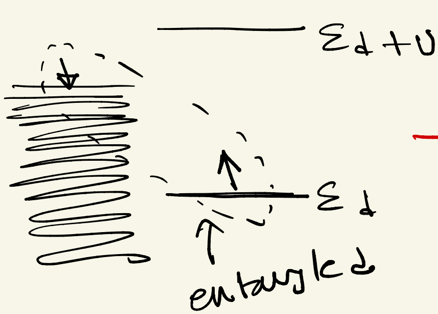
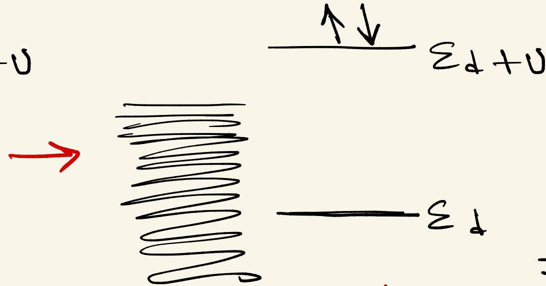
Variational Approach to Anderson's impurity problem.

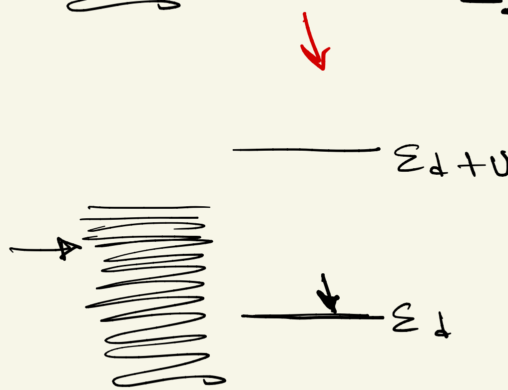
$$H = \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \varepsilon_d c^\dagger_{d\sigma} c_{d\sigma} + U n_{d\uparrow} n_{d\downarrow} + \sum_k \left[V_k c^\dagger_{k\sigma} c_{d\sigma} + h.c. \right]$$

Basic physics when U large, ε_d below fermi energy and $\varepsilon_d + U$ above the fermi energy:





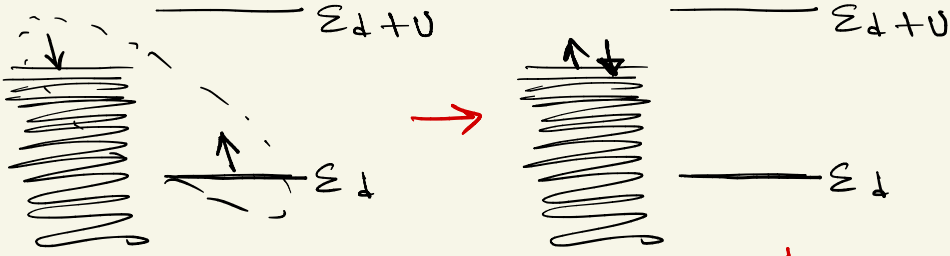
intermediate energy $= 2\varepsilon_d + U$



initial energy $= \varepsilon_F + \varepsilon_d$

$$\Delta E_1 = 2\varepsilon_d + U - (\varepsilon_F + \varepsilon_d)$$

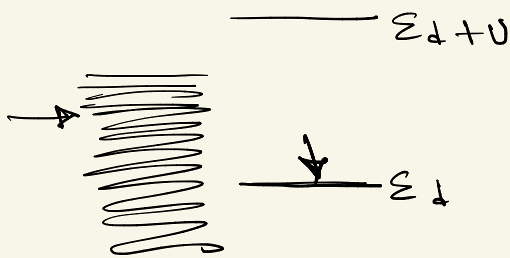
intermediate energy $= 2\varepsilon_F$



initial energy

$= \varepsilon_d + \varepsilon_F$

$\Delta E_2 = 2\varepsilon_F - (\varepsilon_d + \varepsilon_F)$



$$H_{eff} \simeq V^2 \, c^\dagger_k \vec{\sigma} c_{k'} \cdot \vec{S} \left[\frac{1}{\Delta E_1} + \frac{1}{\Delta E_2} \right]$$

$$\Delta E_1 \sim U + \varepsilon_d - \varepsilon_F, \quad \Delta E_2 \sim -\varepsilon_d + \varepsilon_F$$

$$\Rightarrow H_{eff} \simeq J \, c^\dagger \vec{\sigma} c \cdot \vec{S}.$$

$J \simeq \dfrac{V^2}{|\tilde{\varepsilon}_d|}$ = Antiferromagnetic.

where $\tilde{\varepsilon}_d = \varepsilon_d - \varepsilon_F$.

To capture the entanglement between the local moment and the conduction e^-s, consider the following trial wave-f^n:

$$|\psi\rangle = \left[\alpha_0 + \sum_{k<k_F} \alpha_{\vec{k}}\, c_{k\sigma}\, d^\dagger_\sigma\right]|0\rangle$$

where $|0\rangle$ denotes filled-fermi sea $\otimes$ empty d-level.

