Numerical Renormalization Group (NRG)

Invented by Ken Wilson [Wilson 1975], part of Nobel prize citation for development of renormalization group
First readable exposition: [Krishna-murthy 1980 a, b]
Standard review: [Bulla 2008]
In MPS context: [Weidelsbacher 2012 a]

1. Single-impurity Anderson Model (SIAM)

NRG is method of choice for treating "quantum impurity models":
impurity model = "impurity" + "bath"
= discrete states coupled to continuum

\[ \Theta \ldots \Phi \]

SIAM: [Anderson 1961]

\[ H_{\text{SIAM}} = H_{\text{band}} + H_{\text{loc}} + H_{\text{hyb}} \]  

\[ H_{\text{band}} = \sum_{\mathbf{k}, \sigma} \varepsilon_{\mathbf{k}} C_{\mathbf{k}\sigma}^\dagger C_{\mathbf{k}\sigma} \quad (\text{free electrons}) \]

\[ H_{\text{loc}} = \sum_{\mathbf{r}, \sigma} (\varepsilon_{\mathbf{r}} - \varepsilon_{\mathbf{k}}) \hat{n}_{\mathbf{r}\sigma} + \hat{U} \hat{n}_{\mathbf{r}\uparrow} \hat{n}_{\mathbf{r}\downarrow} \quad (\text{local level}) \]

\[ \hat{n}_{\mathbf{r}\sigma} = \hat{d}_{\mathbf{r}\sigma}^\dagger \hat{d}_{\mathbf{r}\sigma} \quad (\text{local occupancy}) \]

\[ H_{\text{hyb}} = \sum_{\mathbf{k}, \mathbf{s}} v_{\mathbf{k}s} (\hat{d}_{\mathbf{s}\uparrow}^\dagger \hat{d}_{\mathbf{s}\uparrow} + \hat{d}_{\mathbf{s}\downarrow}^\dagger \hat{d}_{\mathbf{s}\downarrow}) \quad \text{hybridization between back level and band} \]

\[ \Delta(\varepsilon) = \sum_{\mathbf{k}} v_{\mathbf{k}} \delta(\varepsilon - \varepsilon_{\mathbf{k}}) \quad \text{hybridization function, describes:} \]

\[ \gamma = \pi v^2 \sigma = \text{level width} \]
Some physical background: [vDelft, "Mesoscopic Physics", SoSe 2015] \text{(NRGI. C)}

Tunable experimental realization:

Level occupancy:
\( N_d = \langle N_{d\uparrow} + N_{d\downarrow} \rangle \)

Linear Conductance
\( g = \frac{G}{2e^2/h} \)

Non-linear conductance in local moment regime, where \( N_d = 0 \)

Reason for anomalous behavior in local moment regime:
\text{(NRGI.d)}

- Local spin is "screened" for \( T \leq T_K \)
- Same singlet with spin: \( |S\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle |\downarrow\rangle - |\downarrow\rangle |\uparrow\rangle) \)
- Ground state has total spin \( S = 0 \)

Wilson's goals (1975) for related Kondo model (\( N_d = 1 \), local spin + both): numerically study ground state and low-energy properties

Tools:
- Logarithmic discretization of Land
- Mapping to Wilson chains
- Iterative diagonalization/truncation/mocking
2. Logarithmic discretization

Goal: to resolve low-energy regime.

Tool: log. discretization: \( \omega^+_n = \pm \Lambda^{-n}, \Lambda > 1 \) (e.g. \( \Lambda = 2 \)) \( n = 0, 1, 2, \ldots \)

\[ \begin{array}{cccccccc}
& & & & & & \Lambda^{-1} & \Lambda^{-1} \Lambda^{-2} \Lambda^{-2} \Lambda^{-1} & \Lambda^{-1} & \Lambda^{-2} & \Lambda^{-2} \Lambda^{-1} \\
& & & & -1 & \xi_1^- & \xi_1^- \xi_2^- \xi_2^- \xi_1^- & \xi_1^- & \xi_2^- & \xi_2^- \xi_1^- \\
& & & & & & & & & \text{(D = 1)}
\end{array} \]

Represent each interval \( I_n^\pm = \{ \omega \in (\omega_n^\pm, \omega_{n+1}^\pm) \} \)
in terms of a single state, with energy \( \xi_n^\pm \) and coupling \( \gamma_n^\pm \), such that the hybridization function

\[ \Delta(\epsilon) = \sum_n \gamma_n^\pm \delta(\epsilon - \xi_n^\pm) = \sum_n (\gamma_n^\pm)^2 \delta(\epsilon - \xi_n^\pm) \]

is represented "as well as possible".

