1. What is Numerical RG?

History of SIAM

[Anderson, 1961]	SIAM, local moment formation
[Kondo, 1964]	Kondo's approach, $\log(T)$
[Schrieffer, Wolff, 1966]	SIAM $\rightarrow$ Kondo
[Anderson, 1970]	Anderson's "Poor man's scailing" RG
[Krishna-murthy, Wilkins, and Wilson, 1980]	Numerical RG
[Wiegmann & Tsvelick, 1982-3]	Exact solution by Bethe ansatz

Today's topic!

Standard review paper [Bulla, 2008] for NRG,

What it solves? Quantum impurity model.
Impurity : zero dimensional, small number of degrees of freedom.
Bath : fermions/bosons with continuous excitation spectrum, it can be 1, 2, 3 dimension

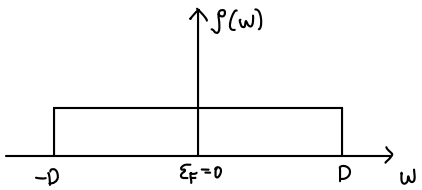
Use tensor network for convenience.

2. NRG techniques

Logarithmic discretization of bath

Assume flat band near Fermi level

$$\rho(\omega) = \frac{1}{2D}\,\Theta(D-|\omega|)$$



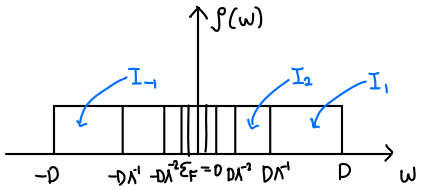
Continuous spectrum $\rightarrow$ discrete spectrum for numerical method.

Why logarithmic discretization?

First, impurity physics lives on small energy scales.
$\Rightarrow$ uniform grid $\sim 10^6$ to resolve tiny scales, but logarithmic grid ~ 20

Second, to avoid $\log(k_BT/D)$ divergence. (This is observed in Poor man's scaling RG)

Third, it gives scale separation.



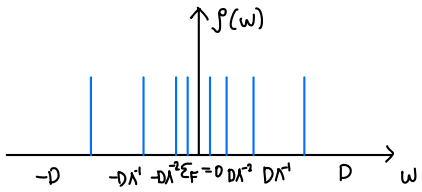
$$H = \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_\sigma \varepsilon_\sigma d^\dagger_\sigma d_\sigma + U d^\dagger_\uparrow d_\uparrow d^\dagger_\downarrow d_\downarrow + \sum_{k\sigma} V_k (d^\dagger_\sigma c_{k\sigma} + c^\dagger_{k\sigma} d_\sigma)$$

$$\Gamma(\omega) = \pi |V|^2 \rho(\omega) = \frac{\pi |V|^2}{2D} \Theta(D-|\omega|) \equiv \Delta_0 \Theta(D-|\omega|)$$

$\Downarrow$

Bin: $I_{\pm k} = [\pm D\Lambda^{-k}, \pm D\Lambda^{-k+1}]$ → single energy level

For each bin, ① representative $\xi_{\pm k}$
② hybridization term for bin I_n, $\gamma_{\pm k}$



$$H = \sum_\sigma \varepsilon_\sigma d^\dagger_\sigma d_\sigma + U d^\dagger_\uparrow d_\uparrow d^\dagger_\downarrow d_\downarrow + \underset{①}{\sum_{\pm,k,\sigma} \xi_{\pm k} a^\dagger_{\pm k\sigma} a_{\pm k\sigma}} + \underset{②}{\sum_{\pm k,\sigma} \left(\gamma_{\pm k} a^\dagger_{\pm k\sigma} d_\sigma + h.c.\right)}$$

① $\xi_{\pm k}$ Wilson's method : center of mass

$$\xi_k = \frac{\int_{D\Lambda^{-k}}^{D\Lambda^{-k+1}} \omega \rho(\omega) d\omega}{\int_{D\Lambda^{-k}}^{D\Lambda^{-k+1}} \rho(\omega) d\omega}$$

However, it is known that this throws away intra-interval bath couplings, there are other methods to calculate ξ_k

