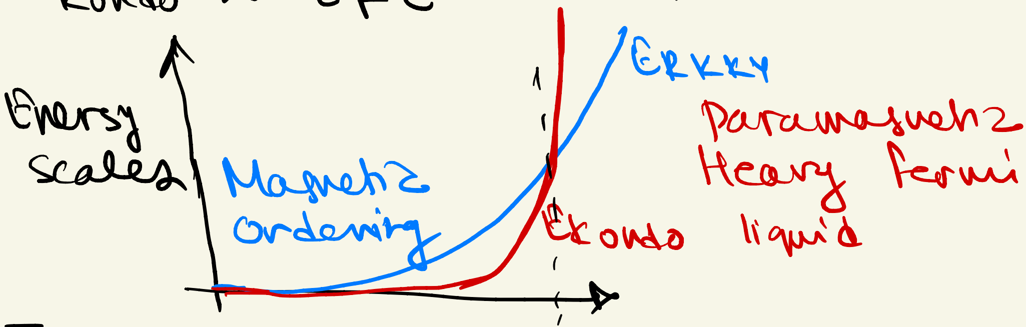
Heavy Fermions and Kondo Lattices

General aspects:

— RKKY Vs Kondo competition:

$$H_{RKKY} = J_K^2 \sum_{rr'} \frac{S(r)\cdot S(r') \cos(2k_F r)\, N(E_F)}{r^3}$$

$$T_{Kondo} \sim E_F\, e^{-1/N(E_F) J_K}.$$



In HFL:

— large effective mass and small Z

— ARPES hard despite large D.O.S. at E_F (related to small Z)

— Often proximity to a quantum critical point with non-fermi liquid behavior in the quantum critical regime.

Mean-field Solution to the Kondo lattice model in the heavy fermion phase.

Consider the Kondo lattice model:

$$H = \sum_{k\sigma} \varepsilon_k \, c^\dagger_{k\sigma} c_{k\sigma} + \frac{J_K}{2} \sum_r c^\dagger_r \vec{\sigma} c_r \cdot \vec{S}_r$$

Lets represent spins $\vec{S}_r$ in terms of spin-1/2 spinons (partons):

$$\vec{S}_r = f_r^\dagger \frac{\vec{\sigma}}{2} f_r$$

where

$f_r = \begin{bmatrix} f_{r\uparrow} \\ f_{r\downarrow} \end{bmatrix}$ is a two component (fermionic) spinor.

In terms of f, the Kondo interaction term is $\frac{J_K}{2}\sum_r f^\dagger_{r\alpha}\frac{\sigma^a_{\alpha\beta}}{2} f_{r\beta}\, c^\dagger_{r\gamma}\sigma^a_{\gamma\delta} c_{r\delta}$

Using $\sigma^a_{\alpha\beta}\sigma^a_{\gamma\delta} = 2\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\beta}\delta_{\gamma\delta}$, the interaction becomes

$$-\frac{J_K}{2}\sum_r c^\dagger_{r\alpha} f_{r\alpha} f^\dagger_{r\beta} c_{r\beta}$$

$$-\sum_r \frac{J_K}{4} c^\dagger_r c_r$$ ← this term can be absorbed in the chemical potential.

Within path-integral, the action is

$$S = \int d\tau \sum_{k\sigma} \bar{c}_{k\sigma}(\partial_\tau - \varepsilon_k) c_{k\sigma}$$

$$+ \int d\tau \sum_{r\sigma} \bar{f}_{r\sigma}(\partial_\tau - i a_0) f_{r\sigma} + i a_0$$

$$-\frac{J_K}{2}\int d\tau \sum_{r\alpha\beta} \bar{c}_{r\alpha} f_{r\alpha} \bar{f}_{r\beta} c_{r\beta}$$

where a_0 is the Lagrange multiplier that enforces $\sum_\sigma f_\sigma^\dagger f_\sigma = 1$.

Crucially, one mus allow a_0 to be a fluctuating field i.e. $a_0 = a_0(r,\tau)$ and therefore it acts like the time-component of a U(1) guage field. 'f' carries guage charge +1 of this gauge field while 'c' is uncharged under this guage field. If spinons acquire a kinetic energy term (which will generically be automatically generated), then the spatial component of $\vec{a}$ will also appear in the action as $\bar{f}_r f_{r'} e^{i a_{rr'}}$.

For now, we ignore the kinetic energy of spinons as its not important deep in the heavy Fermi liquid phase.

In addition, one can write down the kinetic energy for the guage field itself $\int d\tau \int d^d r \ \frac{(\nabla \times a)^2}{e^2}$.

The action is invariant under the following transformations:

global: $U(1)$ charge conservation corresponding to E-M fields: $c \to e^{i\theta} c$.

