DMRG and quantum impurity models

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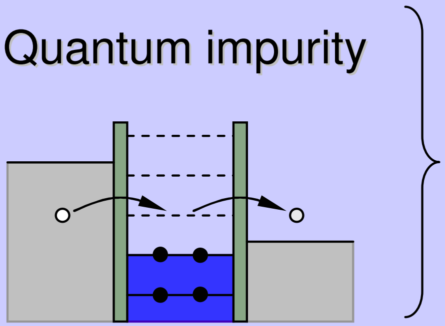
Outline

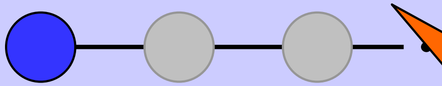
- Motivation
- NRG point of view
  - based on energy scale separation
  - NRG produces matrix product state
- DMRG applied to quantum impurity models
  - variational within the space of matrix product states
  - loosens several strict NRG constraints
  - links to concepts of quantum information
- Correlation functions
- Application to Kondo model in the limit of large B ($B \gg T_K$)
  - DMRG resolves sharp features at finite frequencies *out of reach for NRG*
  - results compare well with analytic results perturbative in $\log[B/T_K]$
- Summary and outlook

Motivation

Quantum impurity

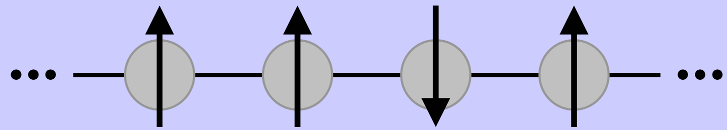


NRG



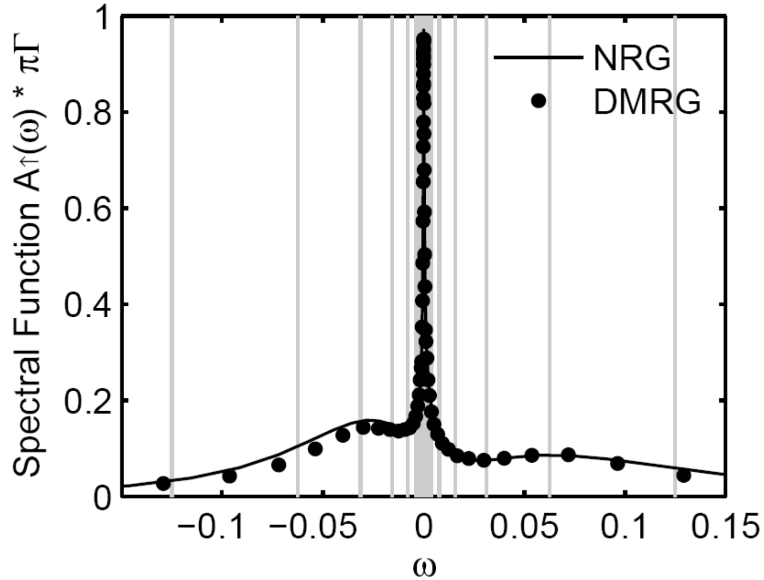
DMRG

quantum chains (spin, Hubbard, …)



Matrix Product States

Verstraete et al. (condmat/2005)



Correlation functions

- NRG has good resolution at ω=0
- Finite resolution at finite frequencies
- sharp features at finite frequency?

NRG = Numerical Renormalization Group (Wilson, 1975)
DMRG = Density matrix Renormalization Group (White, 1992)

Review Bulla et al. (RMP 2008)

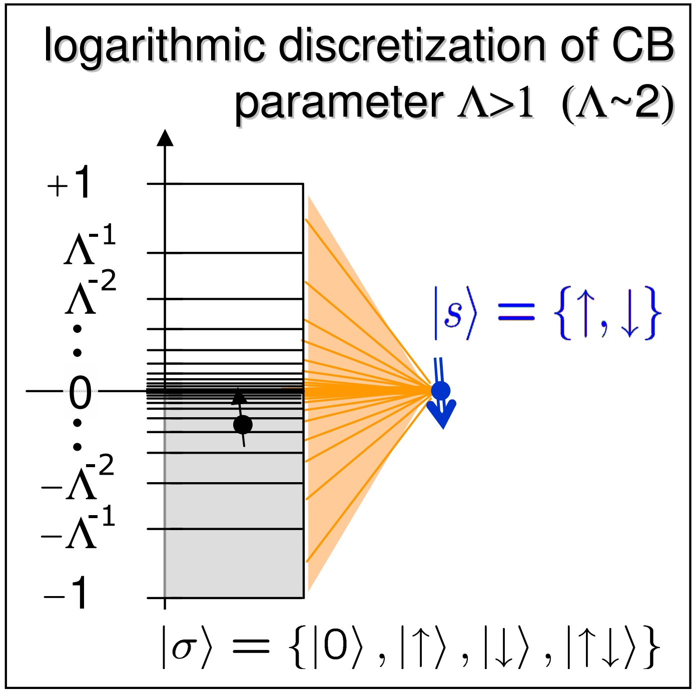
Kondo (1963)

