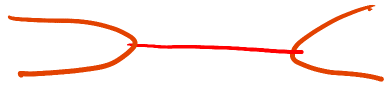
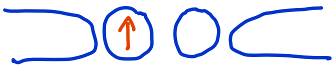
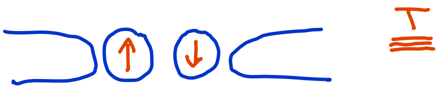
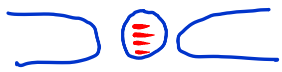
Lecture 4: Numerical Approaches to Quantum Impurity Models

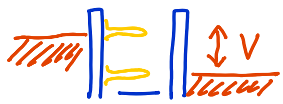
Jan von Delft

N1

Quantum dots opened up a vast set of new, unusual and exotic incarnations of Kondo physics:

- 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 

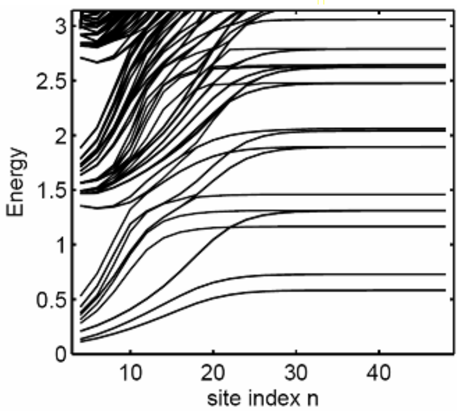
Needed: a generally applicable, flexible, quantitatively accurate tool: NUMERICS

Method of choice: Numerical Renormalization Group (NRG)

N2

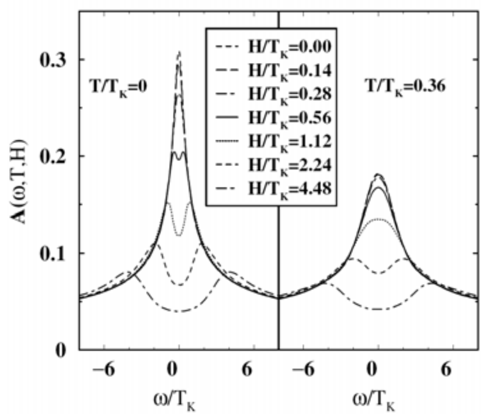
Wilson, Rev. Mod. Phys. 47, 773 (1975); Krishnamurti, Wilkins, Wilson, Phys. Rev. B 21, 1003, (1980); ibid. 1044, (1980).
Hewson, "From Kondo Problem to Heavy Fermions", Cambridge University Press, 1993.
Bulla, Costi, Pruschke, to appear in Rev. Mod. Phys. (2007)
Weichselbaum, von Delft, cond-mat/0607497,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

Finite size spectrum $\{E_n\}$



Wilson, 1975

Dynamical correlation function



Costi, Phys. Rev. Lett, 85, 1504 (2000)

$$F_\sigma := \sum_{k\sigma'} \vec{S}\cdot\vec{\sigma}_{\sigma\sigma'}\, c_{k\sigma'} \qquad \text{(see K12)}$$

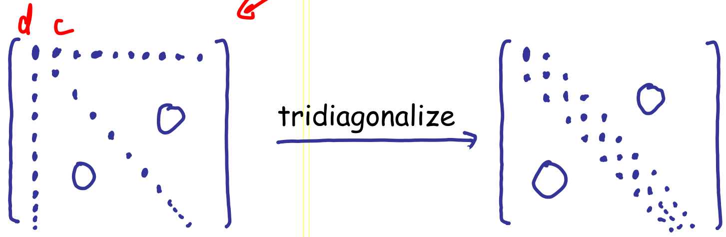
many-body eigenstates of H

$$(1)\quad \sum_{ab} \langle b|\hat{F}_\sigma|a\rangle \left(e^{-\beta E_a}/Z\right)\langle a|\hat{F}_\sigma^\dagger|b\rangle\, \delta(\omega - \underbrace{E_{ba}}_{E_b - E_a}) \overset{\text{Lehmann}}{=} \mathrm{Im}\int_0^\infty \frac{dt}{\pi}\, e^{-i\omega t}(-i)\langle\{F_\sigma(t), F_\sigma^\dagger(0)\}\rangle \quad (2)$$

Mapping to "Wilson chain"

