NRG I: Numerical renormalization group: Wilson chain

NRG was invented by Kenneth Wilson [Wilson1975]. It was part of his Nobel prize citation for development of the renormalization group (RG) concept. It is the first example of an MPS method (but at the time was not formulated in MPS language).

First readable exposition: [Krishna-murthy1980a, Krishna-murthy1980b]

Standard review: [Bulla2008]; in MPS context: [Weichselbaum2012a]

NRG is the method of choice for treating 'quantum impurity models':

impurity model = 'impurity' + 'bath' = discrete states coupled to non-interacting continuum

A canonical example of a quantum impurity model is:

1. Single-impurity Anderson model (SIAM) [Anderson1961]

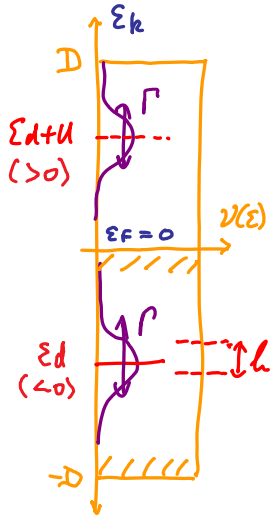
Anderson introduced this model in 1961 to explain formation of local moments in magnetic alloys (metals with magnetic impurities). Starting 1998, it has also been realized in numerous experiments involving transport through quantum dots [Goldhaber-Gorden1998], [Wiel2000].

$$H_{SIAM} = H_{band} + H_{loc} + H_{hyb} \qquad (1)$$

$$H_{band} = \sum_{k} \sum_{s=\uparrow,\downarrow} \varepsilon_k c^\dagger_{ks} c_{ks} \qquad \text{(band of free electrons)} \quad (2)$$

$$H_{loc} = \sum_{s=\uparrow,\downarrow} (\varepsilon_d - \tfrac{1}{2} h s)\, \hat{n}_{ds} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \qquad \text{(local level)} \quad (3)$$

(ε_d: local level position; h: magnetic field; U: Coulomb)



$$\hat{n}_{ds} = d^\dagger_s d_s \quad \text{= local charge for spin } s, \qquad \hat{n}_d = \sum_s \hat{n}_{ds} \qquad (4)$$

$$H_{hyb} = \sum_{ks} v_k \left(c^\dagger_{ks} d_s + d^\dagger_s c_{ks} \right) \qquad \text{(hybridization between local level and band)} \quad (5)$$

take $v_k = v$

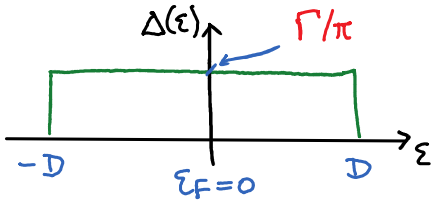
$$\Delta(\varepsilon) = \sum_k v_k^2\, \delta(\varepsilon - \varepsilon_k) \qquad (6)$$

hybridization function, describes 'how strongly does level with energy ω couple to impurity'?

We'll choose 'flat band': $\Delta(\varepsilon) := \frac{\Gamma}{\pi}\, \theta(D - |\varepsilon|)$ (7)

Γ : hybridization strength = level width

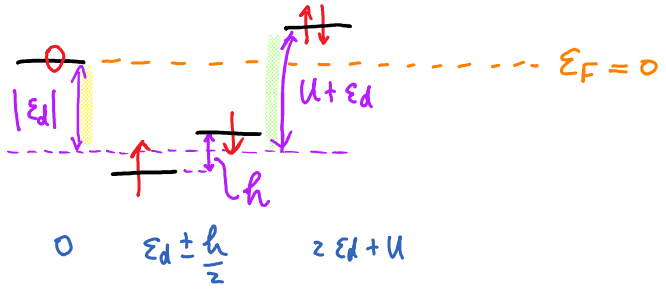
D : half-bandwidth



Local Hilbert space (for impurity):

State	Local energy
$\|0\rangle$	$E_0 = 0$
$\|\uparrow\rangle$	$E_\uparrow = \varepsilon_d - \frac{1}{2}h$
$\|\downarrow\rangle$	$E_\downarrow = \varepsilon_d + \frac{1}{2}h$
$\|\uparrow\downarrow\rangle$	$E_{\uparrow\downarrow} = 2\varepsilon_d + U$

Level scheme for $\varepsilon_d < 0$ $\quad \varepsilon_d + U > 0$



particle-hole symmetry if: $|\varepsilon_d| = U + \varepsilon_d \Rightarrow \varepsilon_d = -U/2$

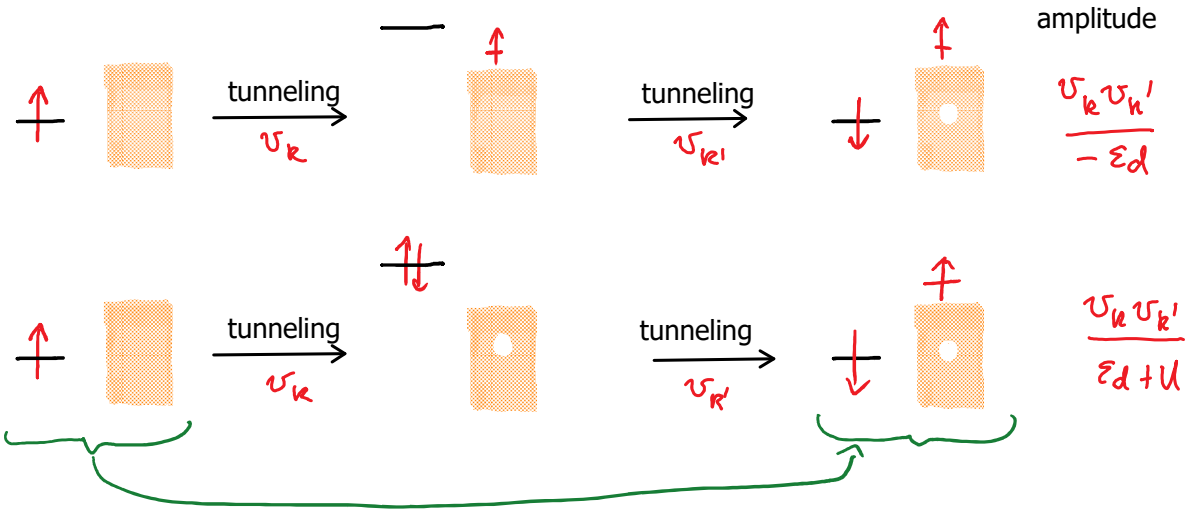
Regime of interest: empty and doubly occupied states of impurity lie far above singly occupied states ('local moment regime'):

$E_0 - E_\sigma > \Gamma$, $E_{\uparrow\downarrow} - E_\sigma > \Gamma$

$0 > \varepsilon_d + \Gamma$, $\varepsilon_d + U > \Gamma \Rightarrow -U + \Gamma < \varepsilon_d < -\Gamma$

Then average occupancy of local level is $n_d = \langle \hat{n}_d \rangle \simeq 1$

