1st Part

Main points

1. Anderson impurity model with an example (quantum dot)
2. Schrieffer-Wolff transformation and Kondo model
3. Limitation of SW transformation, why NRG

2nd Part

Main points

1. What is Numerical RG (NRG)?
2. NRG techniques
3. Compare with Kondo model

1. Anderson impurity model with an example (quantum dot)

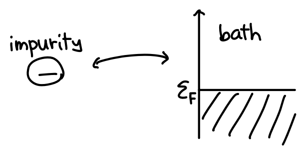
Single Impurity Anderson Model (SIAM)

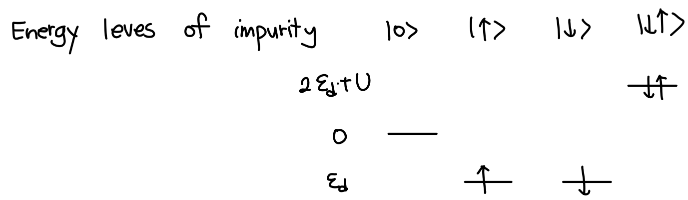
The model describes Kondo effect (resistivity increase logarithmically as temperature $T \to 0K$)

annihilation operator Many body interaction

$$H = \underbrace{\sum_{k,\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma}}_{\text{bath, conduction electron}} + \underbrace{\sum_{\sigma} \varepsilon_0 d^\dagger_\sigma d_\sigma}_{\text{impurity}} + \underbrace{U d^\dagger_\uparrow d_\uparrow d^\dagger_\downarrow d_\downarrow}_{\text{onsite Coulomb repulsion } U} + \sum_{k\sigma} V_k \left(d^\dagger_\sigma c_{k\sigma} + c^\dagger_{k\sigma} d_\sigma\right)$$

hybridization, coupling between impurity and bath.



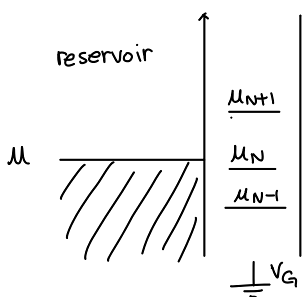


Impurity state – coupled to continuum metalic states.

An example : quantum dot in 2 dimensional electron gas (2DEG)

Realistic example : a quantum dot in semiconductor device.

With 1 reservoir,



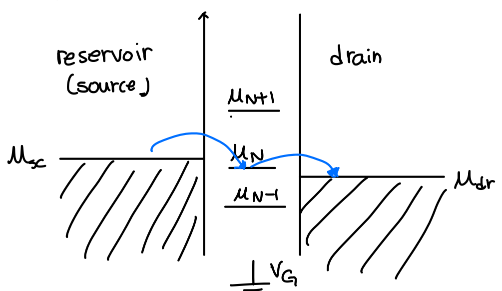
$$H_{QD} = \sum_{n,\sigma} \varepsilon_n d^\dagger_{n\sigma} d_{n\sigma} + \sum_{\{n_i\}\sigma\sigma'} U_{n_1 n_2 n_3 n_4} d^\dagger_{n_1\sigma} d^\dagger_{n_2\sigma'} d_{n_3\sigma'} d_{n_4\sigma}$$

$$H_{reservoir} = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k\sigma} c_k$$

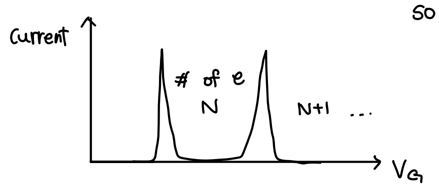
$$H_{coupling} = \sum_{k,n,\sigma} \left(V_{k,n} c^\dagger_{k\sigma} d_{n\sigma} + h.c.\right)$$

tunnel coupling

To get a sense of it, consider 2 reservoirs



so called Coulomb blockade.