N3

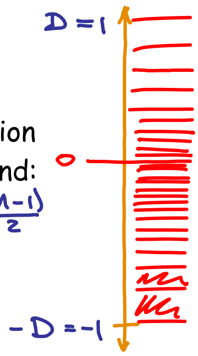
$$H = H_0(d^\dagger_\sigma, d_\sigma) + \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \Big(v \sum_\sigma \sum_k c^\dagger_{k\sigma} d_\sigma + h.c.\Big) \qquad (1)$$



logarithmic discretization of cond. band:

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

$$\Lambda > 1$$



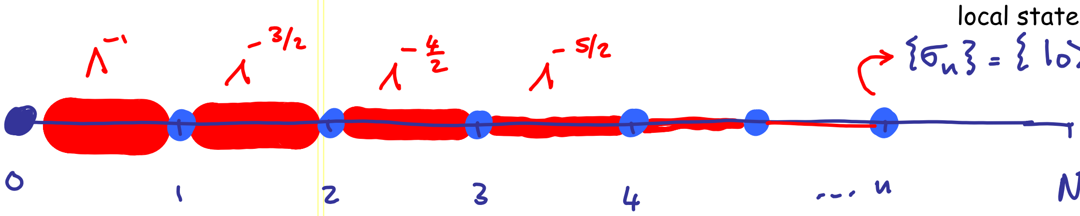
Wilson chain:

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

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

local state space:

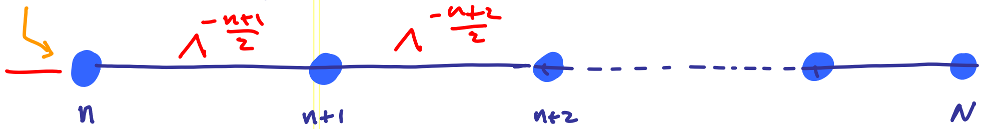
$$\{\sigma_n\} = \{\,|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\}$$