Impurity forms a 'local moment' (= localized spin). Then states with $\langle \hat{n}_d \rangle = 0$ or 2 are accessible only via virtual transitions, involving tunneling into the bath and back, leading (amongst other process) to 'spin-flip transitions':



Netto result: impurity spin is flipped, and particle-hole excitation is created in bath

Effective low-energy model (below the energy scale Γ) describing these spin-flip processes is the Kondo model: [Kondo1964, Schrieffer1966] (= Anderson model projected to $\langle \hat{n}_d \rangle = 1$)

$$H_{Kondo} = H_{band} + H_{loc} + H_{exchange} \qquad (10)$$

$$H_{band} = \sum \varepsilon_k \hat{c}^\dagger_{k\sigma} \hat{c}_{k\sigma} \qquad H_{loc} = h \hat{S}^z \qquad (11)$$

(10)

$$H_{band} = \sum_s \varepsilon_k \hat{c}^\dagger_{ks} \hat{c}_{ks}, \qquad H_{loc} = h \hat{S}^z_d \tag{11}$$

$$H_{exchange} = J \Big(\sum_{kk'} \sum_{ss'} \hat{c}^\dagger_{ks} \tfrac{1}{2} \vec{\sigma}_{ss'} \hat{c}_{k's'} \Big) \cdot \hat{\vec{S}}_d \qquad \text{with} \quad \hat{\vec{S}}_d = |\bar{s}\rangle \tfrac{1}{2} \vec{\sigma}_{\bar{s}\bar{s}'} \langle \bar{s}'| \tag{12}$$

$\sum_{kk'} \sum_{ss'} \hat{c}^\dagger_{ks} \tfrac{1}{2} \vec{\sigma}_{ss'} \hat{c}_{k's'} \equiv \hat{S}_c$

spin-1/2 operators

$$= J \hat{\vec{S}}_c \cdot \hat{\vec{S}}_d$$

States with $n_d = 1$, $\{|\uparrow\rangle, |\downarrow\rangle\}$, have spin $1/2$. The operator $\hat{S}^a_d$ acts on this spin-$1/2$ multiplet, like the matrices $\frac{1}{2}\sigma^a$ on two-component spinors, $\left\{ \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right\}$. (13)

$\hat{S}^a$ $a = x, y, z$ = quantum-mechanical spin-$\frac{1}{2}$ degree of freedom.

'spin-spin exchange interaction', if derived from SIAM:

$$J = \frac{U v^2}{|\varepsilon_d|(\varepsilon_d + U)} = v^2 \left(\frac{1}{-\varepsilon_d} + \frac{1}{\varepsilon_d + U} \right) > 0 \tag{14}$$

SIAM and Kondo model have the same low-energy behavior. We will discuss them interchangeably.

Perturbative treatment of Kondo model breaks down for $T \to 0$ (next section). What is ground state?

In late 1960's, Anderson had hypothesized (correctly!) that ground state of the Kondo model is a spin singlet: the conduction band electrons 'screening' the local spin to give total spin $S = 0$.

$$|g\rangle = |\Uparrow\rangle |\downarrow\rangle - |\Downarrow\rangle |\uparrow\rangle \tag{15}$$

However, no formal proof was available at that time. (In it was proven by Bethe Ansatz in 1983.)

Wilson's goal (1975): numerically study ground state and low-energy properties!

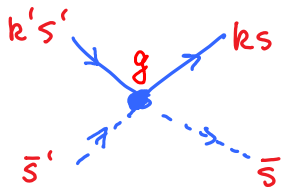
Tools: -logarithmic discretization of band

- mapping to 'Wilson chain'
- iterative diagonalization / truncation / rescaling

2. Kondo model: low-order perturbation theory

NRG-I.2

$H_{Kondo} = H_{band} + H_{exchange}$



$H_{band} = \sum_{ks} \varepsilon_k \hat{c}^\dagger_{ks} \hat{c}_{ks}$, with $\varepsilon_k \in [-D, D]$ (Σ bandwidth)

$H_{exchange} = J \underbrace{\left(\sum_{kk'} \sum_{ss'} \hat{c}^\dagger_{ks} \tfrac{1}{2}\vec{\sigma}_{ss'} \hat{c}_{k's'} \right)}_{\equiv \hat{\vec{S}}_c} \cdot \hat{\vec{S}}_d$ with $\hat{\vec{S}}_d = |\bar{s}\rangle \tfrac{1}{2}\vec{\sigma}_{\bar{s}\bar{s}'} \langle \bar{s}'|$ (1)

spin-1/2 operators

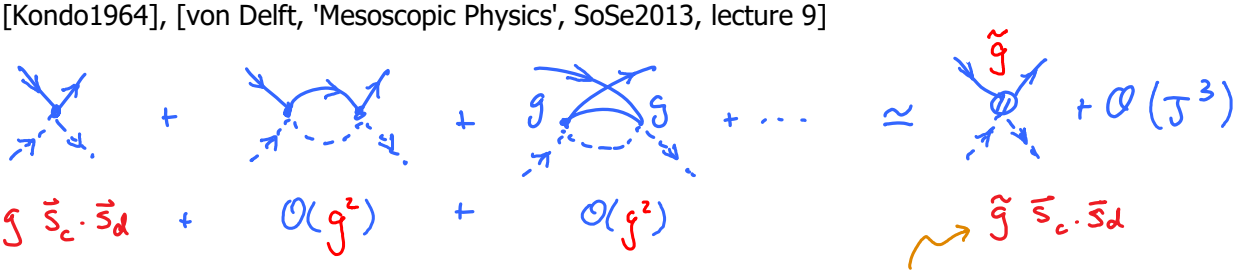
$= J\, \hat{\vec{S}}_d \cdot \hat{\vec{S}}_c$ 'spin-spin exchange interaction' (2)

Dimensionless coupling: $g = J\nu$ where ν = conduction electron density of states at ε_F ($\nu \leftrightarrow \Delta(0)$)

Why does Kondo model require non-perturbative treatment (like NRG)?

Perturbation theory in $H_{exchange}$ leads to logarithmic divergences:

[Kondo1964], [von Delft, 'Mesoscopic Physics', SoSe2013, lecture 9]



(3)

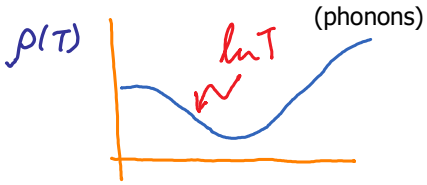
$g\,\vec{S}_c \cdot \vec{S}_d + O(g^2) + O(g^2) \simeq \tilde{g}\,\vec{S}_c \cdot \vec{S}_d$

same form as first-order term, but with modified coupling

One finds: effective vertex is $\tilde{g}\,\vec{S}_c \cdot \vec{S}_d$, with $\tilde{g}(T) = g + g^2 \ln D/T$ (4)

Thus 'effective coupling strength', $\tilde{g}$, computed in 2nd order perturbation theory, grows with decreasing temperature!

This was Kondo's explanation for 'resistivity anomaly' in magnetic alloys, which had been a puzzle since 1934.



Occurrence of $\ln D/T$ implies conceptual problem: effective coupling $\tilde{g}(T)$ grows with decreasing T, hence perturbation theory breaks down for sufficiently small T.