Assumption : level $n=0$ is well separated $\Rightarrow$ truncate to a single orbital
$d_{n\sigma} \to d_\sigma$, $U_{0000} \to U$

$$H_{QD} \to \sum_\sigma \varepsilon_0 \, d_\sigma^\dagger d_\sigma + U d_\uparrow^\dagger d_\uparrow d_\downarrow^\dagger d_\downarrow$$

$\Rightarrow$ it reduces to SIAM

Hybridization / Broadening

Observation: Due to coupling term, $\sum_{k\sigma} (V_k c_{k\sigma}^\dagger d_\sigma + h.c.)$

1. an electron on the dot can leak into continuum states. : finite life time Γ
2. the bath shifts energy level of impurity : energy level shift $\varepsilon_d \to \tilde{\varepsilon}_d$

Recall Fermi's Golden rule, assume $U=0$.
Transition rate, which is probability of transition per unit time
$\Gamma_{i\to f} = 2\pi |\langle f|H'|i\rangle|^2 \delta(E_f - E_i)$, let $\hbar = 1$
where H' : perturbation

Let's calculate $\Gamma(\omega)$, "amplitude" of transition per unit time.

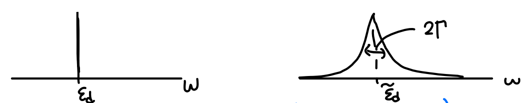
Hence, $2\pi \longrightarrow \pi$ and $|i\rangle$: N electron in the dot (impurity) $|N\rangle$
$|f\rangle$: $N-1$ " , $|N-1\rangle$
$H' = \sum_{k,\sigma} (V_k c_{k\sigma}^\dagger d_\sigma + h.c.)$

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

Density of States (DOS) of Conduction electrons

$\Gamma(\varepsilon_d)$: amplitude transition rate of $|N=1\rangle \to |N=0\rangle$

The DOS of impurity $A_d(\omega) = \delta(\omega - \varepsilon_d) \longrightarrow A_d(\omega) = \frac{1}{\pi} \frac{\Gamma(\omega)}{(\omega - \tilde{\varepsilon}_d)^2 + \Gamma^2(\omega)}$: Lorentzian with width 2Γ



(Indeed, it is local DOS since we neglect higher orbitals)

DOS and Green's function.

Sokhotski – Plemlj theorem : $\lim_{\varepsilon \to 0^+} \frac{1}{x \pm i\varepsilon} = \mp i\pi \delta(x) + \mathcal{P}(\frac{1}{x})$

Note that DOS $\rho(\omega) = \sum_k \delta(\omega - E_k)$
Using the thm, $\rho(\omega) = -\frac{1}{\pi} \mathrm{Im} \left(\sum_k \frac{1}{\omega - E_k + i0^+} \right)$
= Retarded Green's function.

Also, we have Tunnel coupling term : level shift $\Lambda(\omega)$, broadening $\Gamma(\omega)$
Coulomb interaction : self energy $\Sigma_U^R(\omega)$ (Dyson equation $G = G_0 + G_0 \Sigma G$)

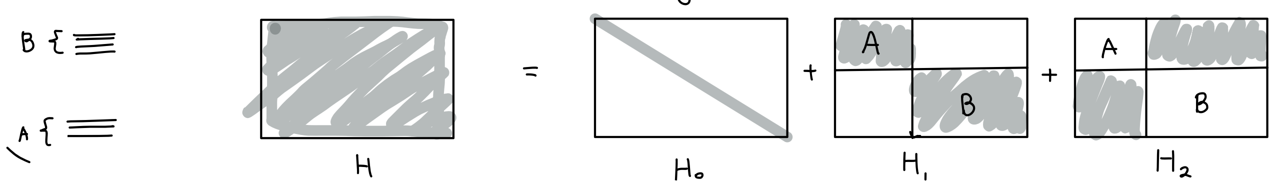
Retarded Green's ftn of impurity: $G_d^R(\omega) = \dfrac{1}{\omega - \varepsilon_d - \Lambda(\omega) + i\Gamma(\omega) - \Sigma_U^R(\omega, T)}$

2. Schrieffer-Wolff transformation and Kondo model

Schrieffer - Wolff transformation

- a unitary transformation used to determine an effective (often low-energy) Hamiltonian by decoupling weakly interacting subspace.
- Operator version of perturbation theory.

