7. NRG iteration scheme from RG perspective

\[ H_{\text{disc}}^N = H_{\text{loc}}(d_s, d_s^t) + \sum_{n=0}^{N-1} \sum_{s} t_n \left( f_n^s f_n^{s+1} + \text{h.c.} \right) \]

\[ = H_{\text{chain}}^N \]

(1) 

\[ t_n = \Lambda^{-(n+\frac{1}{2})} \tilde{t}_n \]  

\[ \tilde{E}_n \rightarrow \frac{1}{2} \left( 1 + \Lambda^{n} \right) = \mathcal{O}(1) \]  

for large \( n \).

(2) 

Therefore, lowest energy splitting of \( H_{\text{chain}}^N \) is \( \mathcal{O} \left( \Lambda^{-(N-1)/2} \right) \).

coupling between sites \( N-1 \) and \( N \)

To resolve this, define new set of \textit{rescaled} Hamiltonians:

\[ \tilde{H}_N = \Lambda^{-(N-1)/2} (H_{\text{disc}}^N - E_{\text{disc}}^{N}) \]

\[ \tilde{H}_N \] chosen to make ground state energy of \( \tilde{H}_N \) equal to zero.

then lowest energy splittings in spectrum of \( \tilde{H}_N \) are \( \mathcal{O}(1) \).

We will use hidden to indicate rescaled quantities.

\[ \text{(3)} \]

(3.3) implies RG recursion formula:

\[ H_{N+1} = \Lambda^{-N/2} \left( H_{\text{disc}}^{N+1} - E_{\text{disc}}^{N+1} \right) \]

\[ = \Lambda^{-N/2} \left( H_N - E_{\text{disc}}^{N} \right) + \Lambda^{-N/2} \left( t_n \sum_{s} \left( f_n^s f_{n+1}^{s+1} + \text{h.c.} \right) \right) - \Lambda^{-N/2} \left( E_{\text{disc}}^{N+1} - E_{\text{disc}}^{N} \right) \]

\[ \equiv S \tilde{E}_{G, N+1} \]

\[ H_{N+1} = \Lambda^{-N/2} H_N + \sum_{s} \tilde{t}_n \left( f_n^s f_{n+1}^{s+1} + \text{h.c.} \right) - S \tilde{E}_{G, N+1} \]

(3)

\[ \text{rescale} \]

\[ \text{enlarge system} \]

\[ \text{set GS. energy to zero} \]

Symbolic notation:\n
\[ H_{N+1} = T \left[ H_N \right] \]

\( T \) denotes RG transformation (4)

Question: what happens under repeated application of \( T \)?

Answer: one moves towards a fixed point!
"Fixed point Hamiltonian" $H^*$ of $T$ remains invariant:

$$ T [H^*] = H^* $$  \hspace{1cm} (1)

Actually, $T$ does not have fixed points, but $T^2$ (operating twice) does:

$$ T^2 [H^*] = H^* $$  \hspace{1cm} (2)

in sense that eigenspectrum of $H^*$, and matrix elements of $T^*$, remain invariant.

Key insight by Wilson: fixed points of $H^*$ and $H^{**}$ can be understood in terms of fixed points of free-electron Hamiltonian.

$$ H_0^* = \sum_{n=0}^{N-1} \sum_{k=0}^{N} \lambda^{(N-1-k)/2} \tilde{e}_n \{ \text{funs}, \text{freqs} \text{ anc \text{hics.}} \} $$  \hspace{1cm} (3)

Eigenvalues of $H_0^*$ can be found by diagonalizing a $(N+1) \times (N+1)$ dimensional matrix, where only non-zero elements are

$$ (H_0^*)^{n,n+1} = (H_0^*)^{n+1,n} = \lambda^{(N-1-n)/2} \tilde{e}_n $$  \hspace{1cm} (4)

Particle-hole symmetry implies: eigenvalues come in pairs, $\pm \eta$:

$$ i \# N+1 \rightarrow \begin{cases} \text{even:} & \pm \eta_j \text{ , } j = 1, 2, 3, \ldots, \frac{1}{2} (N+1) \\ \text{odd:} & \eta_0 = 0, \pm \eta_0 \end{cases} $$  \hspace{1cm} (5)