Kondo Hamiltonian

$$\mathcal{H} = \mathbf{B}\cdot\mathbf{s} + 2J\mathbf{s}\cdot\mathbf{S} + \int_{-D}^{D} d\epsilon\ \epsilon\ c^{\dagger}_{\epsilon\mu} c_{\epsilon\mu}$$

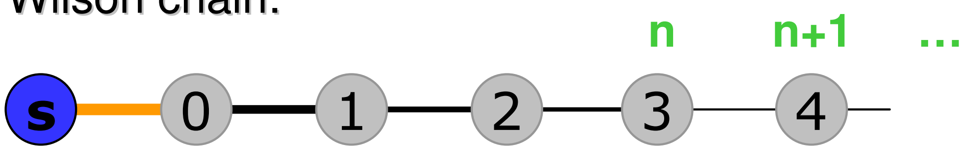
$$\mathbf{S} \equiv \frac{1}{2}\int_{-D}^{D} d\epsilon d\epsilon' \rho\ c^{\dagger}_{\epsilon\mu}\sigma_{\mu\mu'}c_{\epsilon'\mu'}$$

$$T_K = \sqrt{2\rho J}e^{-\frac{1}{2\rho J}}$$



logarithmic discretization + tridiagonalization

→ Wilson chain:



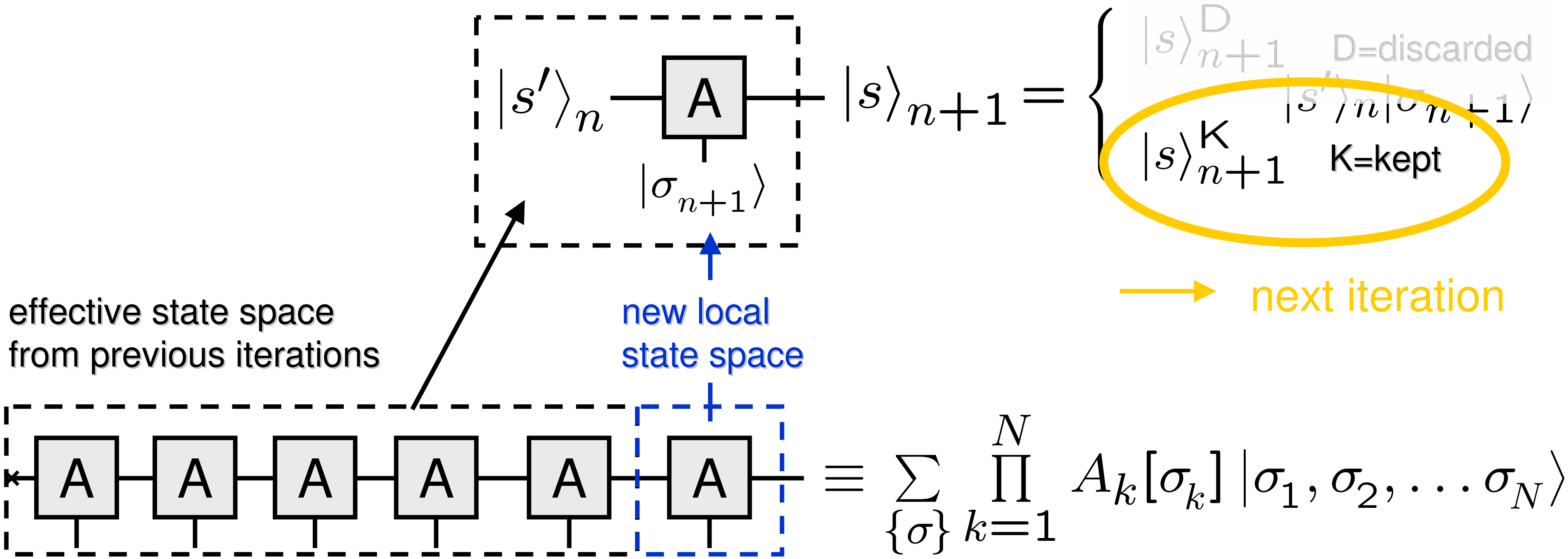
energy scale separation

$$\sim \left(\frac{1}{\Lambda}\right)^{n/2}$$