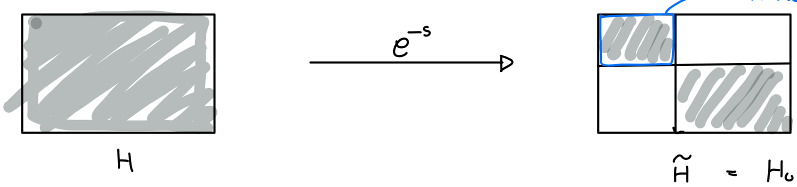
Let $H = H_0 + H_1 + H_2$ $\qquad$ H_0 : diagonal, H_1, H_2 : off-diagonal terms



coupling within subset A and B $\qquad$ coupling between states in A and B

SW transformation $\quad \tilde{H} = e^{-S} H e^{S}$ $\quad$ with $\quad S = -S^{\dagger}$

effective Hamiltonian in subspace A



$$\tilde{H} = H_0 + [H_0, S] + \frac{1}{2}[[H_0, S], S] + \cdots$$

Simple cheet sheet

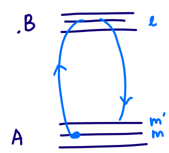
let $|m\rangle \in A$, $\quad |\ell\rangle \in B$, $\quad H' = H_1 + H_2$, $\quad \tilde{H} = \hat{H}^{(0)} + \hat{H}^{(1)} + \hat{H}^{(2)} + \cdots$

$$\langle m|\tilde{H}^{(0)}|m'\rangle = \langle m|H_0|m'\rangle$$

$$\langle m|\tilde{H}^{(1)}|m'\rangle = \langle m|H'|m'\rangle = \langle m|H_1|m'\rangle$$

$$\langle m|\tilde{H}^{(2)}|m'\rangle = \frac{1}{2}\sum_{\ell} \underbrace{\langle m|H'|\ell\rangle}_{=\langle m|H_2|\ell\rangle}\langle \ell|H'|m'\rangle \left[\frac{1}{E_m - E_\ell} + \frac{1}{E_{m'} - E_\ell}\right]$$

$\vdots$



SW transformation of SIAM

In SIAM,

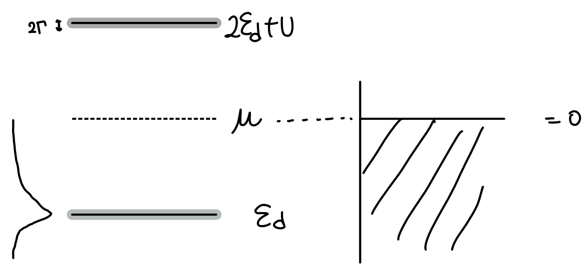
$$H = \underbrace{\sum_{k,\sigma} \varepsilon_k c_{k\sigma}^{\dagger} c_{k\sigma}}_{\text{bath, conduction electron}} + \underbrace{\sum_{\sigma} \varepsilon_d d_\sigma^{\dagger} d_\sigma}_{\text{impurity}} + \underbrace{U d_\uparrow^{\dagger} d_\uparrow d_\downarrow^{\dagger} d_\downarrow}_{\text{onsite Coulomb repulsion } U} + \sum_{k,\sigma} V_k (d_\sigma^{\dagger} c_{k\sigma} + c_{k\sigma}^{\dagger} d_\sigma)$$

hybridization, coupling between impurity and bath.

When $\varepsilon_d < \mu$, impurity is singly occupied most of the time.

In the assumption $|\varepsilon_d|, |U + \varepsilon_d| \gg \Gamma, k_B T$

(well - separated)



$\Rightarrow$ Project the Hamiltonian to N=1 Hilbert space. = subset A.

Coupling between A and B : ① $N=1 \rightarrow N=0 \rightarrow N=1$

② $N=1 \rightarrow N=2 \rightarrow N=1$

$$H_{1\to0\to1} = \frac{1}{\varepsilon_d}\sum_{kk'\sigma\sigma'} V_k^* \underbrace{d_\sigma^\dagger}_{0\to1} c_{k\sigma}\cdot V_{k'} c_{k'\sigma'}^\dagger \underbrace{d_{\sigma'}}_{1\to0} = -\frac{1}{|\varepsilon_d|}\sum_{kk'\sigma\sigma'} V_k^* V_{k'}\cdot d_\sigma^\dagger \underbrace{c_{k\sigma} c_{k'\sigma'}^\dagger}_{=\delta_{kk'}\delta_{\sigma\sigma'} - c^\dagger_{k'\sigma'}c_{k\sigma}} d_{\sigma'}$$

$$= -\frac{1}{|\varepsilon_d|}\sum_{kk'\sigma\sigma'} V_k^*V_{k'}\left[\delta_{kk'}\delta_{\sigma\sigma'} d_\sigma^\dagger d_{\sigma'} - d_\sigma^\dagger c_{k'\sigma'}^\dagger c_{k\sigma} d_{\sigma'}\right]$$