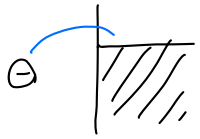
Ex) In, [Campo and Oliveira, 2005]

$$\xi_{\pm k} = \frac{\int_{D\Lambda^{-k}}^{D\Lambda^{-k+1}} \rho(\omega) d\omega}{\int_{\pm D\Lambda^{-k}}^{\pm D\Lambda^{-k+1}} \rho(\omega)/\omega \, d\omega}$$ (This is implemented)

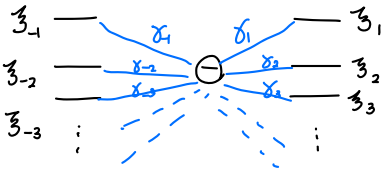
② $\gamma_{\pm k} = \pm \int_{\pm D\Lambda^{-k}}^{\pm D\Lambda^{-k+1}} \Gamma(\omega) d\omega \propto \Lambda^{-k}$: Find # of bins that γ_n is sufficiently smaller than the "smallest" energy scale in the problem. (Here, usually Temp.)

With this discretization, we get "Star" Hamiltonian,

Initial SIAM

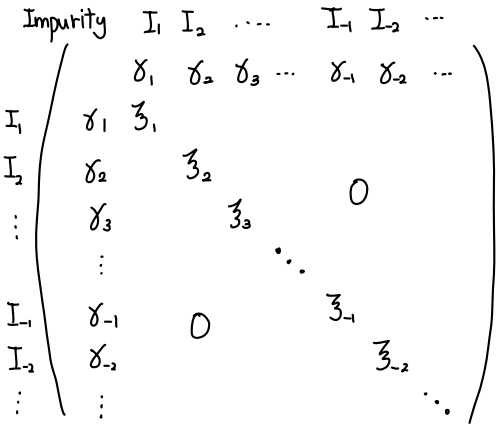


Star geometry

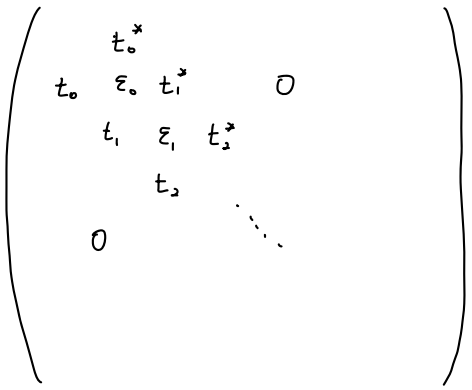


Mapping to "Wilson chain"

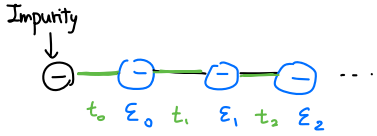
Hamiltonian of star geometry



Lanczos method
Tridiagonization



Wilson chain



$$\hat{H} = \sum_\sigma \varepsilon_0 d_\sigma^\dagger d_\sigma + U d_\uparrow^\dagger d_\uparrow d_\downarrow^\dagger d_\downarrow + \sum_\sigma (t_0 f_{0\sigma}^\dagger d_\sigma + h.c.) + \sum_{n=1}^{N} \sum_\sigma \left(t_n f_{n\sigma}^\dagger f_{n-1,\sigma} + h.c. \right) + \sum_{n=0}^{N} \sum_\sigma \varepsilon_n f_{n\sigma}^\dagger f_{n\sigma}$$

Particle-hole symmetry case, $\varepsilon_0 = -U/2$ PH transformation $f_n \to (-1)^n f_n^\dagger$

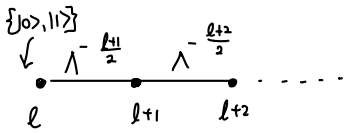
$\Rightarrow f_{n\sigma}^\dagger f_{n-1\sigma} \longrightarrow (-1)^{2n-1} f_{n\sigma} f_{n-1\sigma}^\dagger \to (-1)^{2n} f_{n-1\sigma}^\dagger f_{n\sigma}$