$SU(2)$ spin rotation: $c \to Uc$, $f \to Uf$. $U \in SU(2)$.

gauge redundancy : $f \to f e^{i\theta(r,\tau)}$

$$a_0 \to a_0 + \partial_\tau \theta$$

$$a_{rr'} \to e^{i(\theta_r - \theta_{r'})}$$

In the heavy Fermi liquid phase, $\langle \bar{c}_{r\alpha} f_{r\alpha} \rangle$ forms a Higgs condensate and therefore the gauge field is gapped out. One can describe such a phase within the following mean-field:

$$H_{MF} : \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \mu_f \sum_{k\sigma} f^\dagger_{k\sigma} f_{k\sigma}$$

$$- V \sum_k (c^\dagger_{k\sigma} f_{k\sigma} + h.c.)$$

where $\langle f^\dagger_{r\sigma} f_{r\sigma} \rangle = 1$ ← constrained imposed only on average.

and $V = \frac{J_K}{2} \langle c^\dagger_{r\sigma} f_{r\sigma} + h.c. \rangle$.

$$\Rightarrow H_{MF} = \sum_{k\sigma} \begin{bmatrix} c^{\dagger}_{k\sigma} & f^{\dagger}_{k\sigma} \end{bmatrix} h_k \begin{bmatrix} c_{k\sigma} \\ f_{k\sigma} \end{bmatrix}$$

where $h_k = \begin{bmatrix} \varepsilon_k & -V \\ -V & \mu_f \end{bmatrix}$

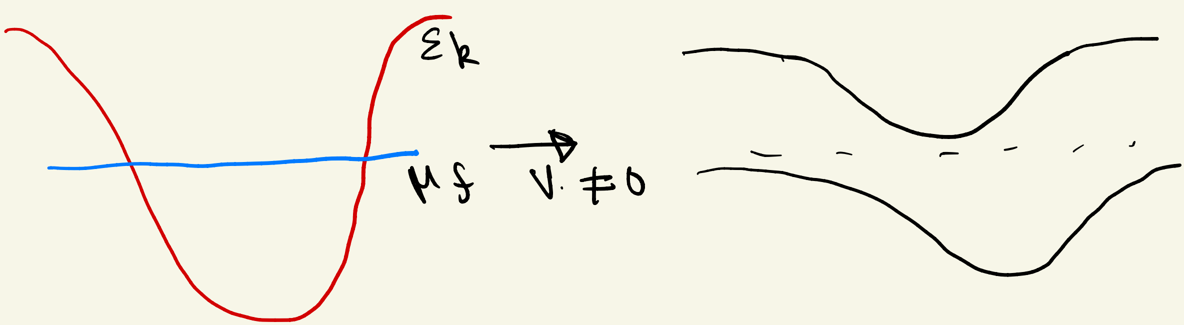
$$= \varepsilon_k \left(\frac{\mathbb{1}+\tau^z}{2}\right) + \mu_f \left(\frac{\mathbb{1}-\tau^z}{2}\right) - V\tau^x$$

$$= \left(\frac{\varepsilon_k+\mu_f}{2}\right)\mathbb{1} + \frac{(\varepsilon_k-\mu_f)}{2}\tau^z - V\tau^x$$

$\Rightarrow$ eigenvalues of h_k

$$= \frac{\varepsilon_k+\mu_f}{2} \pm \sqrt{V^2 + \left(\frac{\varepsilon_k-\mu_f}{2}\right)^2}$$

$$\equiv \epsilon_k^{\pm}$$



Let's determine V self-consistently:

$$V = \frac{J_K}{2} \langle c^\dagger_{r\sigma} f_{r\sigma} + h.c. \rangle$$

$$= \frac{J_K}{2V} \sum_{k\sigma} \langle c^\dagger_{k\sigma} f_{k\sigma} + h.c. \rangle$$

$$= \frac{J_K}{2N_s} - \frac{\partial E_g}{\partial V}$$

where E_g is the ground state energy. Let's assume number of local moments $= N_s$ (no. of sites)

No. of conduction electrons $= N_c < N_s$.

In this situation, the lower band will be partially filled, and the upper band will be completely empty.

$$\Rightarrow V = -\frac{J_K}{2} \int d^d k \; \theta(\varepsilon_F - E_k^-) \frac{\partial E_g}{\partial V}$$

$$= +\frac{J_K}{2} \int d^d k \frac{\theta(\varepsilon_F - E_k^-) V}{\sqrt{V^2 + \frac{(\mu_f - \varepsilon_k)^2}{4}}}$$

$$\simeq \frac{J_K}{2} N(E_F) V \int \frac{d\varepsilon}{\sqrt{V^2 + \frac{\varepsilon^2}{4}}}$$

$$\Rightarrow \frac{2}{J_K} \simeq 2N(E_F) \log\left(\frac{E_F}{V}\right)$$

$$\Rightarrow V \simeq E_F \, e^{-\frac{1}{N(E_F) J_K}} .$$

(Compare with the expression for the 'binding energy' in single impurity problem).

