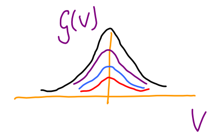
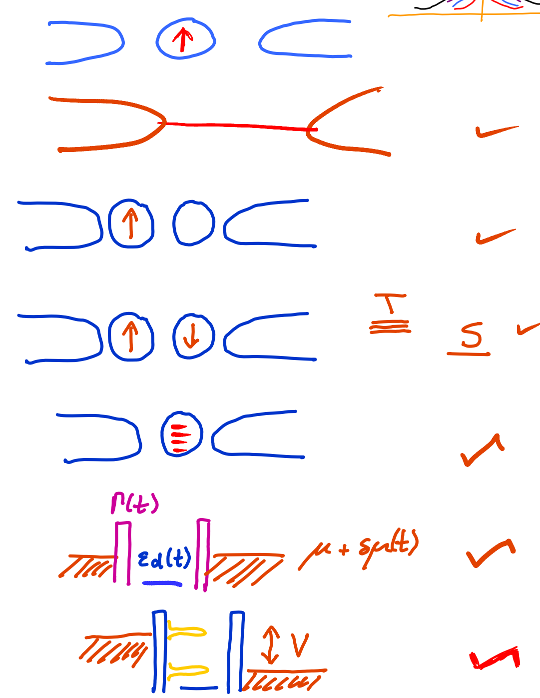
Numerical Renormalization Group for Quantum Impurity Models

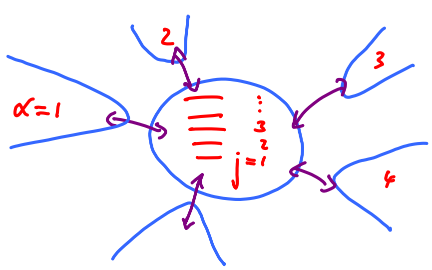


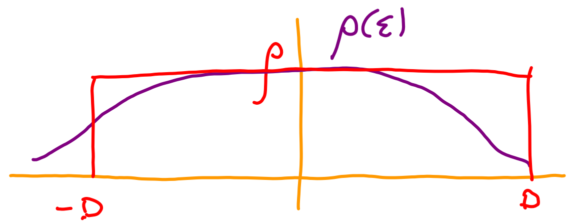
- Kondo effect in Quantum dots
- Kondo effect in carbon nanotubes
- Exotic SU(4) Kondo effects
- Singlet-triplet Kondo effect
- Many-level quantum dots
- Time-dependent problems effect
- Non-equilibrium Kondo effect



Needed: a generally applicable, flexible, quantitatively accurate tool: NUMERICS !

Generic Hamiltonian for Quantum Impurity Models





$$H_{loc} = \sum_{jj'} h_{j\sigma,j'\sigma'} d^\dagger_{j\sigma} d_{j'\sigma'} + \sum_{jj'\sigma\sigma'} U_{j\sigma,j'\sigma'} \underbrace{\hat{n}_{j\sigma}}_{d^\dagger_{j\sigma} d_{j\sigma}} \hat{n}_{j'\sigma'}$$

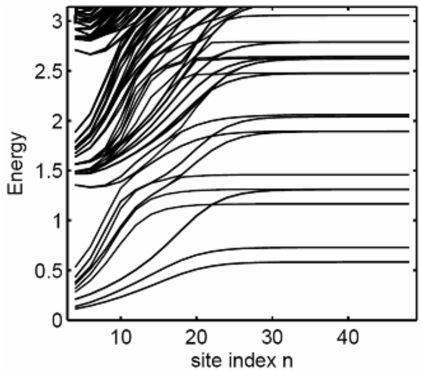
$$H_{lead} = \sum_{k\sigma\alpha} \varepsilon_{k\sigma} c^\dagger_{k\sigma\alpha} c_{k\sigma\alpha}$$

$$H_{tun} = \sum_{k\sigma\alpha j} \left(V_{k\sigma\alpha j} c^\dagger_{k\sigma\alpha} d_{j\sigma} + h.c. \right)$$

Method of choice: Numerical Renormalization Group (NRG)