'Kondo temperature' is the scale where 2nd-order term becomes comparable to 1st-order term, signaling breakdown of pert. theory:

$$g^2 \ln \frac{D}{T_K} \overset{(4)}{\simeq} g \Rightarrow g \ln \frac{D}{T_K} = 1 \Rightarrow T_K = D\, e^{-\frac{1}{g}} \quad (5)$$

T_K is a 'dynamically generated scale', the 'characteristic low-energy scale' of Kondo problem.

Increase of $\tilde{g}(T)$ with decreasing T means: ground state can be understood by considering $\tilde{g} = \infty$

This heuristic argument leads to the conclusion: ground state is a spin singlet.

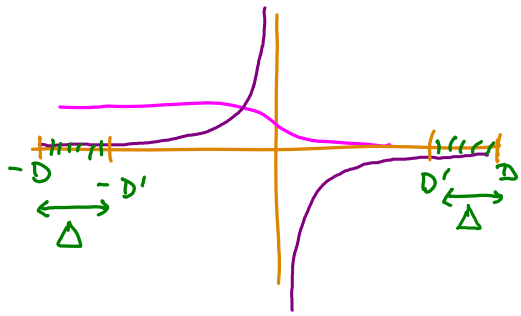
3. Kondo model: poor man's scaling RG

NRG-I.3

[Anderson1970], [Hewson1997]

$\ln(D/T)$ comes from sum over intermediate states in 2nd-order contribution to $\tilde{g} = g + g^2 \ln D/T$

$$\tilde{g}^{(2)} = g^2 \int_{-D}^{D} d\varepsilon \frac{f(\varepsilon)}{-\varepsilon} \simeq g^2 \ln \frac{D}{T} \qquad (1)$$



Anderson's idea: to reduce $\ln D/T$ problem, integrate out only high-energy modes.

Define 'reduced bandwidth', $D' = D - \Delta \qquad (\Delta > 0)$ (2)

and split integral into two parts:

$$g^2 \int_{-D}^{D} d\varepsilon \frac{f(\varepsilon)}{-\varepsilon} = g^2 \left[\int_{-D'}^{D'} d\varepsilon \frac{f(\varepsilon)}{-\varepsilon} + \int_{-D}^{-D+\Delta} d\varepsilon \frac{1}{-\varepsilon} \right] \qquad (3)$$

smaller bandwidth $\ln D'/T$

$\simeq \frac{\Delta}{D}$ if $D \gg T$

If $D \simeq T$, then no ln-divergence occurs, integral yields $\simeq 0$ (4)

Upshot:

$$\tilde{g}(D, g) = g + \tilde{g}^{(2)}(D, g) \qquad (5)$$

$$= g + \tilde{g}^{(2)}(D', g) + g^2 \frac{\Delta}{D} + \mathcal{O}(g^3) \qquad (6)$$

$$\simeq \tilde{g}(D', g') \qquad (7)$$

hence effective vertex can also be described using a reduced bandwidth,

$$D' = D - \Delta \overset{(2)}{=} D + \delta D \qquad (8)$$

and a modified coupling: $g' = g + g^2 \frac{\Delta}{D}$ (9)

Change in coupling: $g' - g \simeq \delta g = -g^2 \frac{\delta D}{D}$ (10)

Differential change:

$$\boxed{\frac{\delta g}{\delta(\ln D)} \simeq -g^2}$$

'scaling equation' (11)

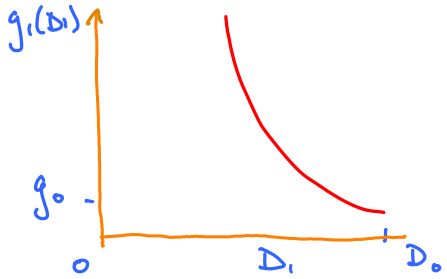
RG-flow of renormalized coupling

$$-\int_{g_0}^{g_1} \frac{dg}{g^2} \overset{(11)}{=} \int_{D_0}^{D_1} d(\ln D) \qquad (12)$$

$$\frac{1}{g_1} - \frac{1}{g_0} = \ln D_1/D_0 \qquad (13)$$

$$g_1(D_1) = \frac{1}{\frac{1}{g_0} - \ln(D_0/D_1)} \qquad (14)$$

$\ln(D_0/D_1) > 0$, grows as $D_1 \to 0$



RG flow has to be stopped when $D_1 \approx T$, so renormalized, T-dependent coupling is given by

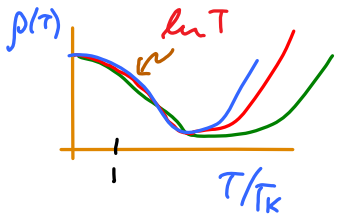
$$g_{eff}(T) = g_1(T) = \frac{1}{\frac{1}{g_0} - \ln(D/T)} \qquad (15)$$

Define Kondo temperature, T_K, as the temperature where $g_{eff}(T_K) = \infty$

$$\frac{1}{g_0} \equiv \ln(D/T_K) \implies T_K = D e^{-\frac{1}{g_0}} \qquad (16)$$

$$g_{eff}(T) \overset{(15)}{=} \frac{1}{\ln D/T_K - \ln D/T} = \frac{1}{\ln(T/T_K)} \quad \text{for} \quad T > T_K. \qquad (17)$$

Consequence: 'universality' - bare parameters D, g_0 occur in effective theory only in the combination $T_K = D e^{-1/g_0}$. Therefore, measurements made for $\rho(T)$ with different bare parameters will show scaling collapse when plotted as function of T/T_K.



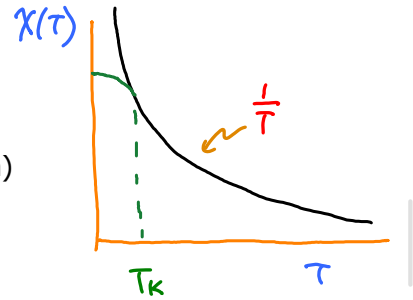
Scaling approach breaks down for $T < T_K$. Lower temperatures, require different approach.
Conjecture for 'strong-coupling regime: If $g_{eff} \to \infty$, then exchange interaction $g_{eff}\ \vec{S}_d \cdot \vec{S}_c$ becomes so strong that $\langle \vec{S}_d \cdot \vec{S}_c \rangle < 0$. Hence ground state is a 'singlet', for which 'impurity spin is screened by conduction electrons.

$$|\uparrow\rangle|\downarrow\uparrow\rangle - |\downarrow\rangle|\uparrow\downarrow\rangle$$

Consequence for spin susceptibility (will be verified numerically):

$$\chi(T) = \left.\frac{\langle S_d^z(h)\rangle_T}{dh}\right|_{h=0}$$

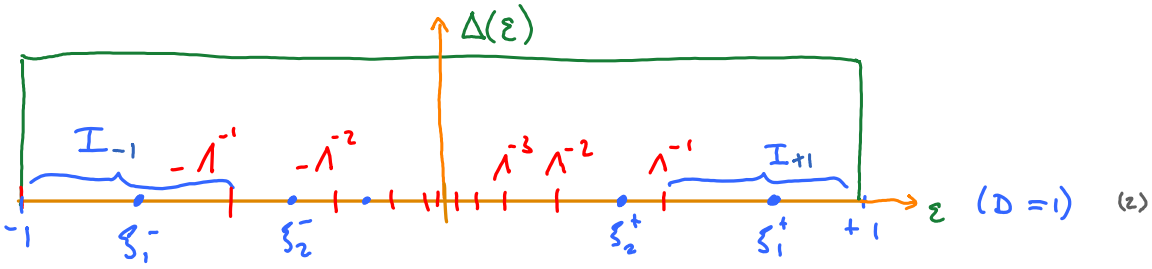
$$= \begin{cases} \frac{1}{T} & \text{for } T \gg T_K \quad \text{(Curie susceptibility of free spin)} \\ \chi_0 & \text{for } T \ll T_K \quad \text{(screened singlet)} \end{cases}$$



4. Logarithmic discretization, Wilson chain

Goal: to resolve low-energy regime. Tool: logarithmic discretization of band.