$$H_{1\to2\to1} = \frac{1}{\varepsilon_d-(2\varepsilon_d+U)}\sum_{kk'\sigma\sigma'} V_k c_{k\sigma}^\dagger \underbrace{d_\sigma}_{2\to1} \cdot V_{k'}^* \underbrace{d_{\sigma'}^\dagger}_{1\to2} c_{k\sigma'}$$

$$= -\frac{1}{|\varepsilon_d+U|}\sum_{kk'\sigma\sigma'} V_k V_{k'}^* c_{k\sigma}^\dagger\left(\delta_{\sigma\sigma'} - d_{\sigma'}^\dagger d_\sigma\right) c_{k\sigma'}$$

$$= -\frac{1}{|\varepsilon_d+U|}\sum_{kk'\sigma\sigma'} V_k V_{k'}^* \left[\delta_{\sigma\sigma'} c_{k\sigma}^\dagger c_{k'\sigma'} - c_{k\sigma}^\dagger d_{\sigma'}^\dagger d_\sigma c_{k'\sigma'}\right]$$

$$\tilde{H}^{(2)} = H_{1\to0\to1} + H_{1\to2\to1} = +\left(\frac{1}{|\varepsilon_d|} + \frac{1}{|\varepsilon_d+U|}\right)\sum_{kk'} V_k^* V_{k'} \sum_{\sigma\sigma'}\left(d_\sigma^\dagger d_{\sigma'}\right)\left(c_{k'\sigma'}^\dagger c_{k\sigma}\right)$$

$$-\frac{1}{|\varepsilon_d|}\sum_k |V_k|^2 \underbrace{\sum_\sigma d_\sigma^\dagger d_\sigma}_{=1} - \frac{1}{|\varepsilon_d+U|}\sum_{kk'} V_k V_{k'}^* \sum_\sigma c_{k\sigma}^\dagger c_{k'\sigma}$$

$*$ $\vec{S} = \sum_{\alpha,\beta} \frac{1}{2} d_\alpha^\dagger \vec{\sigma}_{\alpha\beta} d_\beta$, $\quad \vec{S}_{kk'} = \sum_{\alpha,\beta} \frac{1}{2} c_{k\alpha}^\dagger \vec{\sigma}_{\alpha\beta} c_{k'\beta}$

$d_\sigma^\dagger d_{\sigma'} = \frac{1}{2}\delta_{\sigma\sigma'} n_d + \vec{S}\cdot\vec{\sigma}_{\sigma\sigma'}$, $\quad c_{k\sigma}^\dagger c_{k'\sigma'} = \frac{1}{2}\delta_{\sigma\sigma'}\sum_\alpha c_{k\alpha}^\dagger c_{k'\alpha} + \vec{S}_{kk'}\cdot\vec{\sigma}_{\sigma\sigma'}$

(Similar to $\vec{M} = a_0 I + \vec{a}\cdot\vec{\sigma}$)

Then, $$\sum_{\sigma\sigma'}\left(d_\sigma^\dagger d_{\sigma'}\right)\left(c_{k'\sigma'}^\dagger c_{k\sigma}\right) = \frac{1}{2}\underbrace{n_d}_{=1}\cdot\frac{1}{2}\left(\sum_\alpha c_{k\alpha}^\dagger c_{k'\alpha}\right)\underbrace{\sum_{\sigma\sigma'}\delta_{\sigma\sigma'}\delta_{\sigma\sigma'}}_{=2} + \underbrace{\sum_{\sigma\sigma'}\left(\vec{S}\cdot\vec{\sigma}_{\sigma\sigma'}\right)\left(\vec{S}_{kk'}\cdot\vec{\sigma}_{\sigma\sigma'}\right)}_{=\sum_{ij} S^i S^j_{kk'} \underbrace{\sum_{\sigma\sigma'}\sigma^i_{\sigma\sigma'}\sigma^j_{\sigma'\sigma}}_{=2\delta_{ij}}}$$

$$= \frac{1}{2}\left(\sum_\sigma c_{k\sigma}^\dagger c_{k'\sigma}\right) + 2\,\vec{S}\cdot\vec{s}_{kk'}$$