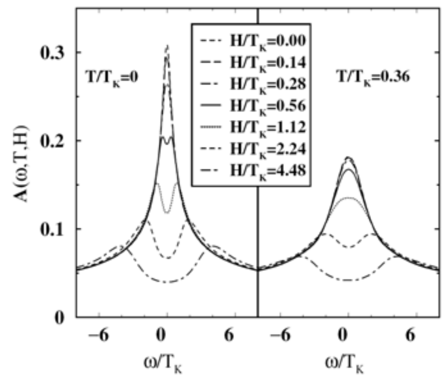
Wilson, Rev. Mod. Phys. 47, 773 (1975); Krishnamurti, Wilkins, Wilson, Phys. Rev. B 21, 1003, (1980); ibid. 1044, (1980).
Hewson, "From Kondo Problem to Heavy Fermions", Cambridge University Press, 1993.
Bulla, Costi, Pruschke, to appear in Rev. Mod. Phys. (2007)
Weichselbaum, von Delft, cond-mat/0607497, to appear in Phys. Rev. Lett. (2007)

Finite size spectrum $\{E_n^s\}$



Wilson, 1975

Dynamical correlation function



Costi, (2000)

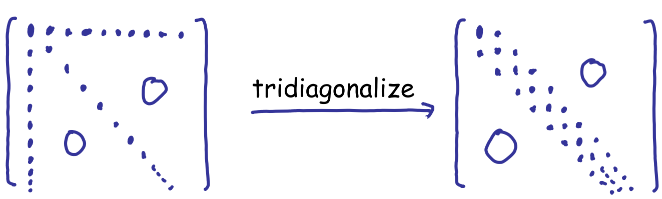
$$A^{BC}(\omega) = \int \frac{dt}{2\pi} e^{i\omega t} \langle \hat{B}(t)\hat{C}(0)\rangle_T = \sum_{ab} \frac{e^{-\beta E_a}}{Z} \langle a|\hat{B}|b\rangle\langle b|\hat{A}|a\rangle \delta(\omega - E_{ba})$$

$E_b - E_a$

many-body eigenstates of H

Mapping to "Wilson chain"

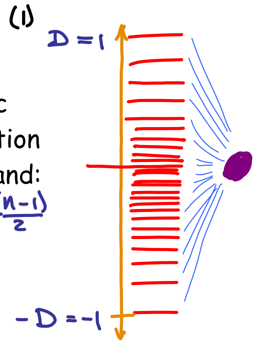
$$H = H_0(\underbrace{d^\dagger_\sigma, d_\sigma}_{\equiv f_{0\sigma}}) + \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \Big(v \sum_\sigma \underbrace{\sum_k c^\dagger_{k\sigma}}_{f^\dagger_{1\sigma}} \underbrace{d_\sigma}_{f_{0\sigma}} + h.c.\Big) \qquad (1)$$



logarithmic discretization of cond. band:

$\omega_n = \Lambda^{-\frac{(n-1)}{2}}$

$\Lambda > 1$



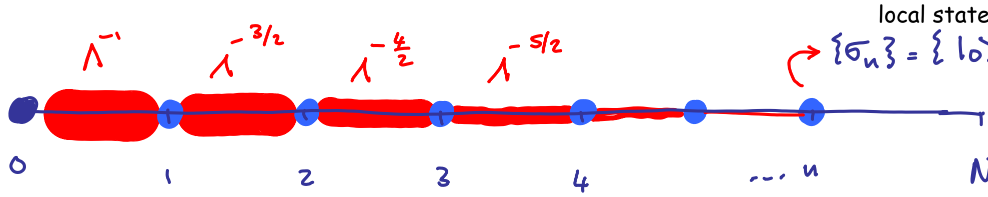
Wilson chain:

$$H = \lim_{N\to\infty} H_N = H_0(f_0^\dagger, f_0) + \sum_{n=1}^{N\to\infty} \lambda_n (f_n^\dagger f_{n-1} + h.c.) \qquad (2)$$

