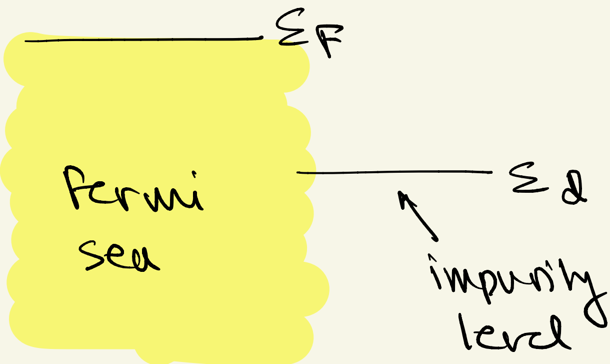
Anderson's impurity model

Consider a magnetic impurity in a metal.



Since the impurity is coupled to a continuum of states, one might expect that an electron that occupies this level will have a finite lifetime and the impurity level will acquire a non-zero width. However, when $\varepsilon_d \ll \varepsilon_F$, all electronic states close to ε_d are already occupied and it is not obvious that the hybridization is enough to quench the magnetic moment. Further, local Coulomb repulsion on the impurity, e.g. a Hubbard term $U n_{d\uparrow} n_{d\downarrow}$ ($U > 0$), will also enhance the tendency to retain the magnetic moment.

To capture the competition between hybridization and onsite Coulomb repulsion Anderson considered the following model:

$$H = \sum \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \varepsilon_d \sum_\sigma d^\dagger_\sigma d_\sigma$$
$$+ U n_{d\uparrow} n_{d\downarrow} + \sum_{k,\sigma} (V_k c^\dagger_{k\sigma} d_\sigma + \text{h.c.})$$

Note that $d^\dagger_\sigma$ does not have any momentum label since it corresponds to a single localized level.

A magnetic solution would correspond to $\langle n_{d\uparrow} \rangle \neq \langle n_{d\downarrow} \rangle$. Physically, this seems impossible since this would imply spontaneous symmetry breaking in 0+1-d. What actually happens is that in the regime of mean-field where such a magnetic solution exists, one may safely replace the local impurity level with a single spin-1/2 and it turns out that the corresponding model (single impurity Kondo model) exhibits physics that explains the Kondo resistivity minimum.

To proceed with the mean-field, we replace

$$U n_{d\uparrow} n_{d\downarrow} \longrightarrow U\left[\langle n_{d\uparrow}\rangle n_{d\downarrow} + n_{d\uparrow}\langle n_{d\downarrow}\rangle - \langle n_{d\uparrow}\rangle\langle n_{d\downarrow}\rangle\right].$$

We would be interested in local density of states at the impurity level. It is useful to carry out the mean-field as follows. The Heisenberg equation of motion for $c_{k\sigma}$ d_σ is

$$i\frac{\partial c_{k\sigma}}{\partial t} = [c_{k\sigma}, H]$$

$$i\frac{\partial d_\sigma}{\partial t} = [d_\sigma, H]$$

Fourier transforming, one obtains,

$$\omega c_{k\sigma} = \varepsilon_k c_{k,\sigma} + V_k d_\sigma$$

$$\omega d_\sigma = \varepsilon_d d_\sigma + U \langle n_{d-\sigma} \rangle d_\sigma + \sum_k V^*_k c_{k\sigma}$$

From these equations, one may obtain the Green's f^n $\langle d^\dagger_\sigma(\omega) d_\sigma(\omega) \rangle \equiv G^\sigma_{dd}$ for the impurity,

$$G^\sigma_{dd} = \frac{1}{\omega - \varepsilon_d - U\langle n_{d-\sigma}\rangle - \sum_k \frac{|V_k|^2}{\omega - \varepsilon_k}}$$

The density of states at the impurity is given by

$$\rho_{d\sigma}(\omega) = \mathrm{Im}\ G^{d}_{\sigma\sigma}(\omega + i\varepsilon)$$

$$\simeq \frac{1}{\pi} \frac{\Gamma}{\Gamma^2 + (\omega - \varepsilon_d - U\langle n_{d-\sigma}\rangle)^2}$$

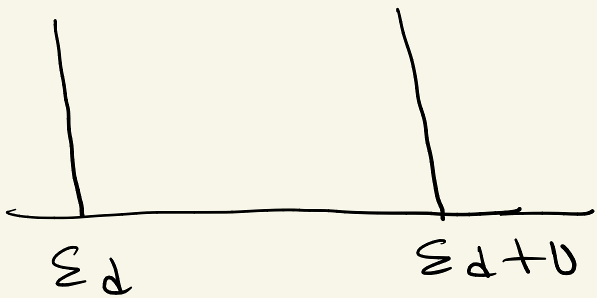
where $\Gamma = \pi \sum_k |V_k|^2 \delta(\omega - \varepsilon_k)$

$$\simeq \pi \overline{|V_k|^2} \rho(\varepsilon_F)$$

and we have dropped the real part of $\sum_k \frac{|V_k|^2}{\omega + i\varepsilon - \varepsilon_k}$ since it can be absorbed as a shift in ε_d.