As $N$ increases, they approach limiting values:

$$ \eta_j \rightarrow \eta_j \stackrel{\text{large } N}{\longrightarrow} \eta_j \Rightarrow \begin{cases} \lambda^{j-1} & \text{if } N+1 \text{ even} \\ \lambda^{j-2} & \text{if } N+1 \text{ odd} \end{cases} $$  \hspace{1cm} (6)

(Not surprising, since $H_0^*$ is rescaled version of discretized Hamiltonian)

Correctly, for $\lambda = 2.5$:

$$ \eta_0^* = 0.746856, \ 2.493206, \ 6.249995, \ (2.5)^3, \ (2.5)^4, \ldots, \ (2.5)^{N-1}, \ldots, \ (N+1) \text{ even } ; $$  \hspace{1cm} (4.4)

$$ \eta_0^{**} = 1.520483, \ 3.952550, \ 9.882118, \ (2.5)^{3/2}, \ (2.5)^{3/2}, \ldots, \ (2.5)^{N-1/2}, \ldots, \ (N+1) \text{ odd } ; $$  \hspace{1cm} (5.5)
\[ N+1 = \text{even}: \]

\[ \eta_j \text{ values define single-particle spectrum of diagonalized } H_N^0: \]

\[ H_N^0 = \sum_j \sum_{\nu_j} \eta_j (\hat{\mathbf{g}}_{j\nu_j} \hat{\mathbf{g}}_{j\nu_j} + \hat{\mathbf{l}}_{j\nu_j} \hat{\mathbf{l}}_{j\nu_j}) \]

Many-body spectrum consists of multiple single-particle excitations:

\[ \begin{array}{cccc}
q^0 & q^{+} & q^{-} & q^{+} + q^{-} \\
\hline
5 & 0 & 0 & 1 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 \\
\end{array} \]

Many-body spectrum at "even fixed point"

At \( T^2 \), say \( H_0^0 \):

\[ \text{Energy } S \quad \text{Degeneracy } = (2.5)^s \]

\[ NRG7.e \]

\[ N+1 = \text{odd}: \]

\[ \eta_j \text{ values define single-particle spectrum of diagonalized } H_N^0: \]

\[ H_N^0 = \sum_j \sum_{\nu_j} \eta_j (\hat{\mathbf{g}}_{j\nu_j} \hat{\mathbf{g}}_{j\nu_j} + \hat{\mathbf{l}}_{j\nu_j} \hat{\mathbf{l}}_{j\nu_j}) \]

Many-body spectrum consists of multiple single-particle excitations:

\[ \begin{array}{cccc}
q^0 & q^{+} & q^{-} & q^{+} + q^{-} \\
\hline
\frac{3}{4} \eta^0 & 0 & 0 & 1 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 \\
\end{array} \]

Many-body spectrum at "odd fixed point"

At \( T^2 \), say \( H_0^0 \):

\[ \text{Energy } S \quad \text{Degeneracy } = (2.5)^{3/2} \]

\[ NRG7.f \]
Fixed points for Kondo model \( (\mathrm{at} \; \lambda = 0) \) [Wilson 1975, VIII] \[ \text{NRG 7.8} \]

\[
H_{\text{Kondo}} = J \hat{S}_c \cdot \hat{S}_d + H_{\text{chain}} \quad (1)
\]

\[\hat{S}_c = \sum_{kk'} \hat{S}_{kk'} \quad (2)\]

\[
\hat{S}_c = \sum_{kk'} \hat{S}_{kk'} \quad (2) \quad \text{since} \quad \hat{S}_{kk'}^+ \hat{S}_{kk'} = \delta_{kk'}
\]

Re-scaled Hamiltonian: \( H_N = \lambda^{(N-1)/N} \sum \hat{S}_c \cdot \hat{S}_d + H_{\text{N-1}} \) \( \square \) \( \square \) \( \square \)

Kondo model has two fixed points, corresponding to \( \lambda = 0 \) and \( \lambda = \infty \)

(i) **Free "local moment" (LM) fixed point:**

\[ H_{LM, N}^* = H_N (\lambda = 0) = \begin{array}{c}
\begin{array}{c}
\text{imp} \ \ 0 \ \ 1 \ \ 2 \ \ \cdots \ \ N
\end{array}
\end{array} \quad (4) \]