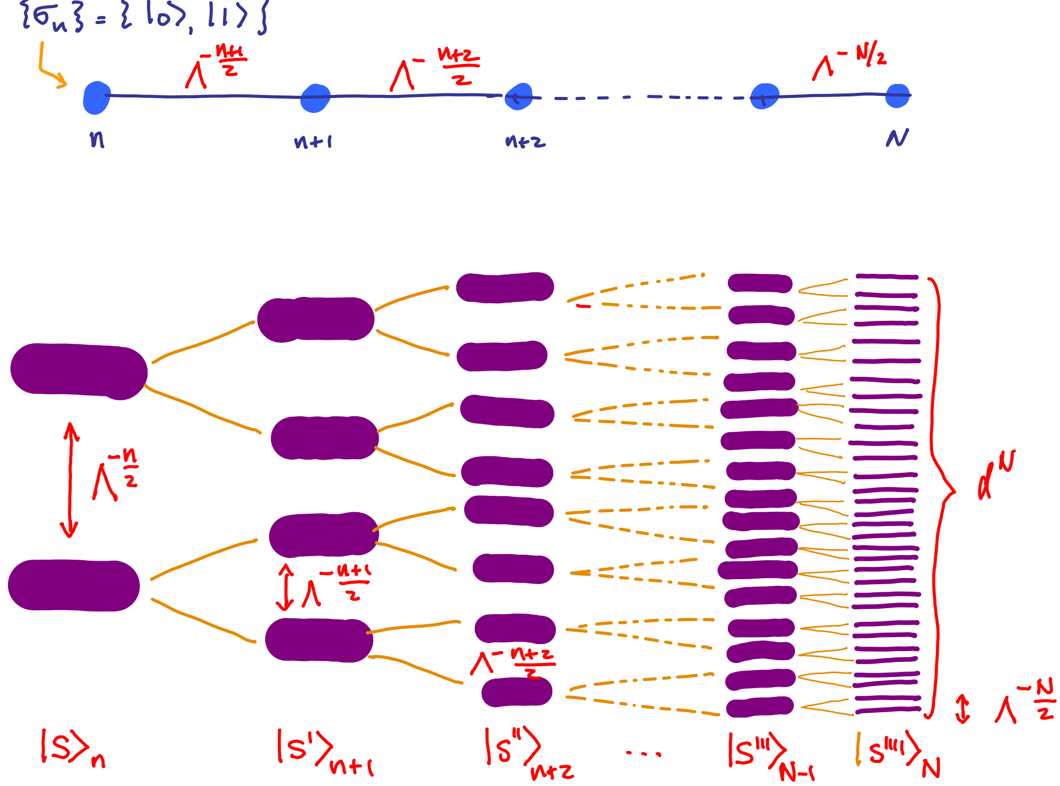
$\lambda_n \simeq \Lambda^{-n/2}$

local state space:

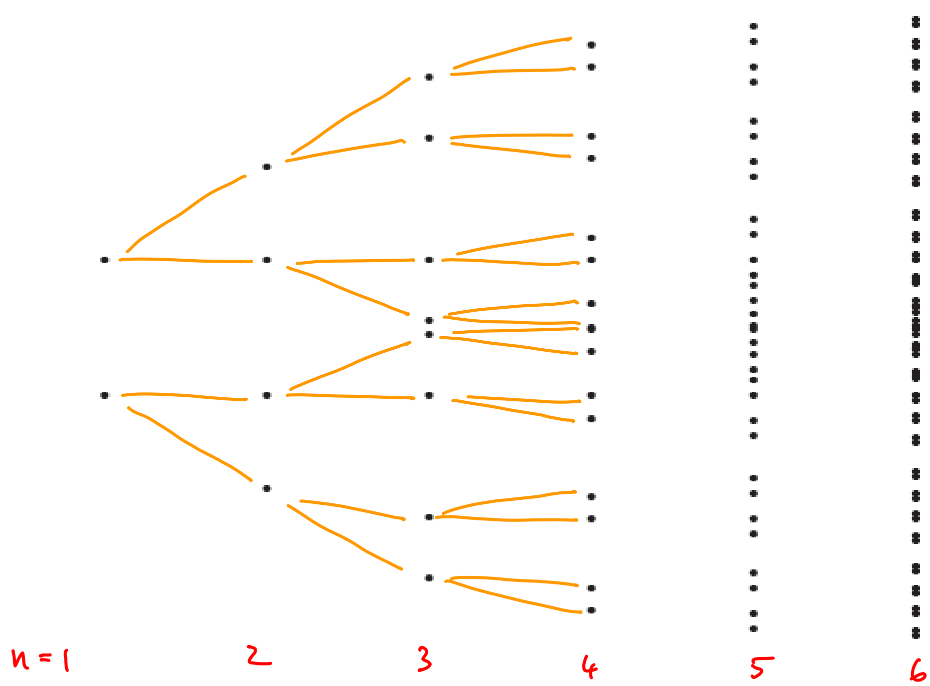
$\{\sigma_n\} = \{|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\}$