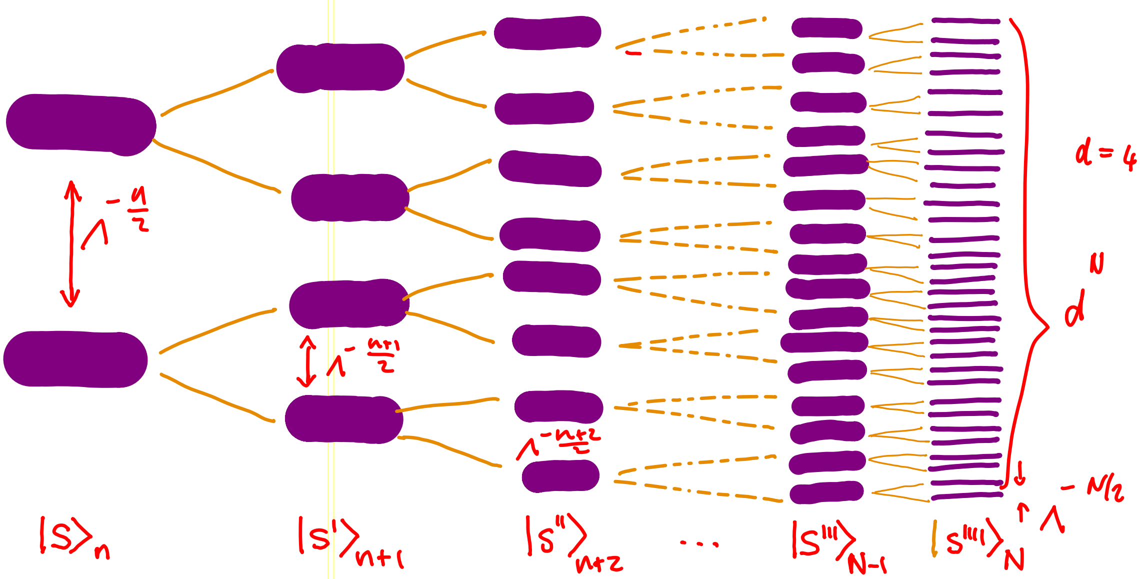


Iterative refinement of resolution of eigenspectrum

N4

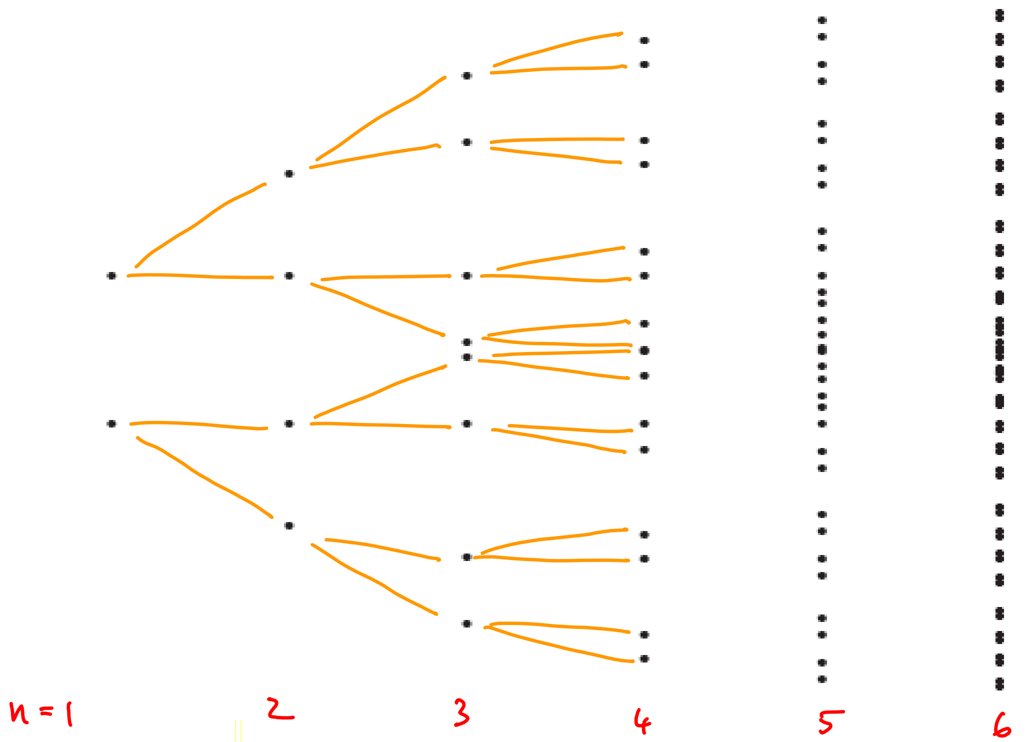
$\{\sigma_n\} = \{\,|0\rangle, |1\rangle\}$: $d=2$





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

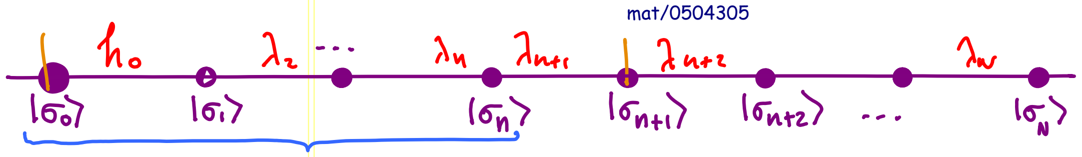
N5



Iteration produces Matrix Product States

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

N6



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

$\downarrow \lambda_{n+1}$

d matrices

$[A^{\sigma_{n+1}}]_{ss'}$ old M × (Md) new states

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

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

λ_{n+2} ... λ_N

$d^{N-1} \times d^N$ matrix

truncation needed !

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

"matrix product state" (MPS)

Wilson's truncation scheme

N7

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

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

$|s'\rangle^D_{n+1} \xleftarrow{\text{disc:}}$, $|s'\rangle^K_{n+1} \xleftarrow{\text{kept: M}}$