As $\Gamma \sim \overline{|V_k|^2} \to 0$, the density of states becomes two delta-fn peaks as expected:

$\Gamma = 0$



In the presence of non-zero Γ, these levels broaden. One expects that when $U \gg \Gamma$, the magnetic solution $\langle n_{d\uparrow} \rangle \neq \langle n_{d\downarrow} \rangle$ will persist. This is indeed the case.

To see, one finds $\langle n_{d\sigma}\rangle$

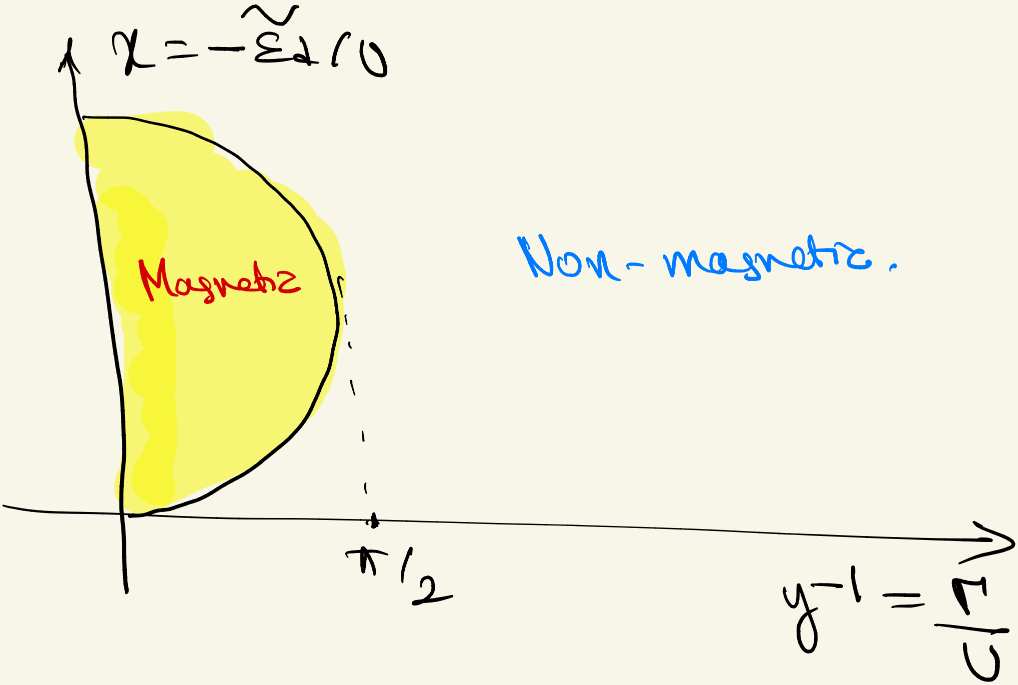
$$= \int_{-\infty}^{\varepsilon_F} \rho_d(\omega)\, d\omega = \frac{1}{\pi} \cot^{-1}\left[\frac{\tilde{\varepsilon}_d + U\langle n_{d-\sigma}\rangle}{\Gamma}\right]$$

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

These are two coupled equations for $\langle n_{d\uparrow}\rangle$ and $\langle n_{d\downarrow}\rangle$. Clearly, when $U = 0$, $\langle n_{d\uparrow}\rangle = \langle n_{d\downarrow}\rangle$. Similarly, when $\Gamma \to \infty$, $\cot^{-1}(\,) \to \frac{\pi}{2}$

$\Rightarrow \langle n_{d\uparrow}\rangle = \langle n_{d\downarrow}\rangle = \frac{1}{2}$.

Writing $x = -\frac{\tilde{\varepsilon}_d}{U}$, $y = \frac{U}{\Gamma}$, one finds the following phase diagram:



$x = -\tilde{\varepsilon}_d / U$
Magnetic
Non-magnetic.
$\pi/2$
$y^{-1} = \frac{\Gamma}{U}$