Iterative refinement of resolution of eigenspectrum

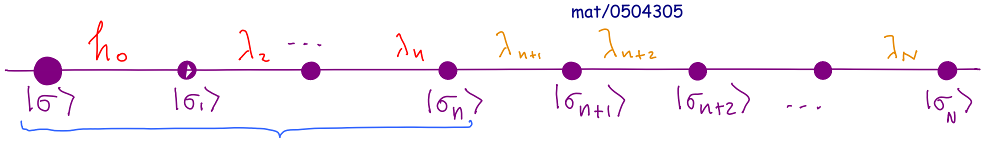


Actual Wilson chain eigenspectra for chains of length n = 1, ..., 6



Iteration produces Matrix Product States

Verstraete, Weichselbaum, Schollwöck, Cirac, von Delft, cond-mat/0504305



$H_n |s\rangle_n = E^n_s |s\rangle_n$ (M eigenstates)

d matrices, M x (Md)

$[A^{\sigma_{n+1}}]_{ss'}$ — old, new states

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

$$|s'\rangle_{n+1} = \sum_{s\sigma_{n+1}} |s\rangle_n |\sigma_{n+1}\rangle \langle \sigma_{n+1}| {}_n\langle s|s'\rangle_{n+1} \qquad (1)$$

$\Downarrow$

$$\boxed{|s'\rangle_{n+1} = \sum_{s\sigma_{n+1}} |s\rangle_n |\sigma_{n+1}\rangle [A^{\sigma_{n+1}}]_{ss'}} \qquad (2)$$

$[d^{N-1} \times d^N \text{ matrix}]$

truncation needed !

$\lambda_{n+2} \neq 0$

$\lambda_N \neq 0$

$$|s''\rangle_{\cancel{n+2}\,N} = \sum |s\rangle_n |\sigma_{n+1}\rangle |\sigma_{n+2}\rangle \ldots |\sigma_N\rangle [A^{\sigma_{n+1}} A^{\sigma_{n+2}} \ldots A^{\sigma_N}]_{ss''} \qquad (3)$$

"matrix product state" (MPS)

Wilson's truncation scheme

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

$|s'\rangle^D_{n+1}$ disc.

$|s'\rangle^K_{n+1}$ kept : M

$$|s'\rangle^X_{n+1} = \sum_{s\sigma_{n+1}} |s\rangle^K_n |\sigma_{n+1}\rangle [A^{\sigma_{n+1}}_{KX}]_{ss'} \qquad (1)$$