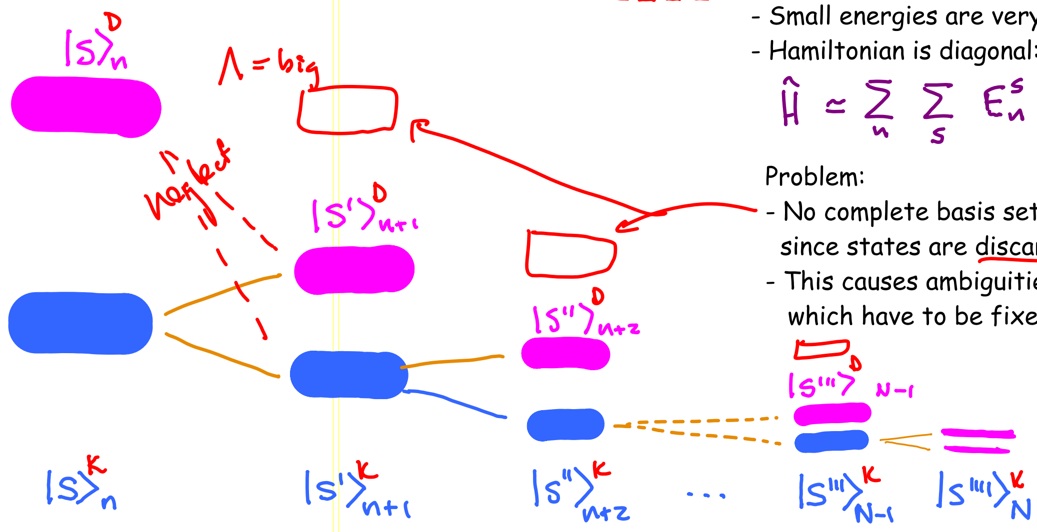
$$|s'\rangle^X_{n+1} = \sum_{s\sigma_{n+1}} |s\rangle^K_n |\sigma_{n+1}\rangle \left[A^{\sigma_{n+1}}_{KX}\right]_{ss'} \qquad X = K, D \qquad (1)$$

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:

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

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

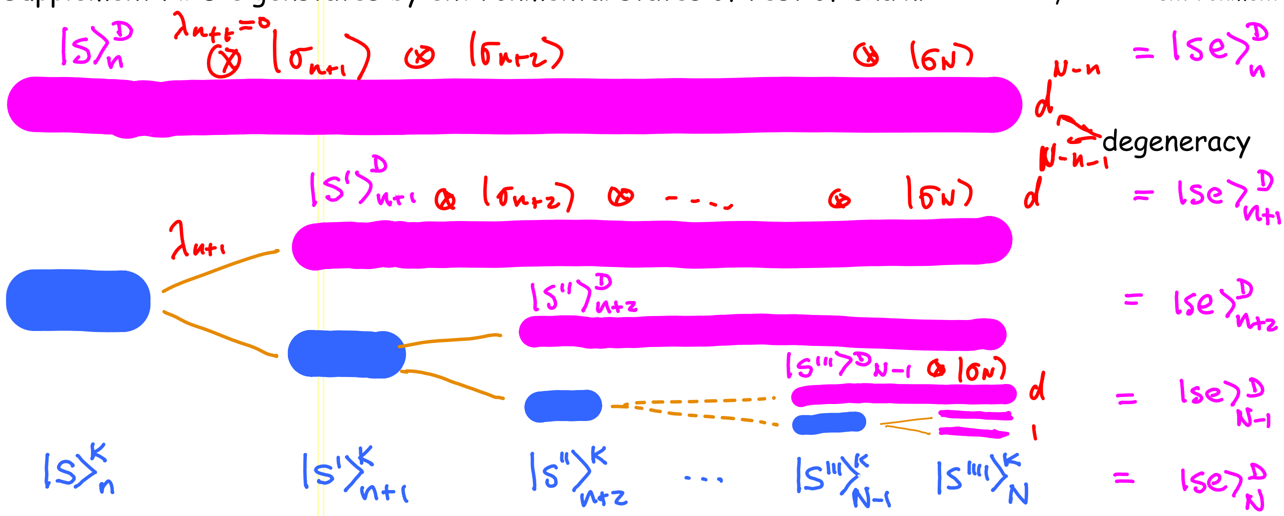


Construction of complete Fock state basis

Anders, Schiller, PRL. 95, 196801, (2005); cond-mat/0604517

N8

Supplement NRG eigenstates by environmental states of rest of chain!



General construction:

$$\left.\begin{matrix}|s\rangle^D_n \\ |s\rangle^K_n\end{matrix}\right\} \otimes |\sigma_{n+1}\rangle \cdots |\sigma_N\rangle = \left\{\begin{matrix}|se\rangle^D_n \\ |se\rangle^K_n\end{matrix}\right. \qquad (1)$$