Define discrete energies: $\omega_n^{\pm} \equiv \pm \Lambda^{-n}$, $\Lambda > 1$ (e.g. $\Lambda = 2$) ('discretization parameter'), $n = 0, 1, 2, 3, \ldots$ (1)



(2)

These partition the band into intervals: $I_{+n} = (\Lambda^{-n}, \Lambda^{-n+1})$, $I_{-n} = (-\Lambda^{-n+1}, -\Lambda^{-n})$

Represent each interval $I_{\pm n}$ in terms of a single state, $|\pm n\rangle$, $n = 1, 2, 3, \ldots$ (3)

with energy $\xi_{\pm n}$ and coupling (to impurity) $\gamma_{\pm n}$, chosen such that the hybridization function,

$$\Delta(\varepsilon) = \sum_k v_k^2 \, \delta(\varepsilon - \varepsilon_k) \simeq \sum_{\pm n} (\gamma_{\pm n})^2 \delta(\varepsilon - \xi_{\pm n}) \quad (4)$$

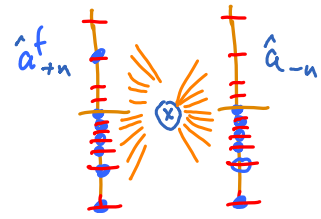
is represented 'as well as possible'. This leads to

Discretized Hamiltonian for SIAM (treatment for Kondo model is analogous)

$$H_{disc} = H_{loc}(\hat{d}_s, \hat{d}_s^\dagger) + H_{bath} + H_{hyb} \quad (5)$$

$$H_{bath} = \sum_{n=1}^{\infty} \sum_{s=\uparrow,\downarrow} \xi_{+n} \hat{a}_{+ns}^\dagger \hat{a}_{+ns} + \xi_{-n} \hat{a}_{-ns}^\dagger \hat{a}_{-ns} \quad (6)$$

particle-like excitations; hole-like excitations



'star geometry'

$$H_{hyb} = \sum_s \Big[d_s^\dagger \underbrace{\Big(\sum_{\pm n} \gamma_{\pm n} \hat{a}_{\pm ns}\Big)}_{\equiv t_{imp} f_{0s}} + \underbrace{\Big(\sum_{\pm n} \gamma_{\pm n} \hat{a}_{\pm ns}^\dagger\Big)}_{\equiv t_{imp} f_{0s}^\dagger} d_s \Big] \quad (7)$$

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

Hybridization function: $\Delta^{dis}(\varepsilon) = \sum_{\pm n} (\gamma_{\pm n})^2 \, \delta(\varepsilon - \xi_{\pm n})$ (8)

Requirements:

preserve weight: $\int_{-1}^{1} d\varepsilon \, \Delta(\varepsilon) = \int_{-1}^{1} d\varepsilon \, \Delta^{dis}(\varepsilon)$ (9)

preserve value at zero energy: $\Delta(0) = \Delta^{dis}(0)$ (10)

Simplest choice that gets weight right (used by Wilson):

$$\gamma_{\pm n}^2 = \int_{I_{\pm n}} d\varepsilon\, \Delta(\varepsilon) \qquad (11)$$

$I_{\pm n}$ interval between $\omega_n^{\pm}$ and $\omega_{n+1}^{\pm}$

$$\xi_{\pm n} = \frac{\int_{I_{\pm n}} d\varepsilon\, \varepsilon\, \Delta(\varepsilon)}{\int_{I_{\pm n}} d\varepsilon\, \Delta(\varepsilon)} \qquad (12)$$

For 'box hybridization function',

$$\Delta(\varepsilon) = \begin{cases} 1 & , \ |\varepsilon| < 1 \\ 0 & \text{otherwise} \end{cases} \qquad (13)$$

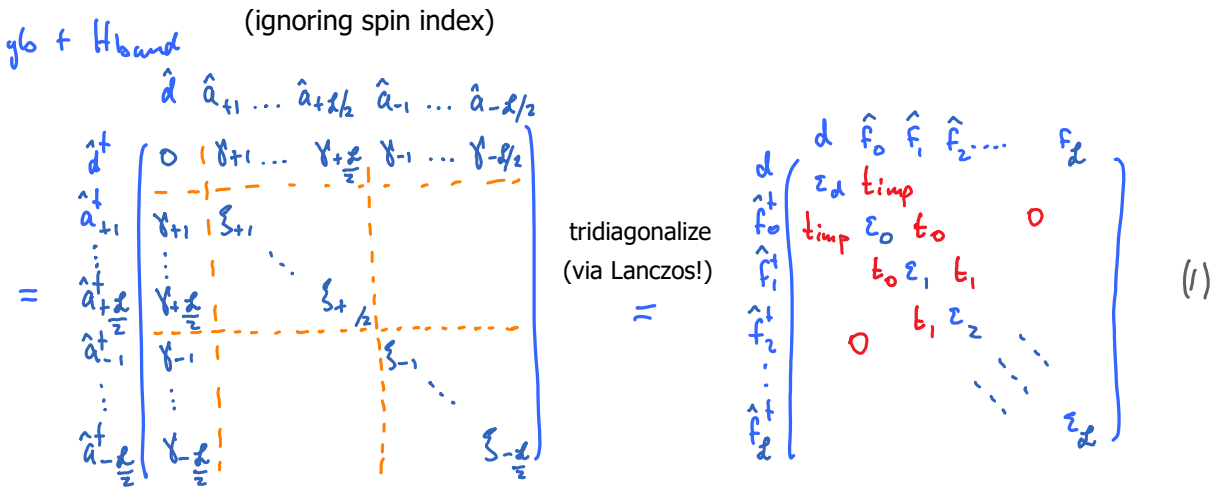
one finds:

$$\left(\gamma_n^{\pm}\right)^2 = \Lambda^{-n}\left(1 - \Lambda^{-1}\right) \sim \Lambda^{-n}$$
$$\xi_n^{\pm} = \pm\frac{1}{2}\Lambda^{-n}\left(1 + \Lambda^{-1}\right) \sim \Lambda^{-n}$$

} decrease exponentially! (14)

For most recent improvement of discretization scheme: [Bruognolo2016a].