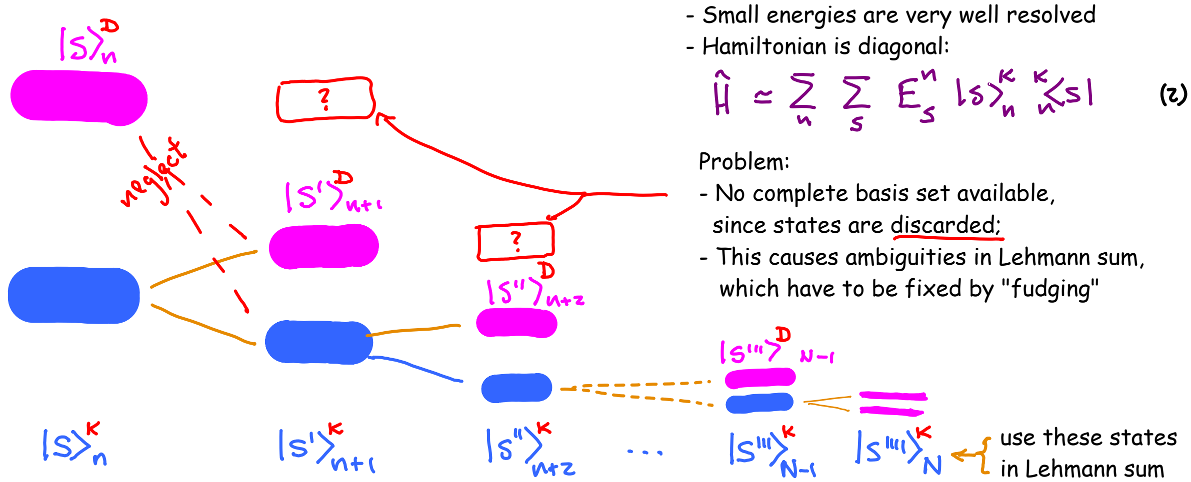
$X = K, D$

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

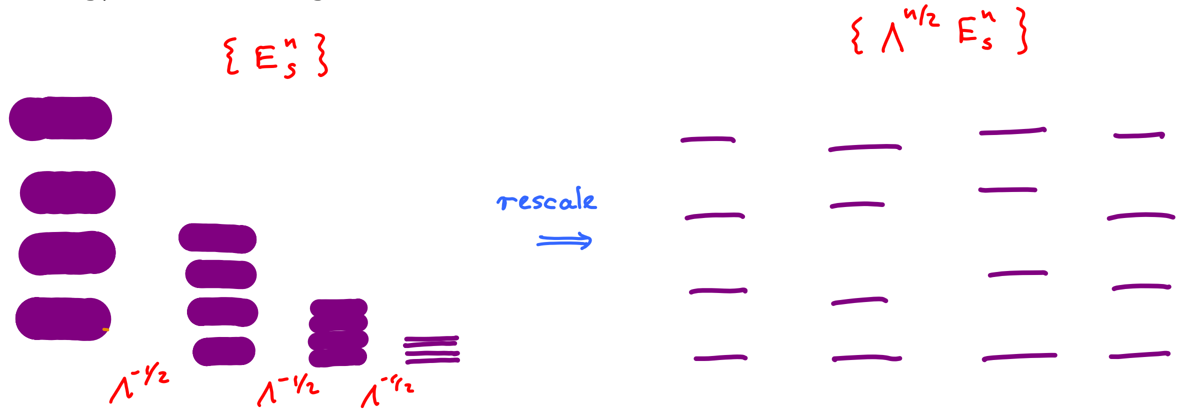
Advantages:
- Managable number of states
- Information obtained from all energy scales
- Small energies are very well resolved
- Hamiltonian is diagonal:

$$\hat H \simeq \sum_n \sum_s E^n_s \, |s\rangle^K_n \, {}^K_n\langle s| \qquad (2)$$

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

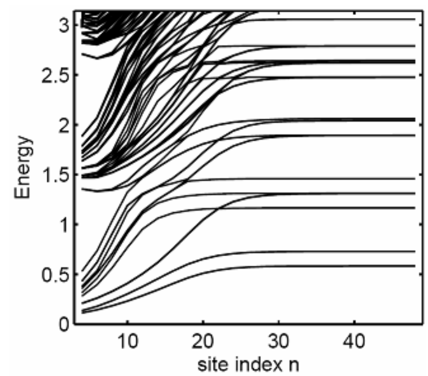


Energy Level Flow Diagram



Finite size spectrum:

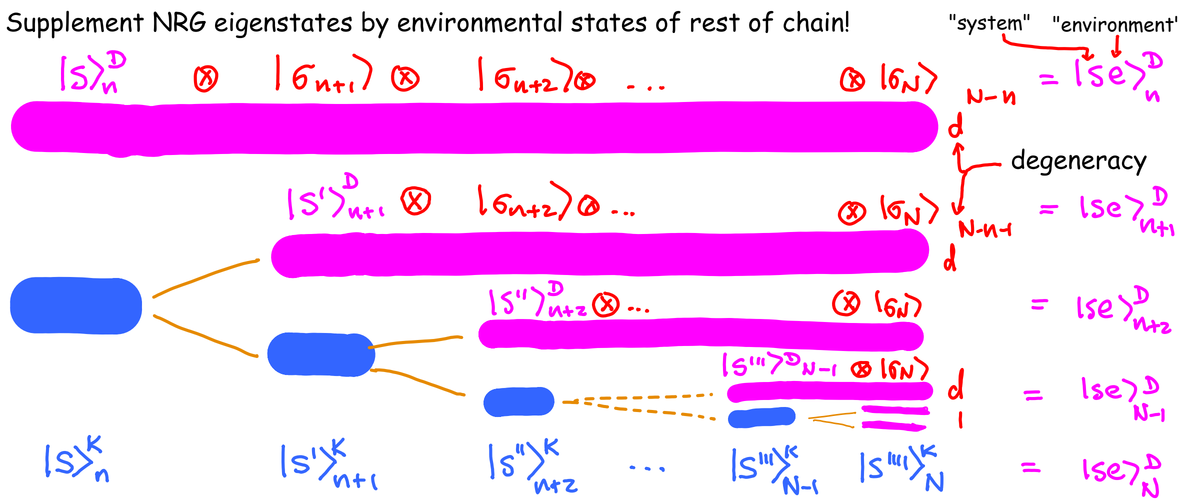
$$\{\Lambda^{n/2} E_s^n\}$$



Construction of complete Fock state basis

Anders, Schiller, PRL (2005); PRB (2006)

Supplement NRG eigenstates by environmental states of rest of chain!