The variational energy is given by,

$$E_{var} = \frac{\langle\psi|\,H|\psi\rangle}{\langle\psi|\psi\rangle}$$

$$= \frac{2\sum_{k<k_F}\left[\alpha^2_k\,(\varepsilon_d - \tilde{\varepsilon}_{\vec{k}}) + 2\alpha_0\,\alpha_k V_{\vec{k}}\right]}{\alpha_0^2 + 2\sum_{\vec{k}} \alpha^2_{\vec{k}}}$$

where we have set the energy of the filled Fermi sea to zero (as a convention).

$$\frac{\partial E_{var}}{\partial \alpha_0} = \frac{\partial E_{var}}{\partial \alpha_k} = 0 \implies$$

$$\alpha_0 E_{var} = 2 \sum_{k<k_F} \alpha_k V_k$$

$$\alpha_k E_{var} = (\varepsilon_d - \tilde{\varepsilon}_k)\alpha_k + \alpha_0 V_k$$

$$\implies E_{var} = 2 \sum_{k<k_F} \frac{|V_k|^2}{E_{var} - \varepsilon_d + \tilde{\varepsilon}_k}$$

One may define the binding energy as $\Delta_K = E_{var} - \varepsilon_d$. If

$\Delta_K < 0$, then the entangled state $|\varphi\rangle$ has a lower energy than the product state $|\text{filled Fermi sea}\rangle \otimes |\text{singly occupied } f\text{-level}\rangle$.

$$\Rightarrow \varepsilon_d + \Delta_K = 2 \sum_{k<k_F} \frac{|V_k|^2}{\Delta_K + \tilde{\varepsilon}_k}$$

$$\simeq 2N(0) \int_{-\varepsilon_F}^{0} \frac{V^2}{\Delta_K + \tilde{\varepsilon}_k}$$

where $N(0)$ = DOS at the fermi energy.

$$\simeq -2N(0)V^2 \log\left[\frac{\varepsilon_F}{|\Delta_K|}\right]$$

(ε_F = Fermi energy)

When $|\Delta_K| \ll \varepsilon_f$,

$$\Delta_K = -\varepsilon_F e^{-\frac{1}{2N(0)V^2/\varepsilon_f}}$$

$$\simeq -\varepsilon_F e^{-\frac{1}{2N(0)J_K}}.$$

One may define a Kondo temperature $T_K \simeq \Delta_K$ and Kondo length scale $\xi_K \simeq v_F/\Delta_K$ that captures the size of the "screening cloud" of the conduction e^-'s around the electrons.

One can show that the occupation level of the impurity

$$\simeq 1 - \frac{\pi \Delta_K}{2 N(0) |V|^2} \simeq 1.$$

Scattering phase shift = occupation
δ / π

$$\delta_\uparrow = \delta_\downarrow = \frac{\pi}{2}. \Rightarrow \text{Resonant scattering.}$$

More on Kondo length scale:

Recall the entangled wave-fn we are considering:

$$|\psi\rangle = \Big[\alpha_0 + \sum_{k<k_F} \alpha_{\vec{k}} \, c_{k\sigma} \, d^{\dagger}_{\sigma} \Big] |0\rangle$$

If we choose the location of the magnetic impurity to be at the origin, then the amplitude corresponding to entanglement between conduction e^- at $\vec{r}$ and the local moment is:

$$\alpha(\vec{r}) = \int_k \alpha_{\vec{k}} \, e^{i\vec{k}\cdot\vec{r}}$$

We now show that $\alpha(\vec{r})$ decays as e^{-r/ξ_K} where ξ_K is the size of the Kondo screening cloud mentioned above.

As shown above, after variational minimization, one obtains,

$$\alpha_{\vec{k}} = \frac{\alpha_0 V_{\vec{k}}}{\Delta_K + \tilde{\varepsilon}_{\vec{k}}}$$

$$\Rightarrow \quad \alpha_{\vec{r}} = \alpha_0 \int_{\vec{k} < k_F} \frac{V_{\vec{k}} \, e^{i\vec{k}\cdot\vec{r}}}{\Delta_K + \tilde{\varepsilon}_{\vec{k}}}$$

Since only e^- close to the Fermi surface are involved in the hybridization, one may assume $V_{\vec{k}} = V = \text{constant}$ and $\tilde{\varepsilon}_{\vec{k}} = -v_F |k - k_F| < 0$

$$\Rightarrow \quad \alpha_{\vec{r}} \simeq -\alpha_0 V \int_{k<k_F} \frac{e^{i\vec{k}\cdot\vec{r}}}{|\Delta_K| + v_F|k-k_F|}$$

where we have used that

$$\Delta_K \left(= -\varepsilon_F\, e^{-\frac{1}{2N(0)|V|^2/\varepsilon_d}} \right) < 0.$$

Due to pole at imaginary k, the above integral decays exponentially as

$$\alpha_{\vec{r}} \sim e^{-|r|/\xi_K}$$

where $\xi_K \sim \dfrac{v_F}{|\Delta_K|}$, as anticipated.