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Discretized Hamiltonian

\[ H_{\text{disc}} = H_{\text{loc}}(d^+, d^-, b^+) + H_{\text{band}} + H_{\text{hyb}} \]

\[ H_{\text{band}} = \sum_{n=0}^{\infty} \sum_{s=t,c} \xi_n^s \eta_n^s d^s_n a_n^s + \eta_n^- b_n^t b_n^s \]

particle-like \quad \text{hole-like}

\[ H_{\text{hyb}} = \sum_s d^s_0 \sum_{n=0}^{\infty} (\gamma_n^t a_n^s + \gamma_n^- b_n^s b_n^s) + \text{h.c.} \]

\[ \equiv \tilde{V}_1 \tilde{f}_1 s \]

Key observation: only a single linear combination couples to minority!

Hybridization function:

\[ \Delta_{\text{hyb}}(\epsilon) = \sum_n (\gamma_n^\pm)^2 \delta(\epsilon - \xi_n^\pm) \]

Requirements:

- preserve weight:
  \[ \int_{-\infty}^{\infty} \Delta(\epsilon) \, d\epsilon = \int_{-\infty}^{\infty} \Delta_{\text{loc}}(\epsilon) \, d\epsilon \]

- low-energy value:
  \[ \Delta(0) = \Delta_{\text{dis}}(0) \]
Simplest choice that gets weight right (used by Wilson):\[ NRG 2.6 \]

\[ G_n^\pm = \int \frac{d\xi}{\pi^+} \Delta(\xi) \] \( (1) \)

\[ \xi_n^\pm = \int \frac{d\xi}{\pi^+} \Delta(\xi) \] \( \frac{\int d\xi}{\xi_n^+} \Delta(\xi) \) 

For "Lax hybridization function", \( \Delta(\xi) = \begin{cases} 1 & \text{if } |\xi| < 1 \\ 0 & \text{otherwise} \end{cases} \) 

one finds:

\[ (\xi_n^\pm)^2 = \lambda^{-n} (1 - \lambda^{-n}) \sim \lambda^{-n} \] 

\[ \xi_n^\pm = \pm \frac{1}{2} \lambda^{-n} (1 + \lambda^{-n}) \sim \lambda^{-n} \] \( \text{decrease exponentially!} \)

For most recent improvement of discretization scheme, [Bronogol et al. 2016].

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3. Wilson chain

\[ NRG 3.1 \]

\[ \text{Hopp's + Hopp's} = d_0 a_0 \cdots a_N b_0 \cdots b_N \]

\[ \begin{pmatrix} a_0^+ & a_1^+ & \cdots & a_N^+ \\ a_0^- & a_1^- & \cdots & a_N^- \\ \vdots & \vdots & \ddots & \vdots \\ b_0^+ & b_1^+ & \cdots & b_N^+ \\ b_0^- & b_1^- & \cdots & b_N^- \end{pmatrix} \]

\[ = \begin{pmatrix} \xi_0^+ & \xi_1^+ & \cdots & \xi_N^+ \\ \xi_0^- & \xi_1^- & \cdots & \xi_N^- \\ \vdots & \vdots & \ddots & \vdots \\ \xi_N^+ & \xi_N^- \end{pmatrix} \]

\[ \equiv \text{Holstein} \]

\[ \text{(ignoring s. index)} \]

\[ \begin{pmatrix} f_0^+ & f_1^+ & \cdots & f_N^+ \\ f_0^- & f_1^- & \cdots & f_N^- \end{pmatrix} \]

\[ \text{By reductions, we can bring this into form of t"uring-induced chain:} \]

\[ \text{Hopp's} + \text{Hopp's} + \equiv \text{Holstein} = \sum_{n=1}^{N} \Sigma \sum_{s} \left[ \xi_n^+ \left( f_n^+ f_{n+1}\ldots f_N \right) + \xi_n^- f_n^+ f_n^- \right] \]

\[ \text{[in literature, chain often starts at } n=0; \text{ we start at } n=1, \text{ to be consistent with code H/t]} \]