Same spectrum as \( H_N^* \), with doubled degeneracy (for impurity \( \pi, \mu \))

For \( N_{\text{tr}} = \text{even} \): \( \text{(2.e)} \)

\[ \begin{array}{c}
\begin{array}{c}
\hat{H}_{LM}^* \quad 0, \quad \hat{\eta}_1^* (12), \quad 3 \hat{\eta}_1^* (14)
\end{array}
\end{array} \quad (5) \]

For \( N_{\text{tr}} = \text{odd} \): \( \text{(2.e)} \)

\[ \begin{array}{c}
\begin{array}{c}
\hat{H}_{LM}^* \quad 0, \quad 2 \hat{\eta}_1^* (12), \quad \hat{\eta}_1^* (14)
\end{array}
\end{array} \quad (6) \]

(ii) **Strong-coupling (SC) fixed point:** \( \lambda = \infty \):

\[ H_{SC, N}^* = \begin{array}{c}
\begin{array}{c}
\text{imp} \ \ 0 \ \ 1 \ \ 2 \ \ \cdots \ \ N
\end{array}
\end{array} \quad (1) \]

To minimize effect of exchange coupling, all low-energy states have \( \langle \hat{S}_c \cdot \hat{S}_d \rangle = 0 \) \( \text{, i.e. impurity and site} \ 0 \ \text{form a singlet} \) \( \text{.} \)

\( \Rightarrow \) \( \langle f_{01}^+ f_{01} f_{12}^+ f_{12} \rangle = 0 \) \( \text{, since hopping to or from site} \ 0 \ \text{will break the singlet} \).

\[ \text{So:} \] \[ H_{SC, N}^* = H_N (\lambda = \infty) = H_{N-1}^* \quad (4) \]

For \( N_{\text{tr}} = \text{even} \): \( \text{(2.e)} \)

\[ \hat{H}_{SC}^* 0, \quad \hat{\eta}_1^* (12), \quad 2 \hat{\eta}_1^* (14), \quad \hat{\eta}_1^* (16), \quad 3 \hat{\eta}_1^* (16). \quad (5) \]

For \( N_{\text{tr}} = \text{odd} \): \( \text{(2.e)} \)

\[ \hat{H}_{SC}^* 0, \quad \hat{\eta}_1^* (4), \quad 2 \hat{\eta}_1^* (6), \quad 3 \hat{\eta}_1^* (4), \quad \hat{\eta}_1^* (4). \quad (6) \]
What happens for general $T$? Low-energy spectrum of $H_N(T \ll 1)$ evolves ("flattens") with $N$ (engines), evolving from $H_L \rightarrow H_{sc}^{+}$ (evaporation), or $H_L \rightarrow H_{sc}^{+}$ (odd injection).

Wilson's railroad analogy:

The basic results of the Kondo calculation can be summarized in a geographical allegory. The sequence of Hamiltonians corresponding to adding successive layers of the onion to the impurity will be represented by a railroad track. The length of track from the beginning to the $n$th tie represents the Hamiltonian containing $n$ conduction band single electron states (that is, the $n$th Hamiltonian contains $n$ particle creation and destruction operators).

There is a separate railroad track for each different strength of coupling to the impurity. The approximate numerical solution of this sequence of Hamiltonians is represented by a railroad car which travels down the track. Solving the $n$th Hamiltonian corresponds to having the railroad car at the $n$th tie on the track. The set of energy levels actually computed corresponds to the length of track covered by the railroad car; as the car moves down the track (i.e., as $n$ increases) it covers a smaller and smaller fraction of the total track up to the $n$th tie.