$$\mathcal{H} = H_{\mathrm{dot}} + (2\rho J\, D)\ \mathbf{s}\cdot\tau + \frac{1}{2}\left(1+\frac{1}{\Lambda}\right)\sum_{n=0}^{\infty}\frac{\xi_n}{\Lambda^{n/2}}\left(f^{\dagger}_{n\mu}f_{n+1,\mu} + f^{\dagger}_{n+1,\mu}f_{n\mu}\right), \quad \tau \equiv f^{\dagger}_{0\mu}\sigma_{\mu\mu'}f_{0\mu'}$$

NRG produces Matrix Product States

- Iterative procedures generate Matrix Product States (MPS)



- NRG generates MPS in a “single swee
- DMRG = variational procedure on MPS structure

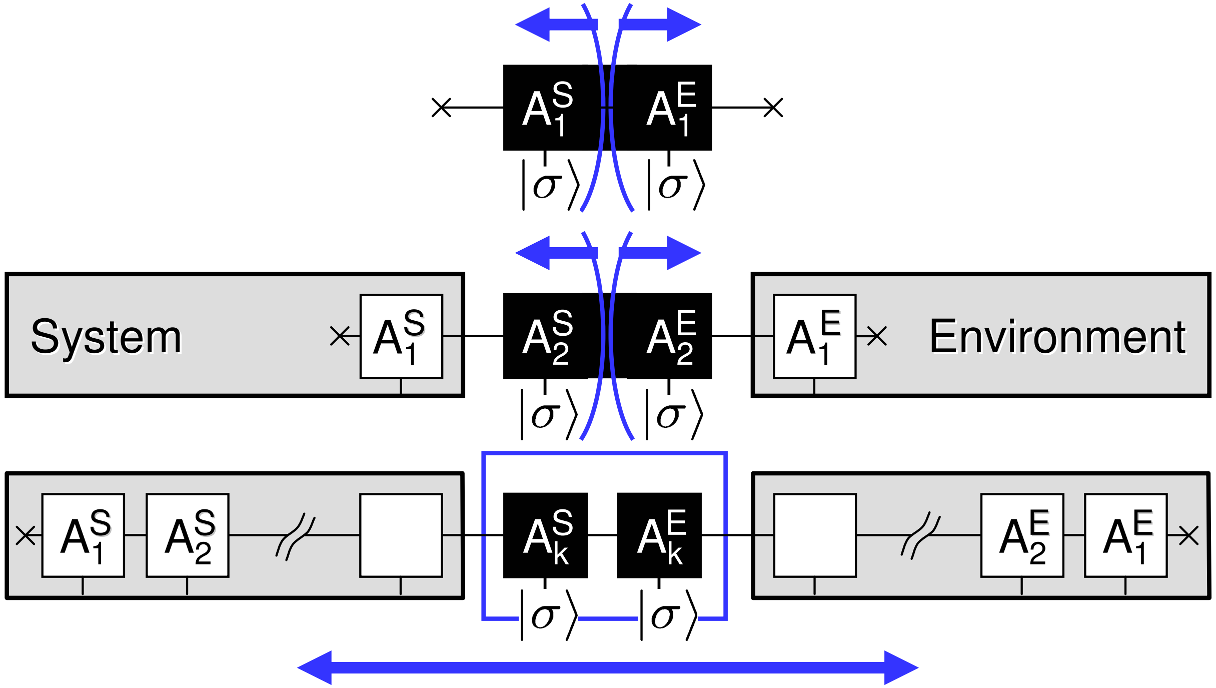
$$\ldots A^{[\sigma_1]}_{s_0 s_1} A^{[\sigma_2]}_{s_1 s_2} A^{[\sigma_3]}_{s_2 s_3} \ldots |\ldots \sigma_1 \sigma_2 \sigma_3 \ldots\rangle$$

Verstraete et al. (2005)
Östlund and Rommer (1995)