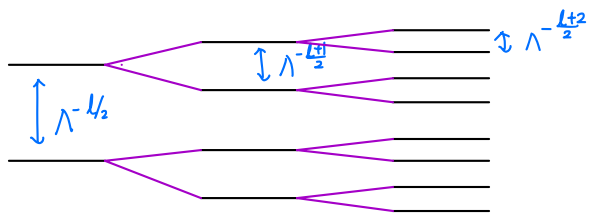
but $f_{n\sigma}^\dagger f_{n\sigma} \to (-1)^{2n} f_{n\sigma} f_{n\sigma}^\dagger \to - f_{n\sigma}^\dagger f_{n\sigma}$: flip sign $\Rightarrow \varepsilon_n = 0$

Hopping terms : $t_n = D \cdot \dfrac{(1+\Lambda^{-1})(1-\Lambda^{-(n+1)})}{2\sqrt{(1-\Lambda^{-2n-1})(1-\Lambda^{-2n-3})}} \Lambda^{-\frac{n}{2}} \propto \Lambda^{-\frac{n}{2}}$

- Hopping/coupling decay exponentially $\longrightarrow$ energy scale separation
- site n+1 perturbs site n "weakly"
- Iteratively solve Hamiltonian, truncate at each step.

Iterative diagonalization and truncation

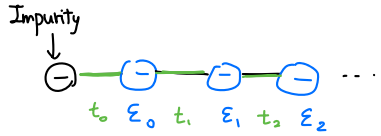




Adding one site l : coupled with hopping term $t_l \propto \Lambda^{-\frac{l}{2}}$,
weakly perturbs the low lying spectrum of $(l-1)$-site chain.

$\Rightarrow$ Iteratively add one site, truncate high energy states.

Wilson chain

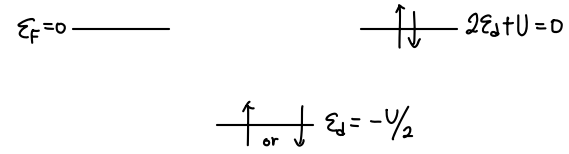


Impurity ($|n_\uparrow\rangle$) + 1 site ($|n_b=0\rangle$)

$$\begin{array}{c} \quad |I\rangle \quad |0\rangle \\ \begin{pmatrix} & t_0^* \\ t_0 & \varepsilon_0=0 \end{pmatrix} \end{array}$$

Indeed, each site has 4 degrees of freedom, ($|0\rangle$, $|1\uparrow\rangle$, $|1\downarrow\rangle$, $|2\uparrow\downarrow\rangle$)

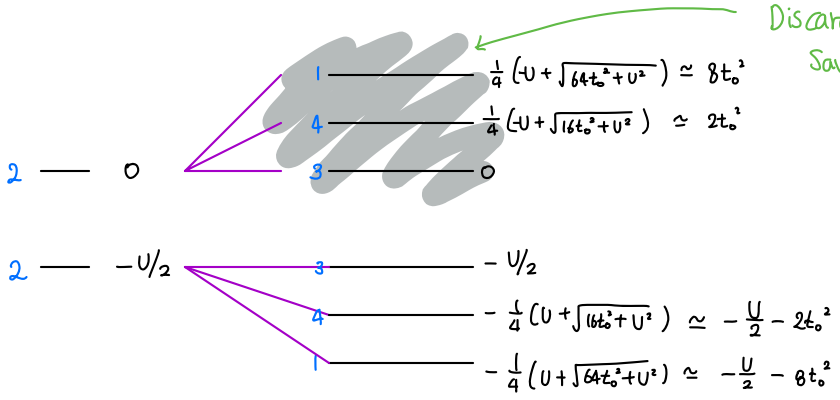
Energy level



$$\begin{array}{c} \quad |0\rangle \quad |1\uparrow\rangle \quad |1\downarrow\rangle \quad |2\uparrow\downarrow\rangle \\ \begin{matrix} |0\rangle \\ |1\uparrow\rangle \\ |1\downarrow\rangle \\ |2\uparrow\downarrow\rangle \end{matrix} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -U/2 & 0 & 0 \\ 0 & 0 & -U/2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \end{array}$$

Add one site : expand Hilbert space : 4 x 4 matrix ⟶ 16 x 16 matrix

Discarded for diagonalization.
Save these states to make "complete set"



If we want to keep N_{keep} states, truncate Hilbert space of high energy levels.