Using conditions:

\[ \left\{ f_{1,5} \equiv \sum_{n=1}^{N} \left( \xi_n^+ a_n^+ + \xi_n^- b_n^+ \right), \right. \]

\[ \left. \left\{ f_{n,5}^+ \equiv \delta_{nn} \xi_n \right\} \right\} \]
Wilson chain

\[ H_{\text{Wilson}} = H_{\text{loc}} + H_{\text{chain}} \]

For "box hybridization function", Wilson finds

\[ \xi_n = \gamma^{-\frac{1}{2}} \frac{1 + \gamma^{-1} (1 - \gamma^{-n+1})}{2 (1 - \gamma^{-2n-1})^{1/2} (1 - \gamma^{-2n-2})^{1/2}} \sim \gamma^{-\frac{n}{2}} \]

Key property:
- endpoint decay exponentially along chain!
- "energy - scale separation"
- site up perturbs site n only weakly!
- solve chain iteratively, truncate at each step.

4. Iterative diagonalization
\[ \{ \sigma_n \} = \{ |0\rangle, |1\rangle \} \] (accords are for spinless fermions, \( d = 2 \))
Actual Wilson chain eigenspectra for chains of length $n = 1, \ldots, 6$

Iteration produces Matrix Product States

$$H_n |\psi_n\rangle = E_n |\psi_n\rangle \quad (M \text{ eigenstates})$$

$$|\psi'_{n+1}\rangle = \sum_{s_{n+1}} |s_n\rangle \sigma_{n+1} |s_{n+1}\rangle |\sigma^{\dagger}_{n+1}\rangle |\psi'_n\rangle$$

$$|\psi'_{n+1}\rangle = \sum_{s_{n+1}} |s_n\rangle \sigma_{n+1} |\sigma_{n+1}\rangle |\psi'_n\rangle$$

$d$ matrices, $M \times (Md)$

$$|\psi'_{n+1}\rangle = \sum_{s_{n+1}} |s_n\rangle \sigma_{n+1} |\sigma_{n+1}\rangle |\psi'_n\rangle$$

$\lambda_{n+1} \neq 0$

$\lambda_n = 0$

$|\psi''_n\rangle = \sum |s_n\rangle |\sigma_{n+1}\rangle |\sigma_{n+1}\rangle \ldots |\sigma_{n+1}\rangle |\psi''_n\rangle$ $\text{truncation needed}$

"matrix product state" (MPS)
Wilson's truncation scheme

Keep only lowest $M$ states of each iteration, Discard the rest!

Justification: "Energy-scale separation":
Highlying states affect low-lying ones only weakly.

$$|S_n^K\rangle = \sum_{s, \sigma_{n1}} \sum_{s, \sigma_{n+1}} \sum_{s, \sigma_{n+2}} \ldots \sum_{s, \sigma_{n+M}} |S_n^K\rangle |S_{n+1}^K\rangle |S_{n+2}^K\rangle \ldots |S_{n+M}^K\rangle$$

Advantages:
- Managable number of states
- Information obtained from all energy scales
- Small energies are very well resolved
- Hamiltonian is diagonal:

$$\hat{H} = \sum_{n} \sum_{s} E_n^s |S_n^K\rangle \langle S_n^K|$$

Problem:
- No complete basis set available, since states are discarded:
- This causes ambiguities in Lehmann sum, which have to be fixed by "fudging"

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Eigenenergy flow diagrams

Eigenstates at iteration $n$ from a "Wilson shell":

$$H_n |S_n^K\rangle = E_n^s |S_n^K\rangle$$

Define rescaled energies, so that average spacing is $O(1)$:

$$E_n^s \equiv \Lambda^{n/2} E_n^s$$

Plot of $E_n^s$ versus $n$ yields "energy level flow diagram":

Various fixed points in flow revealed physical behavior at corresponding energy scales.

Fig. 5 a [Krishnamurthy 1980a]