DMRG Primer

S. White (1992), U. Schollwöck (RMP, 2005)

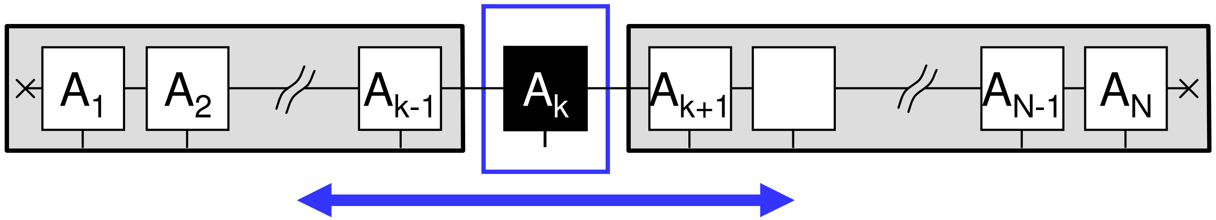
- Infinite-size DMRG (1D-systems with nearest neighbor coupling)



"empty state"

$\rightarrow\!\times \equiv |\rangle$

- Finite-size DMRG
- Variational MPS = 1-site finite-size DMRG

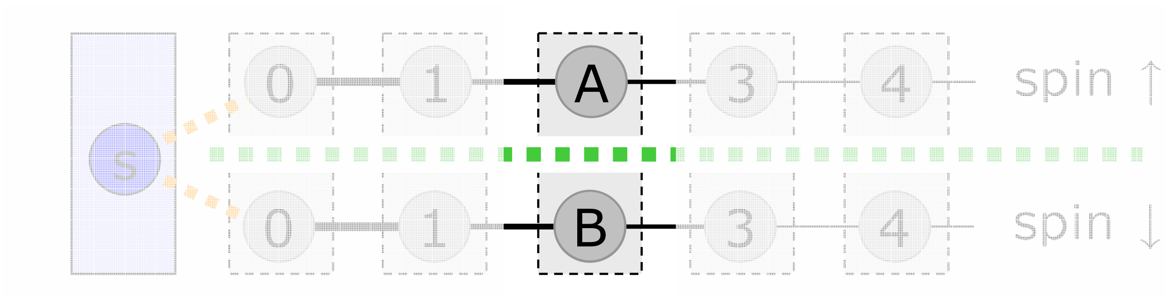


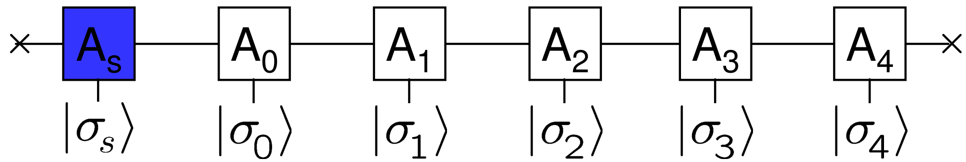
strictly variational within the space of MPS

Unfolding the Kondo model

Variational procedure loosens NRG constraints

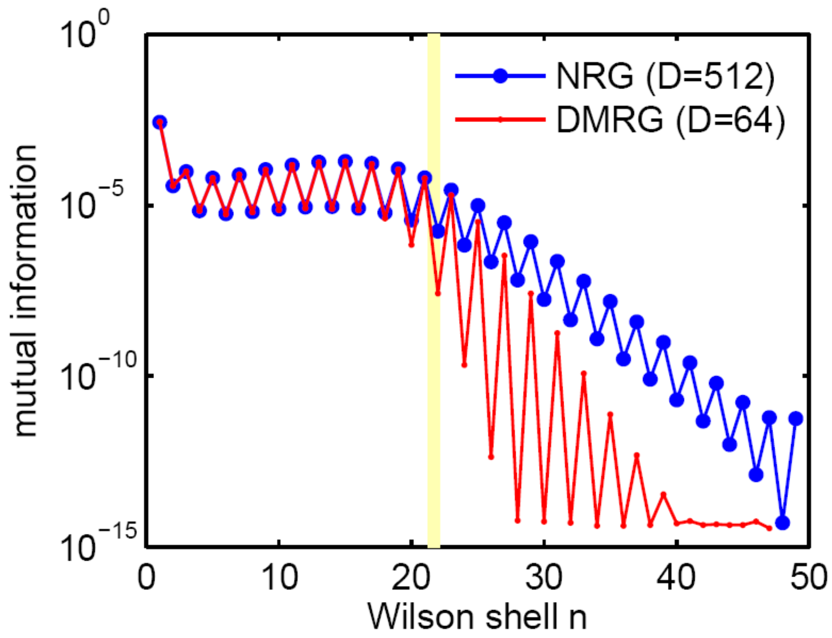
- "Unfolding" spin chains
  [not possible within NRG, energy scale separation!]