NRG-approximation:

$$H|se\rangle^X_n \simeq E^s_n |se\rangle^X_n \qquad (2)$$

Complete basis is formed by: $\{|se\rangle^D_n ; \forall n\}$ $\Leftrightarrow$

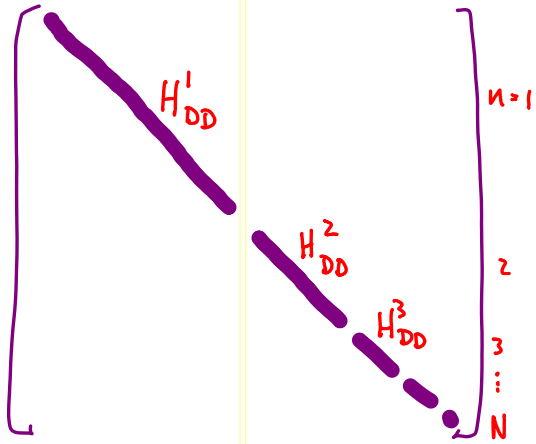
$$\mathbb{1} = \sum_n \sum_{se} |se\rangle^D_n \, {}^D_n\langle se| \qquad (3)$$

Operators

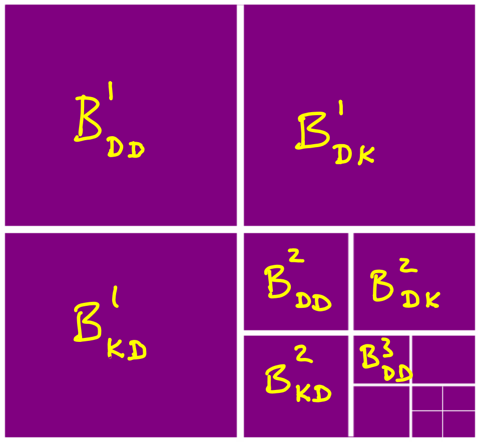
Weichselbaum, von Delft, cond-mat/0607497, to appear in PRL; Peters, Anders, Pruschke, PRB, 74, 245114 (2006)

N9

$\hat{H} \simeq$



$\hat{B} \simeq$



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!

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

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

Density Matrix

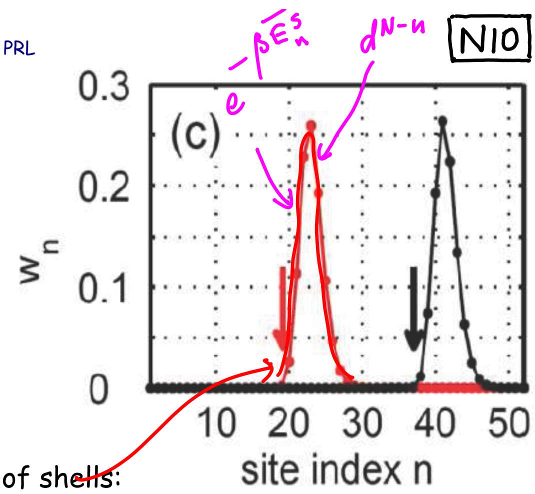
Weichselbaum, von Delft, cond-mat/0607497, to appear in PRL

N10

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

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

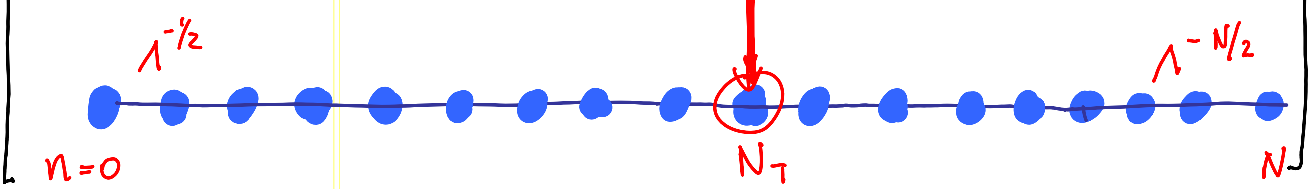
$$=: \sum_n w_n \, \hat{\rho}^{DD}_n \qquad (\mathrm{Tr}\, \hat{\rho}^{DD}_n = 1)$$



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

Shells in range below T contribute consideably!

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



Spectral Functions

Weichselbaum, von Delft, cond-mat/0607497, to appear in PRL

N11

general Lehmann representation:

$$A^{BC}(\omega) = \sum_{ab} \langle b|\hat{C}|a\rangle \frac{e^{-\beta E_a}}{Z} \langle a|\hat{B}|b\rangle \delta(\omega - \overset{E_b - E_a}{E_{ba}})$$

has to be broadened in the end

FDM-NRG:

$$\mathcal{A}^{\mathcal{BC}}_n(\omega) = \sum_{m>n_0}^{n} \sum_{\mathrm{XX'}}^{\neq \mathrm{KK}} \left[\mathcal{C}^{[m]}_{\mathrm{X'X}}\, \rho^{[mn]}_{\mathrm{XX}}\right]_{s's} \left[\mathcal{B}^{[m]}_{\mathrm{XX'}}\right]_{ss'} \delta(\omega - E^m_{s's}),$$