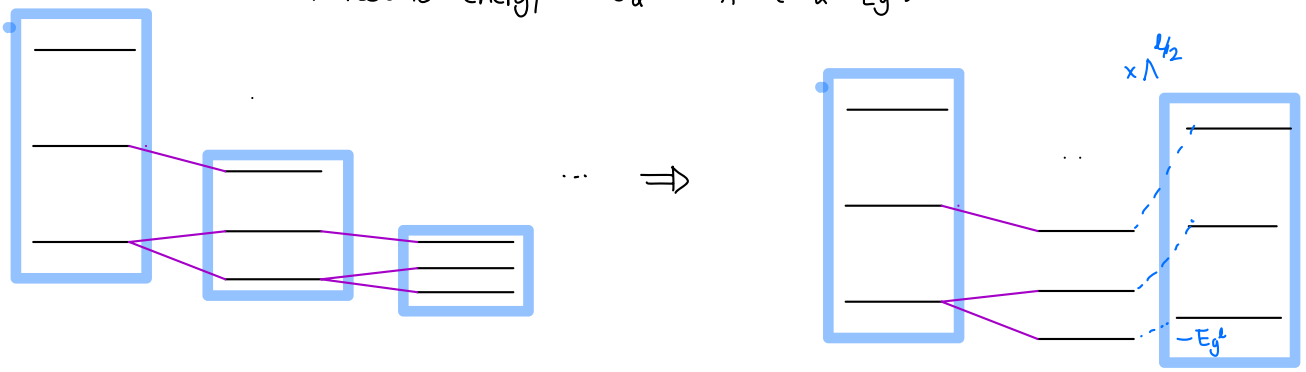
at ℓ th iteration, $H^\ell|\alpha\rangle_\ell = E_\alpha^\ell|\alpha\rangle_\ell$ $\alpha=1, \ldots, N_{keep}$ (rather than $d^{\ell+1}$)

Then, add one site ⇒ H : $4N_{keep}$ x $4N_{keep}$ matrix
Diagonalize ⇒ $4N_{keep}$ energy eigenvalues
Truncation ⇒ N_{keep} low energy eigenvalues/eigenvectors
$3N_{keep}$ " save for later use

Rescaling

We already know at $(l+1)$ th iteration, we will see $t_{l+1} \propto \Lambda^{-\frac{l+1}{2}}$ terms

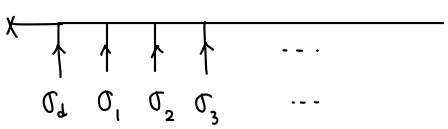
$\Rightarrow$ rescale energy $\varepsilon_l = \Lambda^{\frac{l}{2}} (E_\alpha^l - E_g^l)$



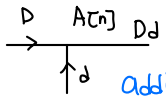
Numerical reason - more stable from floating # error

Physically it is same as RG transformation (zooming in)

Procedures

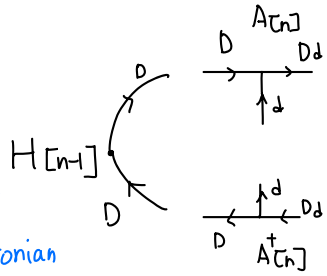


(1) Define Identity tensor $A^{[n]}$



Adding one more site with physical dimension d.