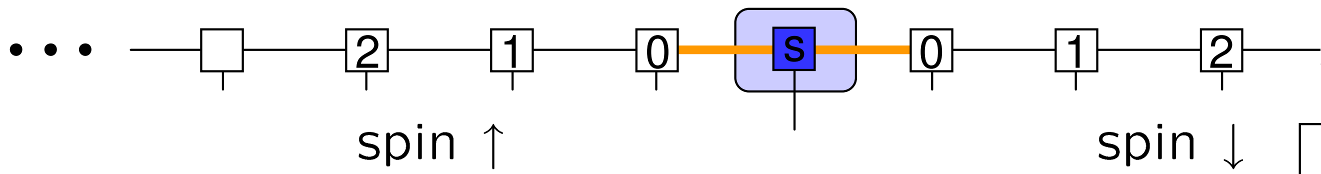


mutual information

$$\mathrm{MI} \equiv -(S_{AB} - S_A - S_B)$$



- mapping onto XY spin Hamiltonian except for impurity (see≃lsd Ra⊗ et l, 2004)

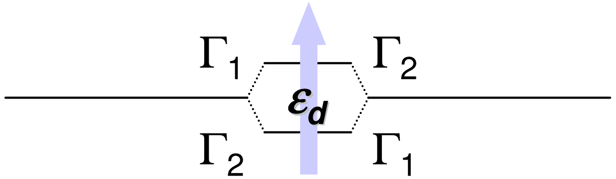


$A_k[\uparrow,\downarrow] \simeq A_k[\uparrow] \otimes A_k[\downarrow]$

NB! computational cost for both, NRG and DMRG is O(D^3) (!!)

$$D_{\mathrm{DMRG}} \simeq d D_{\mathrm{NRG}}^{1/K} \ ?$$

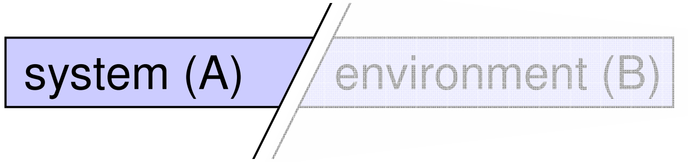
Spinless 2-level 2-channel model



there exists unitary rotation which disentangles channels but depends on non-trivially on ε_d !

QuickTime™ and a
TIFF (Uncompressed) decompressor
are needed to see this picture.