Density matrix of shell n:

$$\left[\rho^{[m=n]}_{\mathrm{DD}}\right]_{ss'} = \delta_{ss'} \frac{e^{-\beta E^n_s}}{Z_n}, \tag{10}$$

Reduced density matrix of shell m:

$$\left[\rho^{[m<n]}_{\mathrm{KK}}\right]_{ss'} = \left[A^{[\sigma_{m+1}]}_{\mathrm{KK}} \dots A^{[\sigma_n]}_{\mathrm{KD}}\, \rho^{[nn]}_{\mathrm{DD}}\, A^{[\sigma_n]\dagger}_{\mathrm{DK}} \dots A^{[\sigma_{m+1}]\dagger}_{\mathrm{KK}}\right]_{ss'},$$

Spectral sum rules: $\int d\omega\, A^{BC}(\omega) = \langle \hat{B}\hat{C}\rangle_T$ hold identically (10^{-15})

Friedel sum rule for peak height at $\omega = 0$: holds to 10^{-3} for $M = 256$

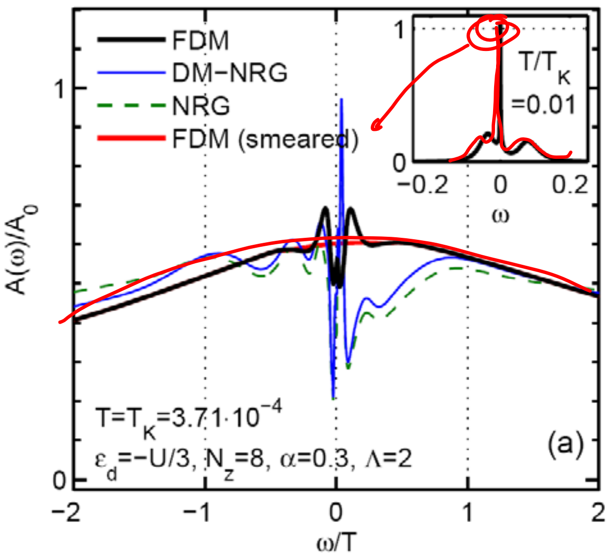
FDM-NRG results for single-impurity Anderson model

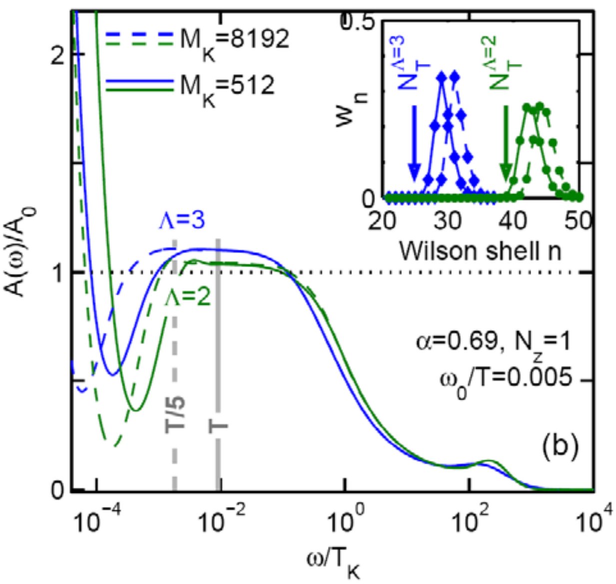
N12

Weichselbaum, von Delft, cond-mat/0607497, to appear in PRL

FMD-NRG spectral functions are better behaved at very small scales than NRG.

Frequencies down to T/5 can be reached. Discretization parameters do affect the final results.