By 'tridiagonalization', we can bring this into form of a 'tight-binding chain':



(1)

$$= \sum_s t_{imp}\left(\hat{d}_s \hat{f}^\dagger_{0s} + \text{h.c.}\right) + \sum_{l=0}^{\mathcal{L}} \sum_s \left[t_l \left(\hat{f}^\dagger_{ls} \hat{f}_{l+1\,s} + \text{h.c.} \right) + \varepsilon_l \hat{f}^\dagger_{ls} \hat{f}_{ls} \right] := H_{chain} \qquad (2)$$

by imposing the conditions:

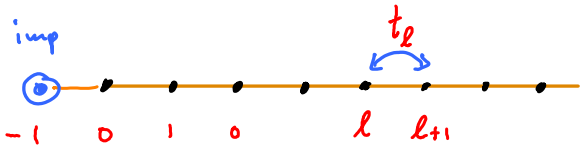
$$t_{imp}\, \hat{f}_{0s} \equiv \sum_{n=1}^{\mathcal{L}/2} \left(\gamma_{+n} \hat{a}_{+ns} + \gamma_{-n} \hat{a}_{-ns} \right), \qquad (3)$$

(normalization fixes t_{imp})

$$\left\{ \hat{f}^\dagger_{ls}, \hat{f}_{l's'} \right\} = \delta_{ll'} \delta_{ss'} \quad , \quad l = 0, \dots, \mathcal{L} \qquad (4)$$

Adding the impurity term, we obtain a 'Wilson chain', with impurity at site $l = -1$:

$$H_{Wilson} = H_{imp} + H_{chain}$$



(5)

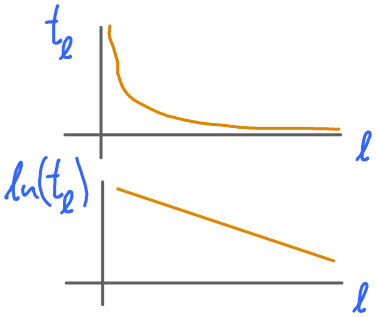
For 'box hybridization function', Wilson finds:

$$\varepsilon_l = 0 \qquad \text{(since band is symmetric around Fermi energy, at } \varepsilon_F = 0\text{)} \qquad (6)$$

$$t_l = \Lambda^{-l/2} \frac{(1+\Lambda^{-1})(1-\Lambda^{-l-1})}{2\,(1-\Lambda^{-2l-1})^{1/2}(1-\Lambda^{-2l-3})^{1/2}} \sim \Lambda^{-l/2} \qquad (7)$$

Key property of Wilson chain:

- couplings decay exponentially along chain!
- 'energy-scale separation'
- site $l+1$ perturbs site l only weakly!
- solve chain iteratively, truncate at each step.



Tridiagonalization can be achieved with the Lanczos method [Lanczos1950, Paige1972]:

iterative method to construct the tridiagonal matrix from general Hermitian matrix M

1st iteration:

1st iteration:

Choose the initial basis vector.

Here we use the basis for the impurity site.

$$\vec{v}_1 := \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix} \quad (8)$$

$$\alpha_1 = \vec{v}_1^{\dagger} M \vec{v}_1 \quad (9)$$

first diagonal element
[i.e., (1,1) element]

$$\vec{v}_2' := \underbrace{(1 - \vec{v}_1 \vec{v}_1^{\dagger})}_{\text{orthogonalize (Gram-Schmidt)}} \underbrace{M \vec{v}_1}_{\text{Act M}} \quad (10)$$

Normalize and register as the 2nd basis vector: $\vec{v}_2 := \vec{v}_2' / \| \vec{v}_2' \|$ (11)

First sub-diagonal element [i.e., (2,1) element]:

$$\beta_1 = \vec{v}_2^{\dagger} M \vec{v}_1 = \sqrt{\vec{v}_1^{\dagger} M^{\dagger} (1 - \vec{v}_1^{\dagger} v_1) M \vec{v}_1} = \| \vec{v}_1' \| \quad (12)$$

Second diagonal element [i.e., (2,2) element]: $\alpha_2 = \vec{v}_2^{\dagger} M \vec{v}_2$ (13)

n-th iteration: basis set $V := (\vec{v}_1, \vec{v}_2, \dots \vec{v}_n)$ $V^{\dagger} V = \mathbb{1}_{n \times n}$ (14)

$$\vec{v}_n' := \underbrace{(\mathbb{1} - V V^{\dagger})}_{\text{orthogonalize (Gram-Schmidt)}} \underbrace{M \vec{v}_n}_{\text{act M}}, \quad \vec{v}_{n+1} := \vec{v}_n' / \underbrace{\| \vec{v}_n \|}_{:= \beta_n}, \quad \alpha_{n+1} := \vec{v}_{n+1} M \vec{v}_{n+1} \quad (15)$$

Result:

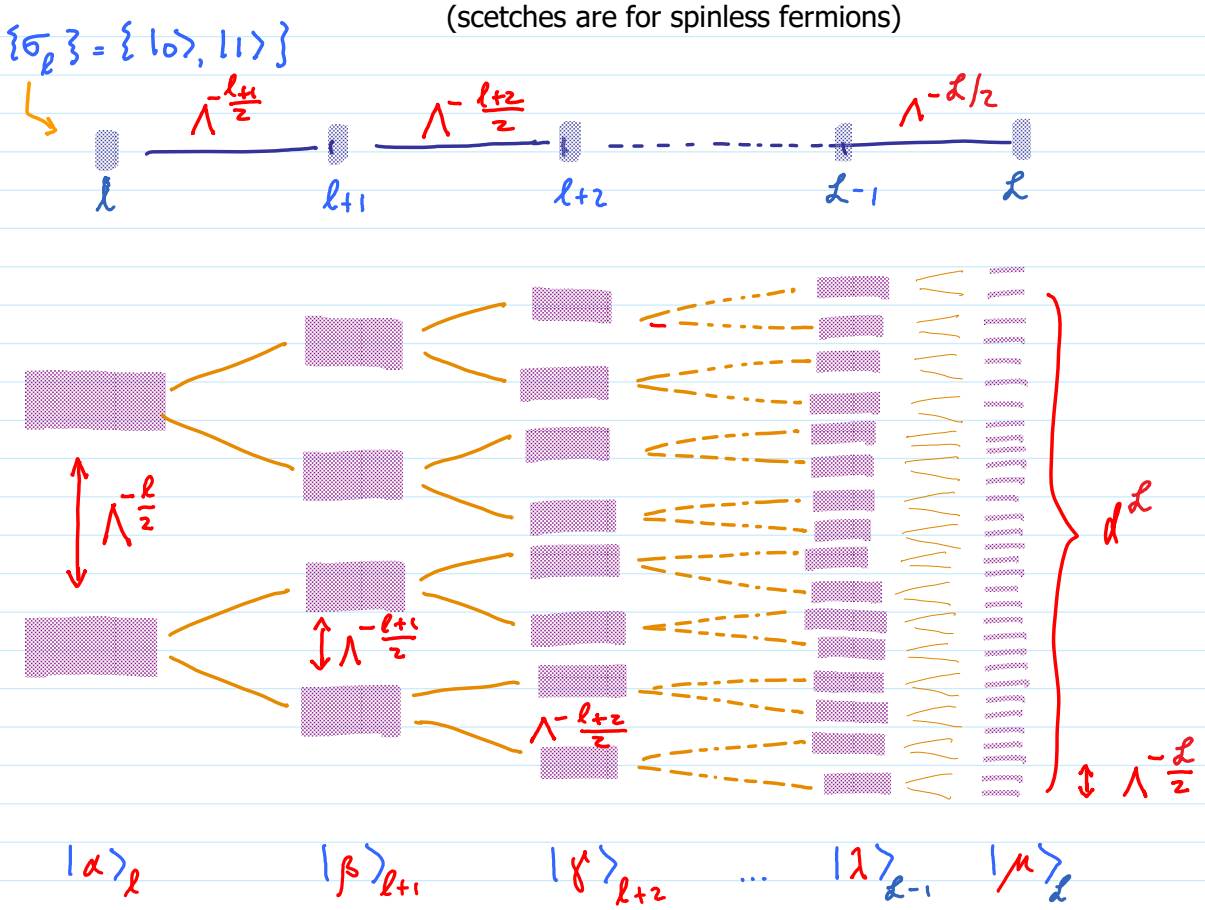
$$V^{\dagger} M V = \begin{pmatrix} \alpha_1 & \beta_1 & & \\ \beta_1 & \alpha_2 & \beta_2 & \\ & \beta_2 & \alpha_3 & \ddots \\ & & \ddots & \end{pmatrix}$$