Resource efficiency

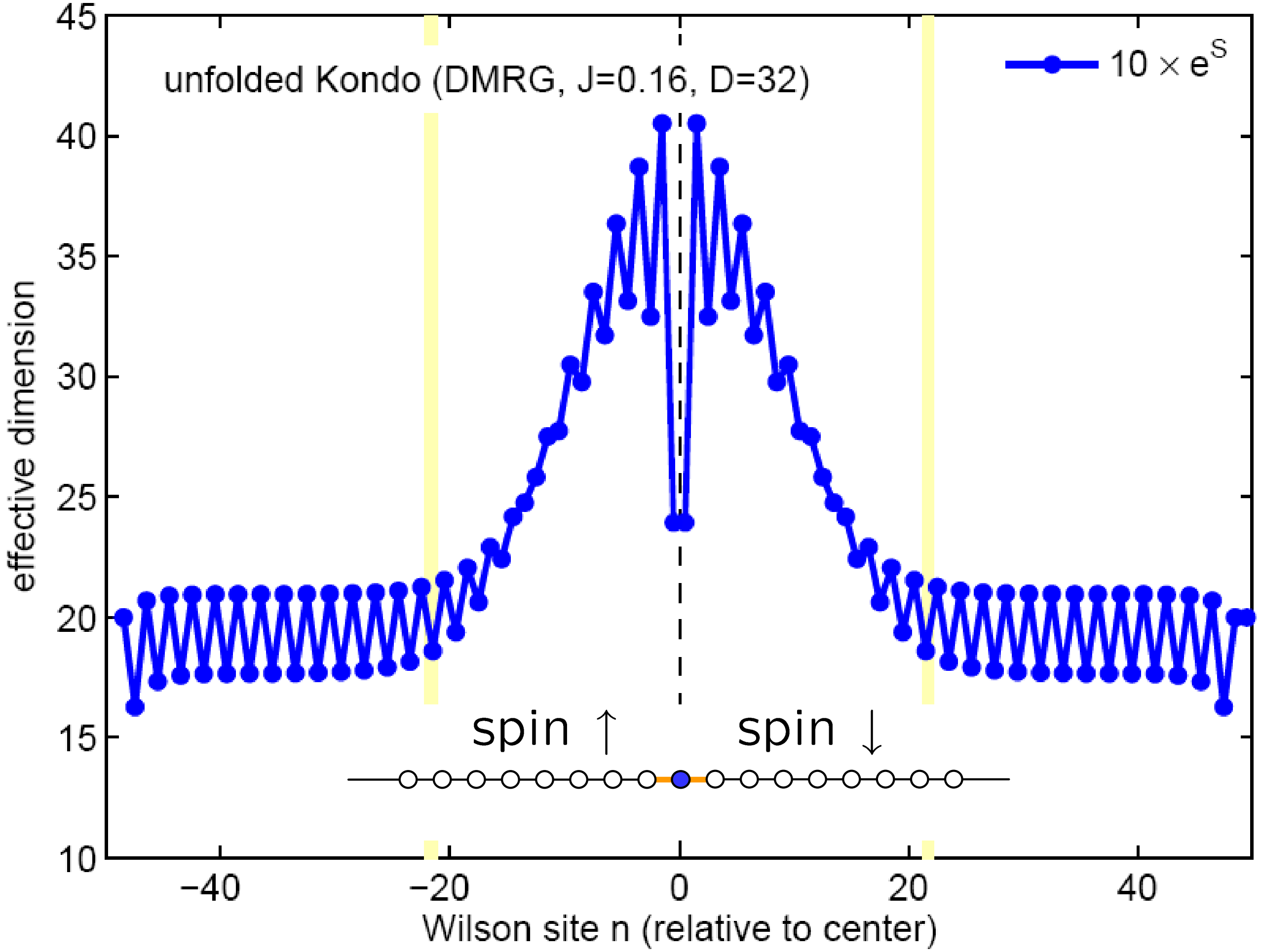


bond entropy

$$S = -\sum_i \rho_i \, \log \rho_i$$

effective dimension

$$D^* \sim e^S$$

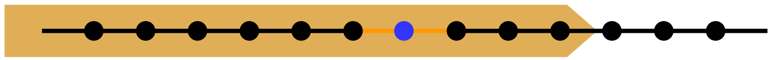


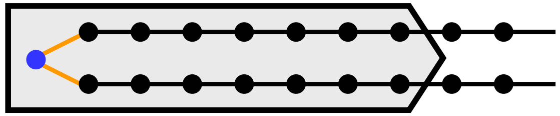
numerical resources can be adjusted dynamically!