General construction: $$\left.\begin{matrix}|s\rangle_n^D\\ |s\rangle_n^K\end{matrix}\right\}\otimes|\sigma_{n+1}\rangle\otimes\ldots\otimes|\sigma_N\rangle \equiv \left\{\begin{matrix}|se\rangle_n^D\\ |se\rangle_n^K\end{matrix}\right. , \quad (1)$$

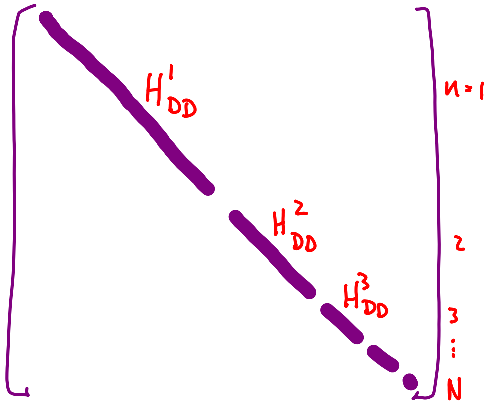
NRG-approximation: $$H|se\rangle_n^X \simeq E_n^s\,|se\rangle_n^X \quad (2)$$

Complete basis is formed by: $$\{|se\rangle_n^D\,;\ \forall n\} \iff \mathbb{1} = \sum_n \sum_{se} |se\rangle_n^D\,{}_n^D\langle se| \quad (3)$$

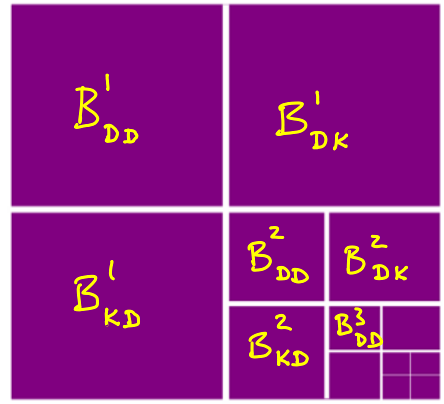
Operators

Weichselbaum, von Delft, PRL (2007); Peters, Anders, Pruschke, PRB (2006)

$\hat{H} \simeq$



$\hat{B} \simeq$



Hamiltonian is diagonal:

$$\hat{H} \simeq \sum_n \sum_{se} E^s_n \, |se\rangle^D_n \, {}^D_n\langle se|$$

NRG - approximation

General: exclude KK to avoid overcounting!

$$\hat{B} \simeq \sum_n \sum_{XX'}^{\neq KK'} \sum_{ss'} \sum_e |se\rangle^X_n \left[\hat{B}^n_{XX'}\right]_{ss'} {}^{X'}_n\langle s'e|$$

All operators are diagonal in "environment" states! Hence it can easily be traced out!

Density Matrix

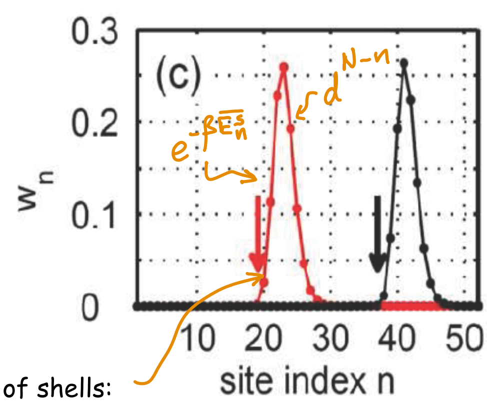
Weichselbaum, von Delft, PRL (2007)

$$\hat{\rho} \simeq \sum_n \sum_{se} \left(e^{-\beta E^s_n}/Z\right) |se\rangle^D_n \, {}^D_n\langle se|$$

all shells contribute: FDM-NRG
(full density matrix NRG)

$$=: \sum_n w_n \, \hat{\rho}^{DD}_n \qquad \left(\mathrm{Tr}\, \hat{\rho}^{DD}_n = 1\right)$$

weight of shell n, $d^{N-n} \frac{Z^D_n}{Z}$, is nonzero over a range of shells:



Shells in range below T contribute consideably!

Conventional NRG uses "single-shell approximation: $w_n = \delta_{nN_T}$ with $\Lambda^{-N_T/2} = T$