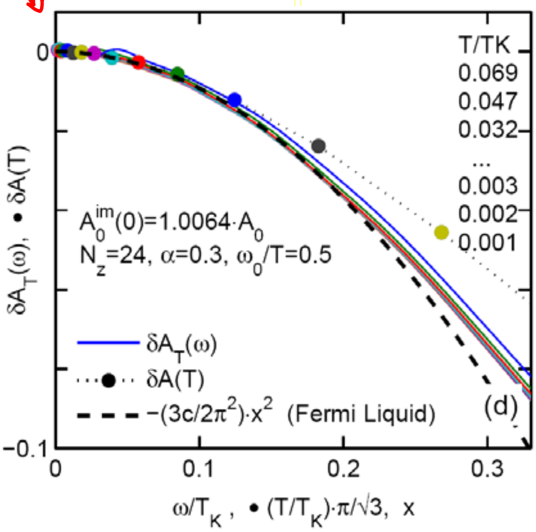


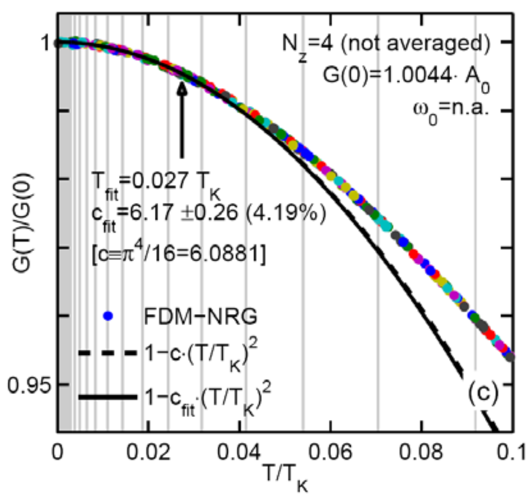


FDM-NRG reproduces exact Fermi liquid results at low energies (ω, $T \ll T_K$) N13

$$A_T(\omega) \simeq A_0 \left[1 - \frac{c}{2}\left(\frac{T}{T_K}\right)^2 - \frac{3c}{2\pi^2}\left(\frac{\omega}{T_K}\right)^2\right], \qquad \chi_0\big|_{T=0} \equiv \frac{1}{4T_K}$$

$$G(T) \equiv \int_{-\infty}^{\infty} d\omega\, A(\omega,T)\left(-\frac{\partial f}{\partial \omega}\right) \simeq A_0\left[1 - c\left(\frac{T}{T_K}\right)^2\right] \qquad \boxed{A_0 \equiv \frac{1}{\pi\Gamma}, \quad c \equiv \frac{\pi^4}{16}}$$





$$\left.\begin{aligned} \delta\mathcal{A}_T(\omega) &= [A_T^{\rm im}(\omega) - A_T^{\rm im}(0)]/A_0^{\rm im}(0) \text{ vs. } \omega/T_K \text{ (curves)} \\ \delta\mathcal{A}(T) &= [A_T^{\rm im}(0)/A_0^{\rm im}(0) - 1] \text{ vs. } (T/T_K)\pi/\sqrt{3} \text{ (dots)} \end{aligned}\right\}$$

Should go like $-\frac{3c}{2\pi^2}x^2$ vs. x.
they do !!

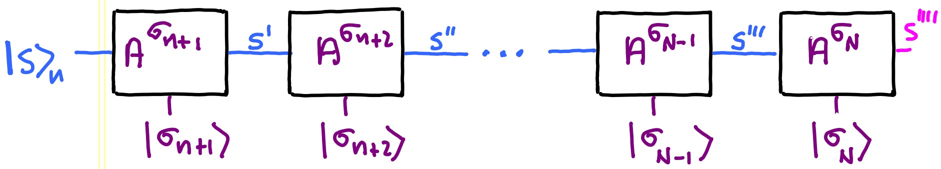
Relation between NRG and DMRG

(see poster: Hamed Saberi) N14

NRG yields MPS:

$$\sum_{s\,\sigma_{n+1}} |s\rangle_n |\sigma_{n+1}\rangle|\sigma_{n+2}\rangle \ldots |\sigma_{N-1}\rangle|\sigma_N\rangle \left[A^{\sigma_{n+1}} A^{\sigma_{n+2}} \ldots A^{\sigma_{N-1}} A^{\sigma_N}\right]_s = |s''''\rangle_N \qquad (1)$$

Graphical representation:



(2)

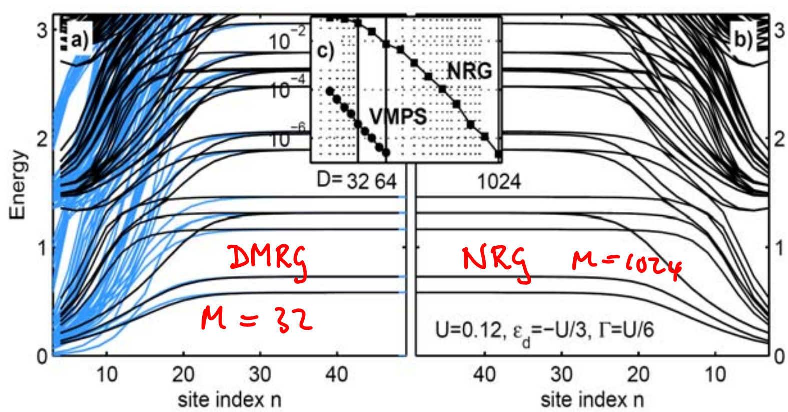
NRG $\rightarrow$ MPS

DMRG (variational approach)