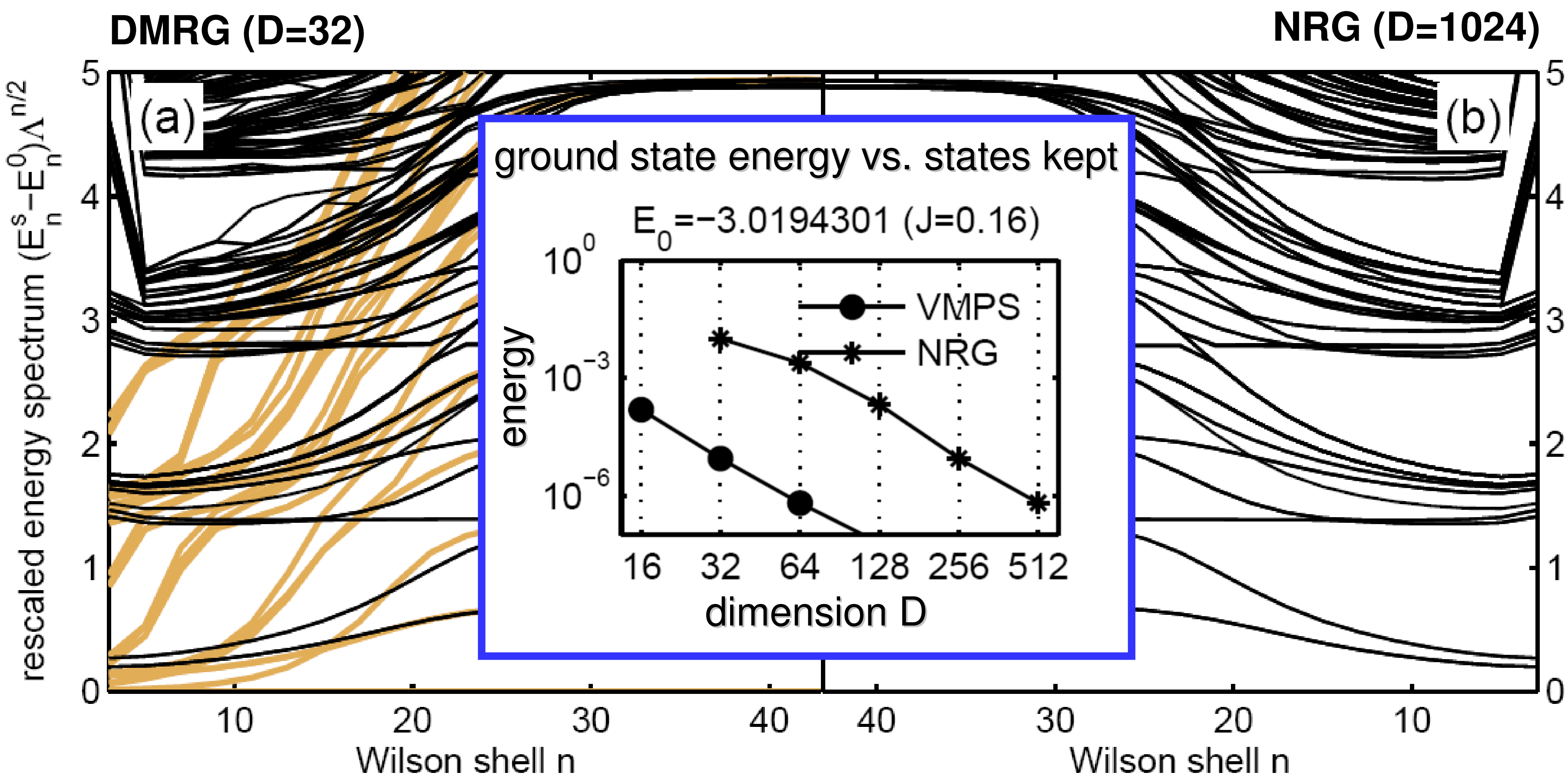
Kondo: Energy flow diagram

cond-mat/0504305

H. Saberi et al. (cond/mat 0804.0193)







D = effective number of states kept per iteration

$$D_{\mathrm{DMRG}} \simeq 2\sqrt{D_{\mathrm{NRG}}}$$

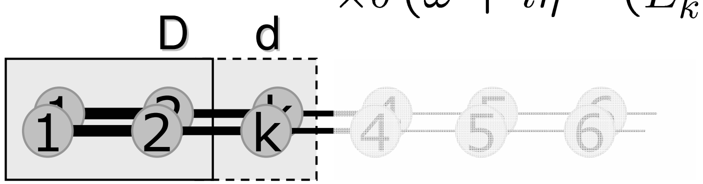
Correlation functions (T=0)

$$G(\omega) = \langle 0|\, c_\sigma \frac{1}{\widehat{H} - \left(E_0^N + \omega + i\eta\right)}\, c_\sigma^\dagger \,|0\rangle$$

NRG

$$G(\omega) = \langle 0|\, c_\sigma \,[1]\, \frac{1}{\widehat{H} - \left(E_0^N + \omega + i\eta\right)} \,[1]\, c_\sigma^\dagger \,|0\rangle$$

$$\Rightarrow \frac{1}{\pi}\mathrm{Im}G(\omega) = \sum_k \langle 0|\, c_\sigma \,|k\rangle \langle k|\, c_\sigma^\dagger \,|0\rangle \times \delta\left(\omega + i\eta - (E_k - E_0)\right)$$