$\vec{v}_m^{\dagger} M \vec{v}_n = 0$ for $|m-n| > 1$

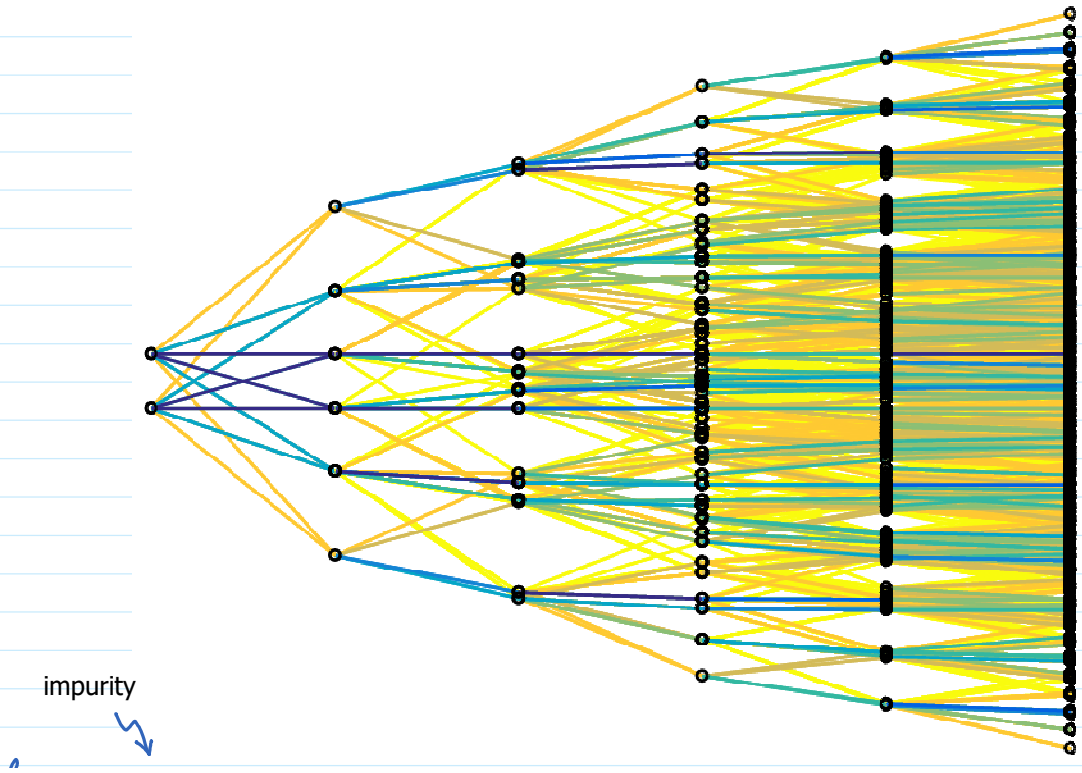
(due to orthogonalization) (16)

6. Iterative diagonalization

(scetches are for spinless fermions)



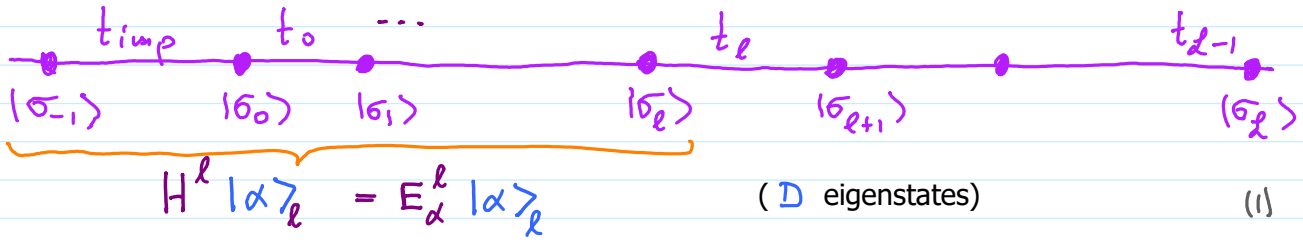
Below is the result of the iterative diagonalization of the Wilson chain for $\mathcal{L}$ = 4, keeping all the states. Circles indicate the energy eigenvalues at each iteration. Color of lines indicate the magnitude of the overlap between the eigenstates at consecutive iterations. Darker (brighter) line means that the eigenstate at the previous iteration contributes more (less) to the eigenstate at the current iteration.