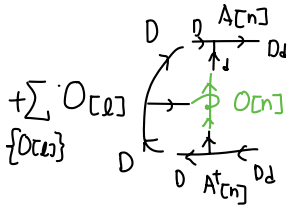
(2) Expand Hamiltonian in new basis



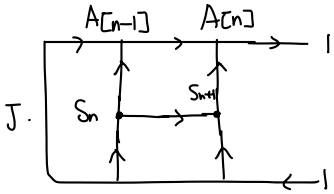
Hamiltonian up to $n-1$ iteration. $D \times D$ matrix

$(\times \sqrt{\Lambda}$ for rescale$)$

(3) Add terms

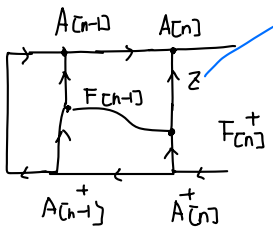


For example



$: J \vec{S}_n \cdot \vec{S}_{n+1}$

$H^{hop}_{[n]} = \Lambda^{\frac{n}{2}} \cdot t_{n-1} \cdot$

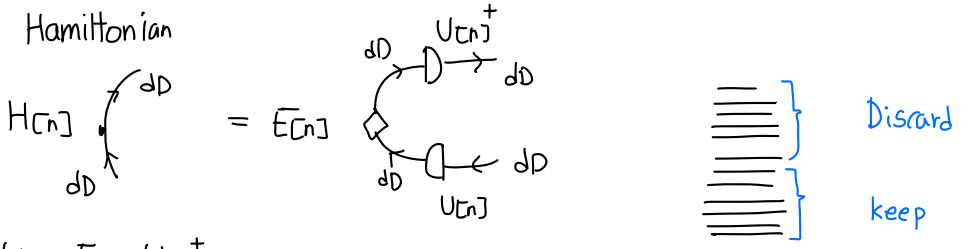


Jordan-Wigner string

$+$ h.c. $+$ onsite term

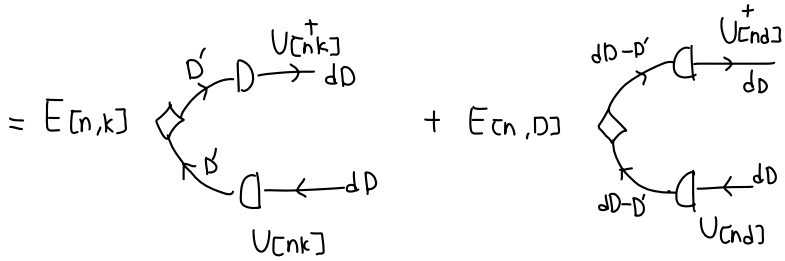
$= \sum_\sigma \hat{f}^\dagger_{n\sigma} \hat{f}_{n+1\sigma}$

(4) Diagonalize Hamiltonian

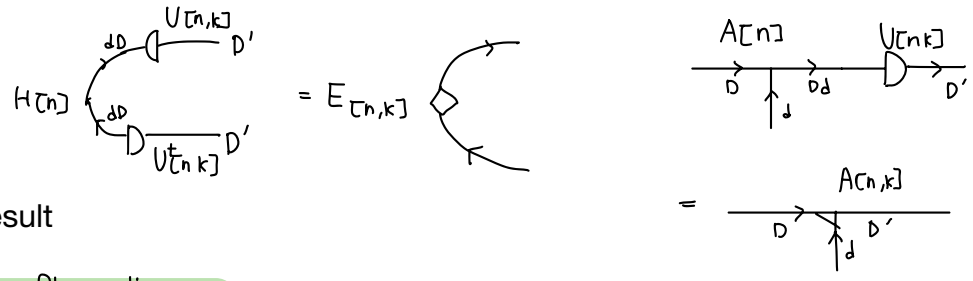


$$H_{[n]} = U_{[n]}\, E_{[n]}\, U_{[n]}^{\dagger}$$

(5) Truncate Hilbert space



(6) Update isometries



Analyzing result

Energy flow diagram

- Rescaled energy
- Even/odd oscillation : finite size effect
- Plateau (C-like) regime
  : $E_n \simeq E_{n+2}$ up to rescaling
  adding "sites" doesn't affect