Hence,
$$\tilde{H}^{(2)} = \underbrace{2\left(\frac{1}{|\varepsilon_d|} + \frac{1}{|\varepsilon_d+U|}\right)\sum_{kk'} V_k^* V_{k'}}_{J_{kk'}} \vec{S}\cdot\vec{s}_{kk'} + \underbrace{\frac{1}{2}\left(\frac{1}{|\varepsilon_d|} - \frac{1}{|\varepsilon_d+U|}\right)\sum_{kk'} V_k^* V_{k'}}_{K_{kk'}} \sum_\sigma c_{k\sigma}^\dagger c_{k'\sigma} - \frac{1}{|\varepsilon_d|}\sum_k |V_k|^2$$

Combining these term,

$$H = \sum_{k\sigma}\varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_\sigma \varepsilon_d d_\sigma^\dagger d_\sigma + U d_\uparrow^\dagger d_\uparrow d_\downarrow^\dagger d_\downarrow + \sum_{k\sigma} V_k\left(d_\sigma^\dagger c_{k\sigma} + c_{k\sigma}^\dagger d_\sigma\right)$$

$$\Longrightarrow \tilde{H} = \sum_{k,\sigma}\varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_{kk'} J_{kk'} \underbrace{\vec{S}\cdot\vec{s}_{kk'}}_{\text{Spin in impurity}} + \sum_{kk'} K_{kk'} \underbrace{\left(\sum_\sigma c_{k\sigma}^\dagger c_{k'\sigma}\right)}_{\text{bath term}} + \text{const.}$$

If V_k is "smooth" near Fermi level, $V_k \to V$ (tiny window near Fermi level),

$$J = 2 \cdot \left(\frac{1}{|\varepsilon_d|} + \frac{1}{|\varepsilon_d + U|} \right) |V|^2 \quad > 0$$: antiferromagnetic

spin-flip scattering

$$K = \frac{1}{2} \left(\frac{1}{|\varepsilon_d|} - \frac{1}{|\varepsilon_d + U|} \right) \cdot |V|^2$$: constant local potential

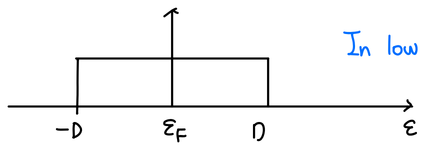
$\varepsilon_d = -U/2$: p-h symmetry point

$$\Rightarrow \quad H = \sum_{k,\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + J \vec{S} \cdot \vec{s}$$: called "Kondo model"

which explains "kondo effect," logarithmic increase in electrical resistivity as temperature is lowered with perturbation up to 3rd order or RG technique.

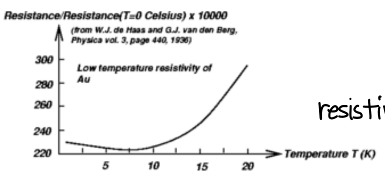
(localized magnetic moment of impurity plays a role when $T \ll T_K$)

With DOS of bath (2D Metal):



In low temp., only ε near ε_F matters

$\rho(\omega) \approx \rho(\varepsilon_F = 0)$



resistivity $R \propto J^2 \left[1 - 4J \rho_0 \log\left(\frac{k_B T}{D}\right) \right]$ ($\because$ diverges for $T \to 0$, $D \to \infty$)

it yields Kondo temperature $T_K \sim D e^{-1/\rho J}$ where $\rho = \rho(\varepsilon_F)$

D : Bandwidth cutoff

3. Limitation of SW transformation, why NRG

SW transformation

- It gives "effective" Hamiltonian in local moment regime ($\varepsilon_d < 0$, $\Gamma \ll |\varepsilon_d|, \varepsilon_d + U$)

limitation

- charge fluctuation is not captured (integrated out)
- nonuniversal crossover.

NRG

- Non-perturbative
- with full-density-matrix NRG, it gives local density of states (LDOS)
  - $\Rightarrow$ possible to calculate thermodynamic quantities, S_{imp}, χ_{imp}, C_{imp} ...
  - $\Rightarrow$ we can find Kondo peak $\omega \approx 0$ (many body peak)
    Hubbard sideband at $\omega \approx \varepsilon_d, \varepsilon_d + U$ (single-particle peaks)
- Works on all regime (not only on local moment regime, $\Gamma \ll |\varepsilon_d|, \varepsilon_d + U$)
- It is used in Dynamical Mean Field Theory (DMFT)
  - model each lattice site as SIAM