$\ell =$ -1 0 1 2 3 4

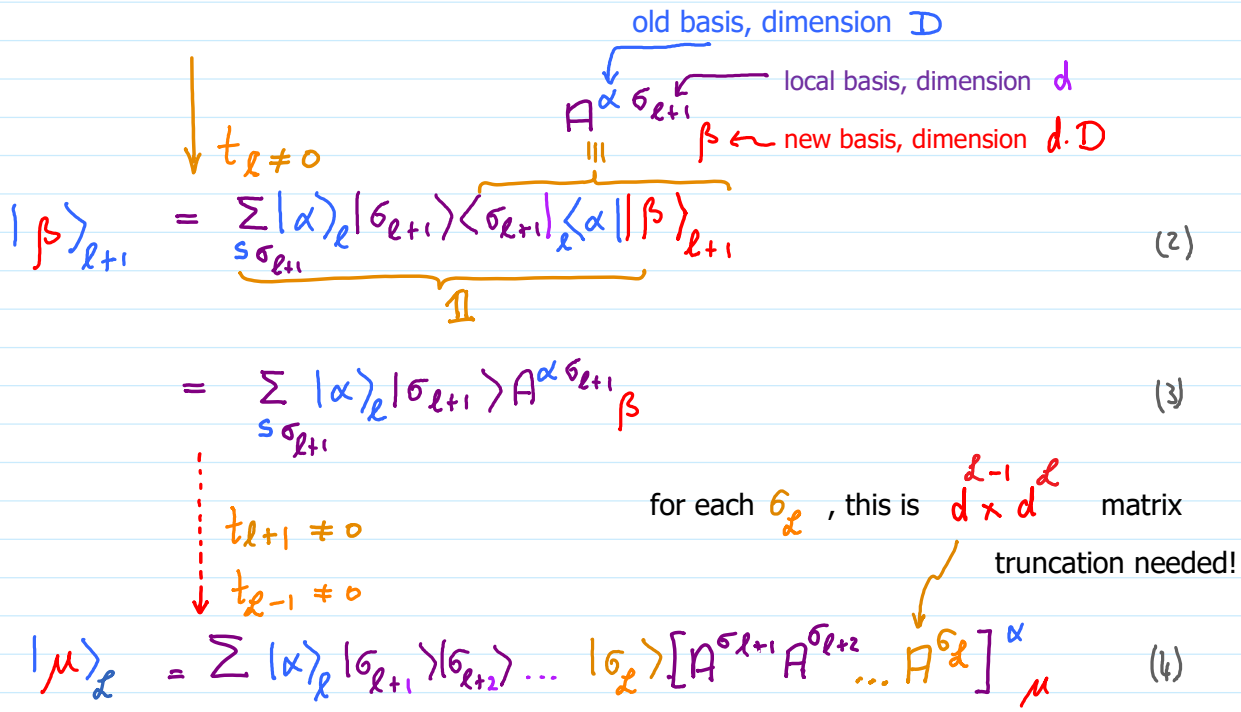
Level spacing decreases, $\sim \Lambda^{-\ell/2}$, number of state increases, $\sim d^{\ell}$

Iteration produces matrix product states [Weichselbaum2009]



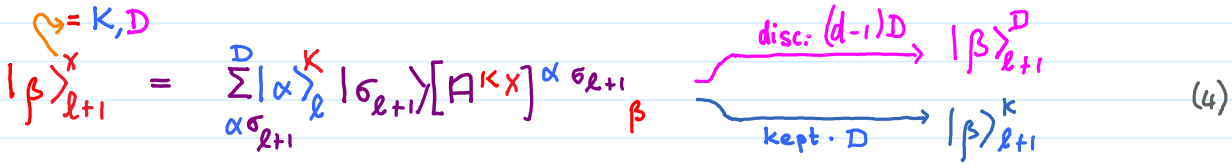
(D eigenstates) (1)

Suppose chain of length ℓ has been diagonalized numerically. Continue by adding one site at a time.



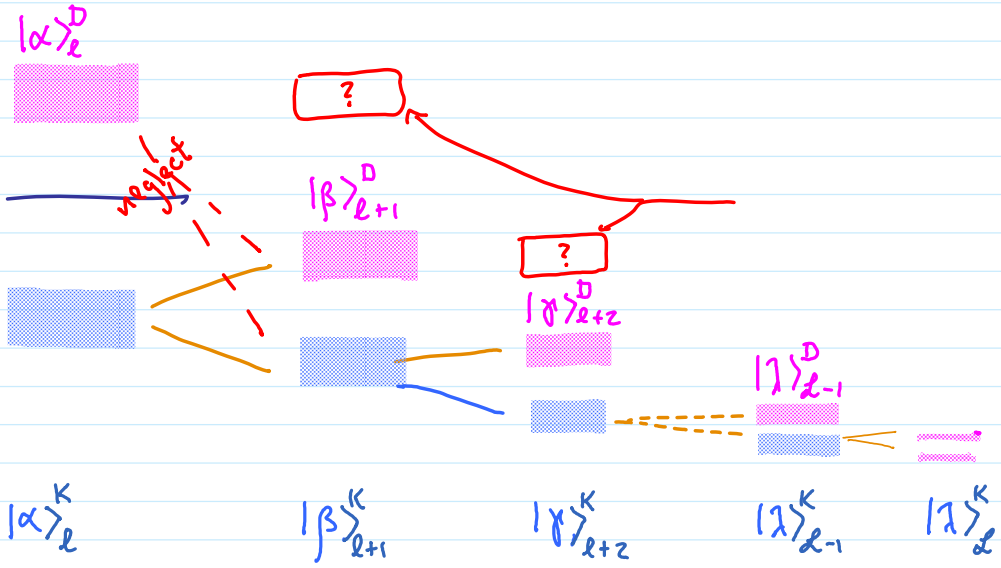
Wilson's truncation scheme:

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



(4)

Justification: 'energy-scale separation": high-lying states affect low-lying ones only weakly, since terms in perturbation expansion contain 'energy denominators' of the form $\sim \sum_\alpha \frac{(t_\ell)^2}{\epsilon - E_\alpha}$ (5)



Advantages of Wilsonian truncation:

- Manageable number of states
- Information obtained from all energy scales
- Small energies are very well resolved
- Hamiltonian of each iteration is diagonal: $\hat{H}^{\ell} = \sum_{\beta \in K} E_{\beta}^{\ell} \, |\beta\rangle_{\ell}^{K\,K} \langle\beta|$ (6)

Problem:

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

(Solution to problem, to be discussed in a later lecture: construct complete basis from discarded states!)

Energy flow diagrams

Eigenstates at iteration ℓ form a 'Wilson shell': $\hat{H}^{\ell} |\alpha\rangle_{\ell} = E_{\alpha}^{\ell} |\alpha\rangle_{\ell}$, $\alpha = 1, \ldots, D$ (7)

Define rescaled energies, so that average level spacing is $O(1)$: $\varepsilon_{\alpha}^{\ell} \equiv \Lambda^{\ell/2} \left(E_{\alpha}^{\ell} - E_{G}^{\ell} \right)$ (8)

Plot of versus yields 'energy level flow diagram':
Various 'fixed points' in flow reveal physical behavior at corresponding energy scales.

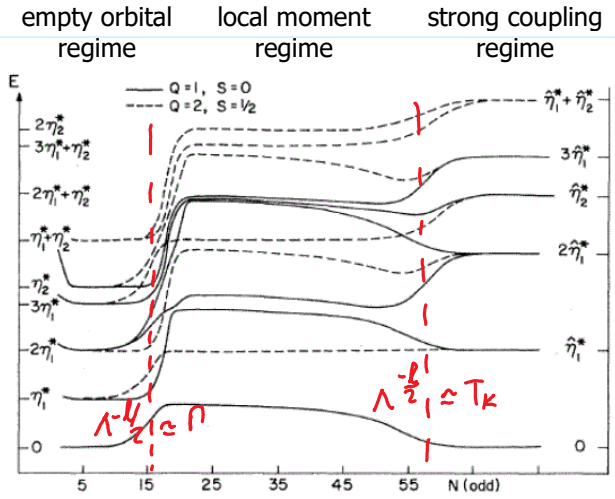
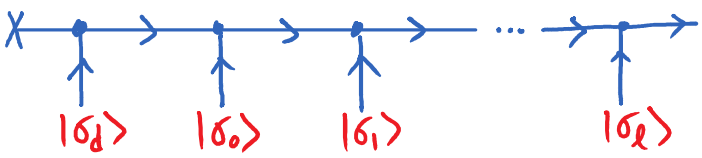
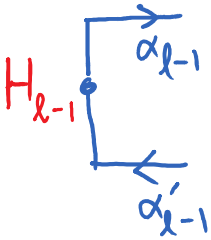