**FIG. 14.** Railroad track analogy for the Kondo calculation. Different tracks correspond to different initial values of $J$. A track from the top of the figure to the $n$th tie corresponds to the Kondo Hamiltonian with $n$ electron states kept. The railroad cars illustrate the subset of energy levels actually kept in the numerical calculations.

\[ J = 0.11, \Lambda = 2, \text{SU}(2)_{\text{charge}} \otimes \text{SU}(2)_{\text{spin}} \text{ symmetry} \]
Fixed points of $\Sigma$ (at $U=0$) \cite{Kishita-murthy1980, Sec. III} \cite{NRG2.3}

$$
H_{\Sigma AM} = \sum_5 \epsilon_d d_5 d_s + U \hat{N}_d \hat{N}_d + \frac{J}{\pi V} \sum_5 \epsilon_d \phi_d \phi_c + H_{\text{chain}} \tag{0}
$$

For $U=\Gamma=\epsilon_d=0$:

Free-orbital (FO) fixed point:

$$
\hat{H}_{\text{FO}} = \hat{H}^{*} \otimes \mathbb{I}_4, \quad \hat{H}_{\text{FO}} = \hat{H}^{*} \otimes \mathbb{I}_4
$$

For $\epsilon_d < -\Gamma$ and $\Gamma < \epsilon_d$:

Local moment fixed point:

$$
\hat{H}^{*}_{\text{LM}} = \hat{H}^{*} \otimes \mathbb{I}_2, \quad \hat{H}^{*}_{\text{LM}} = \hat{H}^{*} \otimes \mathbb{I}_2
$$

For $\Gamma \rightarrow \infty$ at fixed $U$:

Strong-coupling fixed point:

$$
\hat{H}^{*}_{\text{SC}} = \hat{H}^{*}, \quad \hat{H}^{*}_{\text{SC}} = \hat{H}^{*}
$$

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{NRG2.3.png}
\caption{Low-lying energy levels of $H_{\Sigma}$ as a function of odd $N$ for $U/D = 10^{-3}$, $U/\pi\Gamma = 12.66$, and $\Lambda = 2.5$. On the left-hand vertical scale are the lowest-lying free-electron fixed-point levels for $N$ odd, while on the right-hand side are the equivalent levels for $N$ even. The following fixed-point regimes obtain: free orbital $3 < N < 15$, local moment $23 < N < 51$, strong coupling $61 < N$.}
\end{figure}

The fact that the level structure of $\hat{H}_{\text{FO}}$, $\hat{H}^{*}_{\text{LM}}$ and $\hat{H}^{*}_{\text{SC}}$ show up as regions of near-stationarity, proves numerically that there are fixed points!\n
Conversely from even-type $\phi_d^{\uparrow}$ levels to odd-type $\phi_c^{\uparrow}$ levels proves screening, i.e. singlet-bosonization between spin-up and spin-down.
No local moment forms, since there is no region where \( \langle N_{d} \rangle \approx 1 \). However, if \( \gamma \to \infty \), we have \( \langle Q_{d} S_{0} + \text{h.c.} \rangle = 0 \), so site 0 again decouples, so flow is again toward \( H_{s}^{\uparrow} \), \( H_{s}^{\downarrow} \).

8. Thermodynamic observables

Thermal expectation values:

\[
\langle \sigma \rangle_{T} = \lim_{M \to \infty} \frac{\text{Tr} \left[ e^{-\beta H_{M}^{\text{disc}}} \right]}{\text{Tr} \left[ e^{-\beta H_{M}} \right]}
\]

\[
\text{(1)}
\]

Recall:

\[
H_{M} = \Lambda^{(N-1)/2} \left( H_{M}^{\text{disc}} - E_{g_{M}} \right)
\]

\[
\text{(2)}
\]

\[
H_{M}^{\text{disc}} = \Lambda^{-(M-1)/2} H_{M} + E_{g_{M}}^{\text{disc}}
\]

\[
\text{(3)}
\]

\[
\langle \sigma \rangle_{T} = \lim_{M \to \infty} \frac{\text{Tr} \left[ e^{-\beta M H_{M}^{\alpha}} \right]}{\text{Tr} \left[ e^{-\beta M H_{M}} \right]}
\]

\[
\text{(4)}
\]

With rescaled temp:

\[
\beta_{M}^{\alpha} = \Lambda^{-(M-1)/2} \beta = \frac{\Lambda^{-(M-1)/2}}{T}
\]

\[
\text{(5)}
\]
At each energy scale $\Lambda^{-N/2}$, we have a "Wilson shell" of eigenstates, satisfying

$$H_N |j_N\rangle = E_j |j_N\rangle,$$

$$j = 1, \ldots, D_N.$$ (1)

But we don't have a complete set of states for entire chains for $M > e$.