Heaviness of the bands :

Density of state at the Fermi level $N(E_F)$

$$= \int d^d k \;\; \delta(E_F - E_{\bar{k}})$$

for $E_{\bar{k}}$ close to E_F ($\simeq \mu_f$)

$$E_{\bar{k}} \simeq \mu_f - \frac{V^2}{\varepsilon_k - \mu_f}$$

$$\Rightarrow N(E_F) \simeq \int d\varepsilon \; \rho_c(\varepsilon) \, \delta\left(E_F - \mu_f + \frac{V^2}{\varepsilon - \mu_f}\right)$$

where $\rho_c(\varepsilon)$ is the density of states of the non-interacting conduction e^-s. Approximating E_f as,

$$E_{\cancel{F}} \simeq \mu_f - \frac{V^2}{\varepsilon(k_F) - \mu_f}$$

$$\Rightarrow N(E_F) \simeq \int d\varepsilon\, \rho_c(\varepsilon)\, \delta\left[\frac{V^2}{\varepsilon - \mu_f} - \frac{V^2}{\varepsilon(k_F) - \mu_f}\right]$$

$$= \frac{\rho_c(\varepsilon_{k_F})}{\left|\frac{\partial}{\partial \varepsilon}\left[\frac{V^2}{\varepsilon - \mu_f}\right]\right|_{\varepsilon_F}} = \rho_c(\varepsilon_{k_F})\, \frac{(\varepsilon(k_F) - \mu_f)^2}{V^2}$$

$[\varepsilon(k_F) - \mu_f]$ would be typically of the order of the band-width of the non-interacting e^-s. (let's denote it as t)

$$\Rightarrow N(E_F) \simeq \rho_c(\varepsilon_{k_F})\, \frac{t^2}{V^2} \gg \rho_c(\varepsilon_{k_F}).$$

$$\Rightarrow \quad \frac{m^*}{m} \sim e^{\frac{2}{N(E_f) J_K}}$$

Quasiparticle residue Z :

Following Fermi-liquid arguments, one expects that $Z_1 \sim \frac{m}{m^*} \sim \frac{V^2}{t^2}$

$$\sim e^{\frac{2}{N(E_F) J_K}} \ll 1.$$

Let's show this explicitly.

Residue Z_1 is defined as the strength of the pole in the Green's f^n at the Fermi energy :

$$G(k_F, i\omega) = \frac{Z}{i\omega - E(k_F)}$$

where $G(k, i\omega)$ is the Fourier transform of $\langle c(k,\tau)\, c^\dagger(k, \tau=0)\rangle$.

Recall the mean field Hamiltonian derived above:

$$H_{MF} = \sum_{k\sigma} \begin{bmatrix} c^{\dagger}_{k\sigma} & f^{\dagger}_{k\sigma} \end{bmatrix} h_k \begin{bmatrix} c_{k\sigma} \\ f_{k\sigma} \end{bmatrix}$$

where $h_k = \begin{bmatrix} \varepsilon_k & -V \\ -V & \mu_f \end{bmatrix}$

One may diagonalize h_k using a unitary matrix $U_k = \begin{bmatrix} \cos\theta_k & \sin\theta_k \\ \sin\theta_k & -\cos\theta_k \end{bmatrix}$:

$$\begin{bmatrix} c_{k\sigma} \\ f_{k\sigma} \end{bmatrix} = U_k \begin{bmatrix} \gamma_{k,+,\sigma} \\ \gamma_{k,-,\sigma} \end{bmatrix}$$, so that

$$H = E_k^{+} \gamma^{\dagger}_{k,+,\sigma} \gamma_{k,+,\sigma}$$

$$+ E_k^{-} \gamma^{\dagger}_{k,-,\sigma} \gamma_{k,-,\sigma}$$

Solving for $\cos(\theta_k)$ one finds,

$$\cos^2\theta_k \simeq 1 - \frac{v^2}{t^2}$$

$$\Rightarrow \quad \sin^2\theta_k \simeq \frac{v^2}{t^2}.$$

The Green's fn is then given by,

$$\langle c(k,\tau)\, c^\dagger(k,\tau=0)\rangle$$

$$= \cos^2\theta_k \langle \gamma_+(k,\tau)\, \gamma_+^\dagger(k,\tau=0)\rangle + \sin^2\theta_k \langle \gamma_-(k,\tau)\, \gamma_-^\dagger(k,\tau=0)\rangle$$

$$= \cos^2\theta_k\, e^{-\epsilon_k^+ \tau} + \sin^2\theta_k\, e^{-\epsilon_k^- \tau}$$

$$\Rightarrow \langle c(k,i\omega)\, c^\dagger(k,i\omega)\rangle$$

$$= \frac{\cos^2\theta_k}{i\omega - \epsilon_k^+} + \frac{\sin^2\theta_k}{i\omega - \epsilon_k^-}$$

Since the Fermi energy lies in the E_k^- band,

$$Z_1 = \sin^2\theta_k \simeq \frac{V^2}{t^2}$$

$$= \frac{m}{m^*} \ll 1.$$