Fig. 5 of [Krishna-murthy1980a]

Iteration produces matrix product states [Weichselbaum2009]



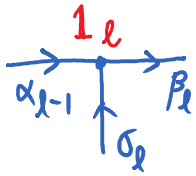
At each iteration:



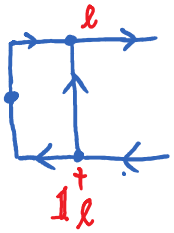
Hamiltonian in the Hilbert space spanned by $\{|\alpha_{\ell-1}\rangle\}$

Diagonal: $[H_{\ell-1}]^{\alpha'}_{\alpha} = \begin{cases} E_{\ell\alpha} & \text{if } \alpha=\alpha' \\ 0 & \text{if } \alpha\neq\alpha' \end{cases}$ (1)

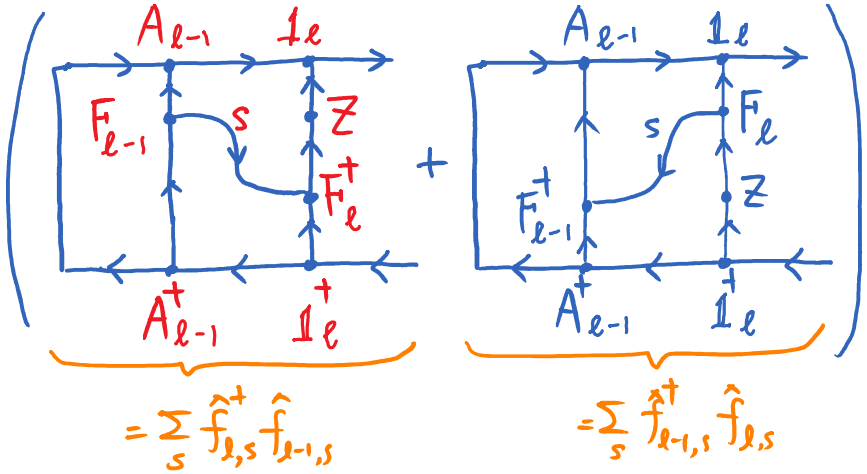
① Create the identity tensor for the product space $\{|\alpha_{\ell-1}\rangle\otimes|\sigma_\ell\rangle\}$



② Update the Hamiltonian $H_{\ell-1}$ for the product space, and rescale by multiplying $\sqrt{\Lambda}$

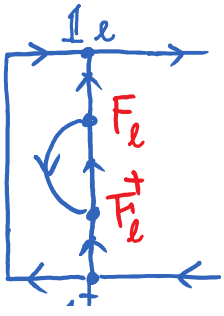
$H'_{\ell-1} := H_{\ell-1}$  $\times\sqrt{\Lambda}$ (2)

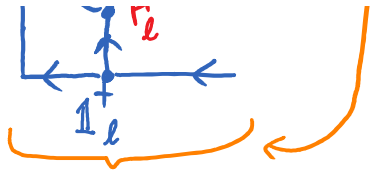
③ Add the hopping term between site $\ell-1$ and ℓ

$H^{\text{hop}}_\ell := \Lambda^{\ell/2} t_{\ell-1} \times$  (3)

$= \sum_s \hat{f}^\dagger_{\ell,s}\hat{f}_{\ell-1,s}$ $\quad$ $= \sum_s \hat{f}^\dagger_{\ell-1,s}\hat{f}_{\ell,s}$

④ Add on-site term at site ℓ, if any

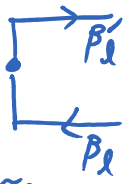
$H^{\text{on}}_\ell := \Lambda^{\ell/2}\varepsilon_\ell \times$  $= \sum_s \hat{f}^\dagger_{\ell s}\hat{f}_{\ell s}$ (4)



(4)

⑤ Diagonalize the Hamiltonian

$$H_\ell = H'_{\ell-1} + H_\ell^{hop} + H_\ell^{on} := \tag{5}$$



$$[H_\ell]^{\beta}_{\beta'} = [U_\ell]^{\beta}_{\tilde{\beta}} [E_\ell]^{\tilde{\beta}}_{\tilde{\beta}'} [U_\ell^\dagger]^{\tilde{\beta}'}_{\beta'} \tag{6}$$

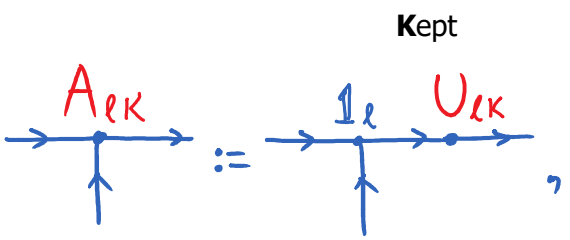
$$[E_\ell]^{\tilde{\beta}}_{\tilde{\beta}'} = \begin{cases} E_{\ell\tilde{\beta}} & \text{if } \tilde{\beta}=\tilde{\beta}' \\ 0 & \text{otherwise} \end{cases} \tag{7}$$

Shift the energy eigenvalues so that the lowest value is 0 (for the rescaling at the next iteration)

$$E_{\ell\tilde{\beta}} \leftarrow E_{\ell\tilde{\beta}} - \min(E_{\ell\tilde{\beta}}) \tag{8}$$

⑥ "Keep" the D lowest-lying eigenvalues and their corresponding eigenstates

$$H_\ell = \underbrace{U_{\ell K} E_{\ell K} U^\dagger_{\ell K}}_{\textbf{K}\text{ept}} + \underbrace{U_{\ell D} E_{\ell D} U^\dagger_{\ell D}}_{\textbf{D}\text{iscarded}} \tag{9}$$



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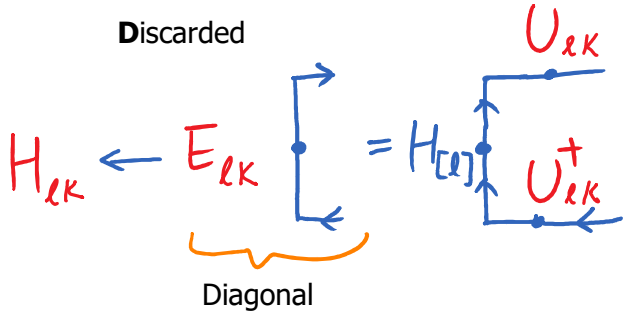

(10)

⑦ Use the tensors $A_{\ell K}$ and $H_{\ell K}$ for the next iteration

Iterative diagonalization result with rescaling, shiting, and truncation:

Color of the line connecting $|\alpha_{\ell-1}\rangle$ and $|\beta_\ell\rangle$ is given by $\sum_\sigma |[A_\ell]^{\alpha\sigma}_{\beta}|^2 \in [0,1]$