Simplification:

$$\langle e^{-\beta M H_M} \rangle \approx \sum_j e^{-\beta M E_j^M} \frac{1}{\sum_j e^{-\beta M E_j^M}}$$ (2)

Trace over shell $M$ with $M$ drawn at the value $M_T$ for which $\beta M_T = 1 \Rightarrow \Lambda^{- (M_T - 1)/2} = T$

- For $M < M_T$ (high-energy states), $\beta M > 1$, $e^{-\beta M} \approx 0$
- For $M > M_T$ (low-energy states), $\beta M < 1$, it doesn't matter for $T$-dependence

(there are comparatively less of them...)

**Physical quantities:**

**Susceptibility:**

$$\chi = \frac{\partial \langle S_0^2 \rangle \tau}{\partial H} \bigg|_{H=0}$$ (1)

$$= \frac{N}{4 \beta H} \frac{\text{Tr} \left[ e^{-\beta H} (S_0^2) S_0^2 \right]}{\text{Tr} e^{-\beta H}}$$ (3)

$$= \beta \frac{\text{Tr} \left( e^{-\beta H} S_0^4 \right)}{\text{Tr} e^{-\beta H}} - \beta \left( \frac{\text{Tr} \left( e^{-\beta H} S_0^2 \right)^2}{\text{Tr} e^{-\beta H}} \right)$$ (4)

In NRW context:

$$\chi(T_N) = \frac{\text{Tr} \left( S_0^2 \right)^2 e^{-\beta N H_N}}{\text{Tr} e^{-\beta N H_N}}$$ (5)

**Impurity contribution:**

$$\chi_{\text{imp}} = \chi_{\text{tot}} - \chi_{\text{band}}$$

**FIG. 9.** Plots of $k_B T x(T)/(g_{\mu_B})^2$ vs $\ln(k_B T/D)$ for the symmetric Anderson model for $U/D = 10^{-3}, U/\pi T = 12.66(A)$ and 1.013(B). The dashed curves correspond to the universal susceptibility curve for the Kondo model (see Fig. 11 and Sec. V). The vertical arrows on the abscissa mark the effective Kondo temperature (5.16) for the two plots. Note that the curves mirror the pattern of energy levels in Figs. 5 and 6. For $U >> \pi T$, there is a well-developed local-moment regime ($T x = \frac{1}{2}$) between the free-orbital regime ($T x = \frac{1}{3}$) and the strong-coupling regime ($x = \text{constant}$), whereas for $U \sim \pi T$, there is a direct transition from the free-orbital to strong-coupling regime. The labels $\rho_{SW}$ are deduced from Eq. (5.14).
Partition function: \( Z = \text{Tr} \ e^{-\beta H} = e^{-\beta F} \)  

\[ (1) \]

Free energy: \( F = -T \ln Z \)

\[ (2) \]

Entropy: \( S = -\frac{\partial F}{\partial T} = \ln Z + T \left[ \frac{\partial}{\partial T} \left( \frac{\partial \ln Z}{\partial T} \right) \right] \)

\[ (3) \]

\[ \frac{1}{T^2} \]

\( S = \ln Z + T \beta, \quad U = \langle H \rangle_T \)

\[ (4) \]

Specific heat: \( C = \frac{\partial U}{\partial T} = \frac{\partial}{\partial T} \left[ \frac{\text{Tr} e^{-\beta H} H}{\text{Tr} e^{-\beta H}} \right] = \beta^2 \left( \langle H^2 \rangle - \langle H \rangle^2 \right) \)

\[ (5) \]

\[ \text{alternative:} \quad C = \frac{\partial}{\partial T} \left[ T (S - \beta \ln Z) \right] \]

\[ (6) \]

Impurity contributions: \( S_{\text{imp}} = S_{\text{tot}} - S_{\text{band}}, \quad C_{\text{imp}} = C_{\text{tot}} - C_{\text{band}} \)

\[ (7) \]

Wilson ratio: \( R = \frac{X_{\text{imp}} / X_{\text{band}}}{C_{\text{imp}} / C_{\text{band}}} \quad \xrightarrow{T=0} \quad Z \quad \text{for Kondo model}. \)

\[ (8) \]