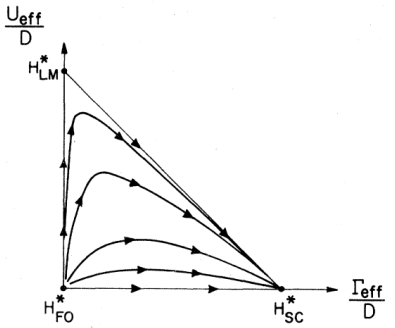
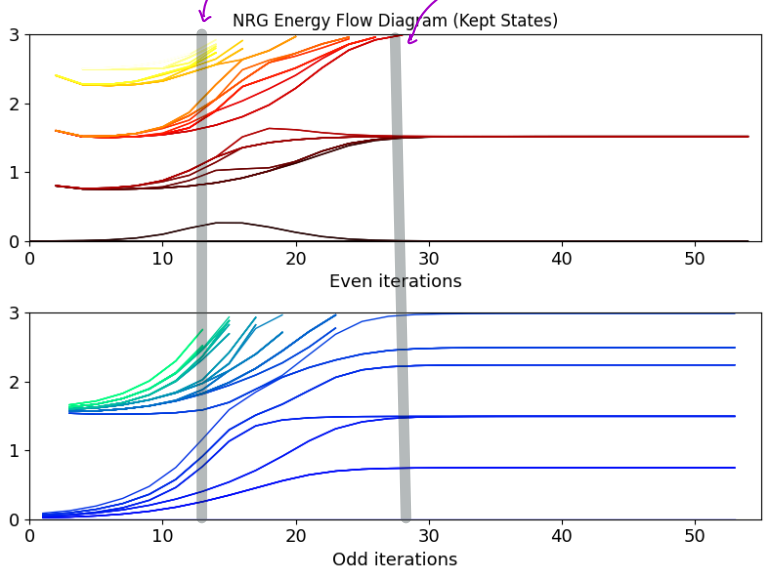


FIG. 8. Schematic renormalization-group flow diagram. Each H_N is thought of as associated with a $U_{\rm eff}$ and $\Gamma_{\rm eff}$. Trajectories depict the flow of H_N with increasing N. Note that only the strong-coupling fixed point is stable.

[Krishna-murthy, Wilkins, and Wilson, 1980]

SIAM

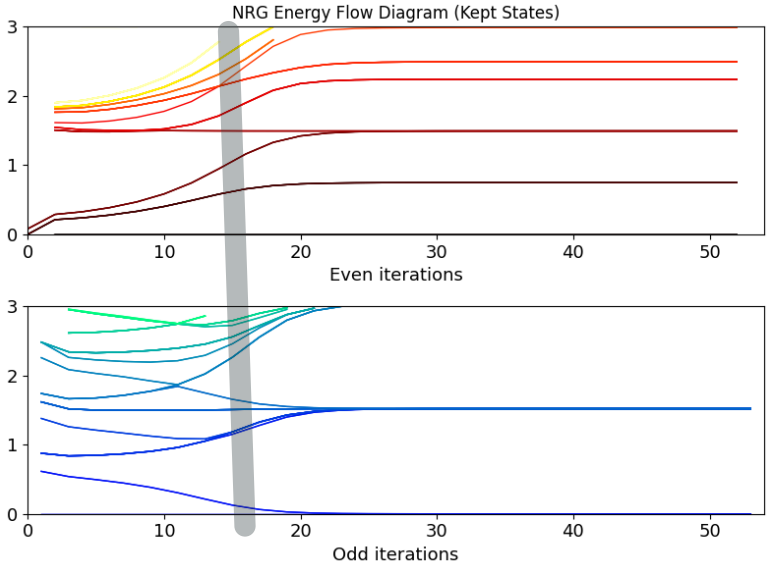
$\Lambda^{-\frac{l}{2}} \sim \Delta_0$ $\Lambda^{-\frac{l}{2}} \sim T_K$ (Kondo temperature)



Free orbital Local moment Strong coupling

Kondo model (Actually SWT to impurity and only first bath site on Wilson chain Hamiltonian)

$$\hat{H} = J \vec{S}_d \cdot \vec{S}_s + \sum_{n=1}^{N} \sum_{\sigma} \left(t_n f_{n\sigma}^{+} f_{n-1,\sigma} + \text{h.c.} \right) + \sum_{n=0}^{N} \sum_{\sigma} \varepsilon_n f_{n\sigma}^{+} f_{n\sigma}$$



No free orbital regime due to SWT