(density matrix renormalization group, White 1992)

So, variationally minimize energy:

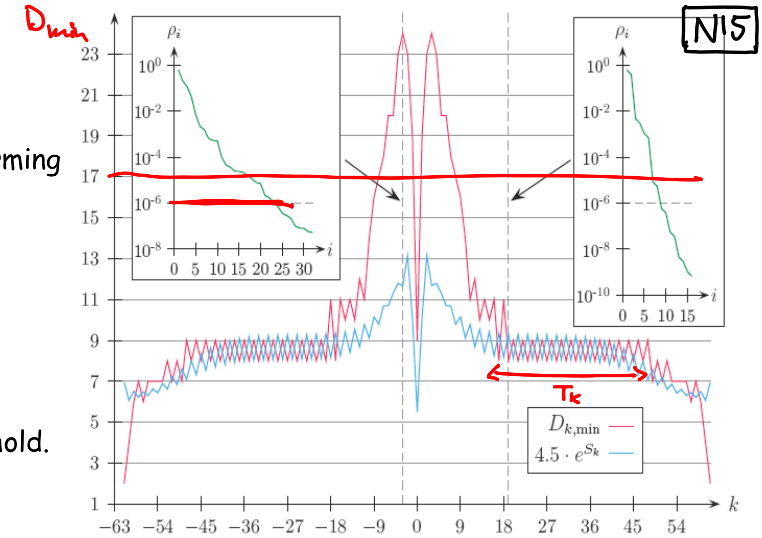
$$\frac{\partial}{\partial A}\ {}_{MPS}\langle\psi|H|\psi\rangle_{MPS} = 0$$



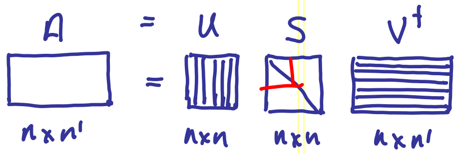
<u>Optimize Numerical Resources</u>

(see poster: Andreas Holzner)

$\boxed{\text{N15}}$

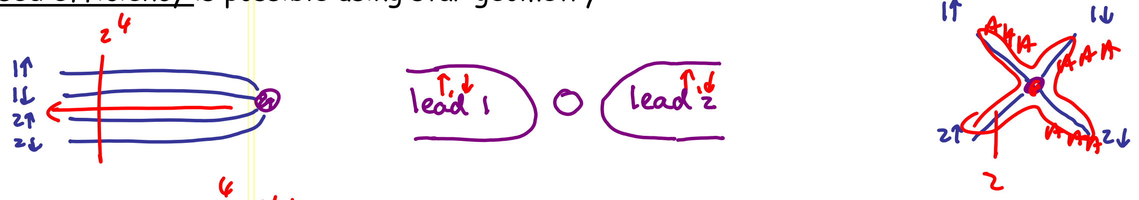


1. Optimize <u>size</u> of A-matrices, by performing "singular value decomposition" on each:



Keep only diagonal elements ➤ set threshold.

2. For more complex geometries, strongly <u>increased efficiency</u> is possible using star geometry:



local state space: $2^4 = 64$

local state space: 2

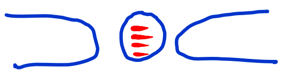
$$M_{NRG}^{1/n} = M_{DMRG}$$

<u>Future Prospects</u>

$\boxed{\text{N16}}$

- Flexibility in discretizing the conduction band
  - variational structure implies:no strict reliance on energy scale separation!
  - any discretization scheme is possible $(\Lambda \to 1)$
  - models with arbitrary band structure can be treated more accurately
  - great potential for dynamical mean field theory applications

- Complex many-level models



- Time-dependence via DMRG
  (NRG: Anders, Schiller)

$$|\psi(t)\rangle = e^{-iHt}\,|\psi(0)\rangle$$

- Out-of-equilibrium ?