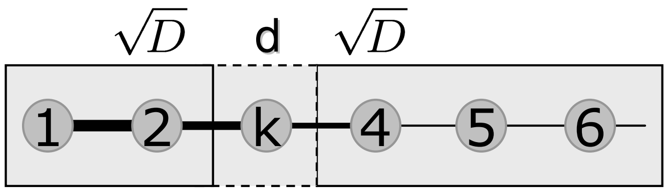
complete (approximate) eigenbasis (Anders et al. 2005)

AW et al. (2007)

all information already carried in NRG basis; evaluate matrix elements; broaden

DMRG

$$G(\omega) = \langle 0|\, c_\sigma \underbrace{\frac{1}{\widehat{H} - \left(E_0^N + \omega + i\eta\right)}\, c_\sigma^\dagger \,|0\rangle}_{\equiv |\chi_\sigma\rangle}$$



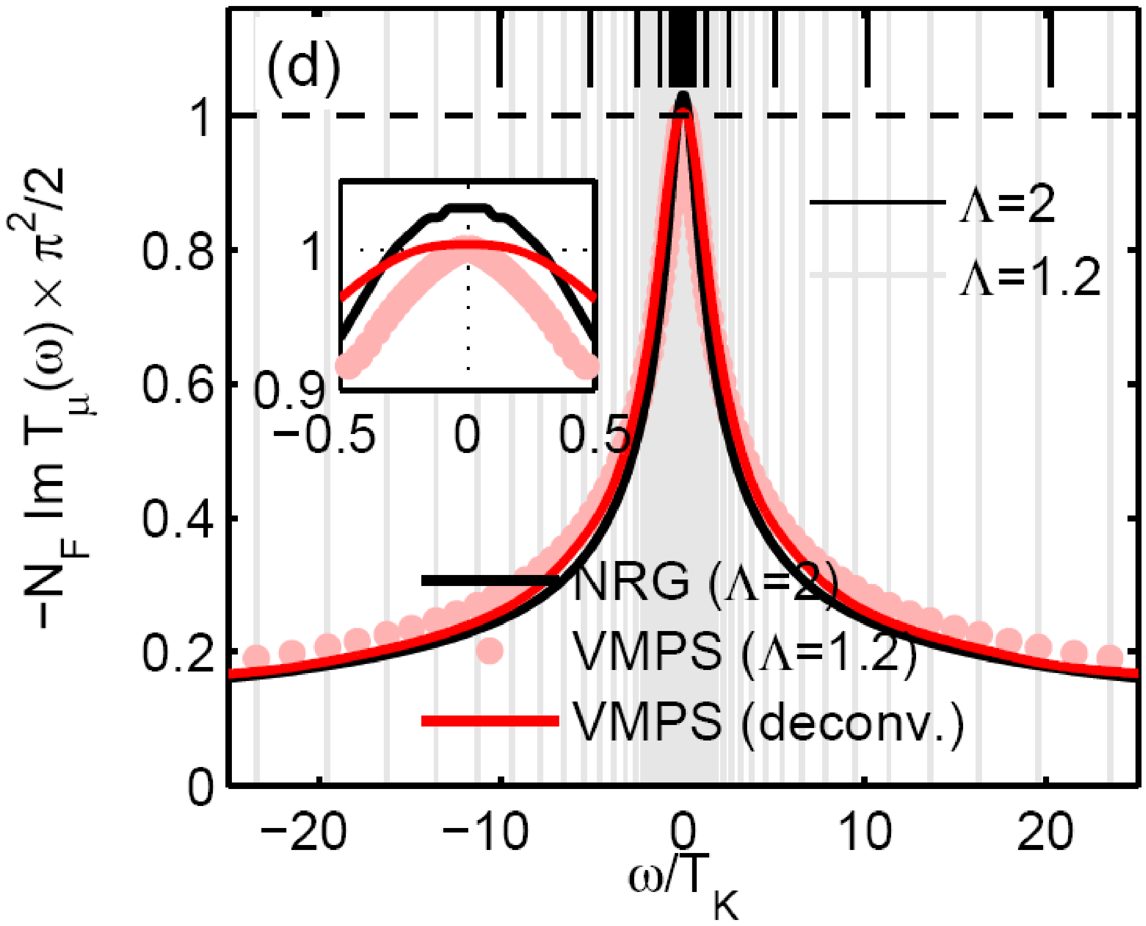
correction vector method

(Kuhner and White, 1999; Ramasesha et al., 1997 Jeckelmann, 2002)

best results but rather expensive as full run is required for every ω_i; deconvolute

Kondo: T-matrix with no magnetic field

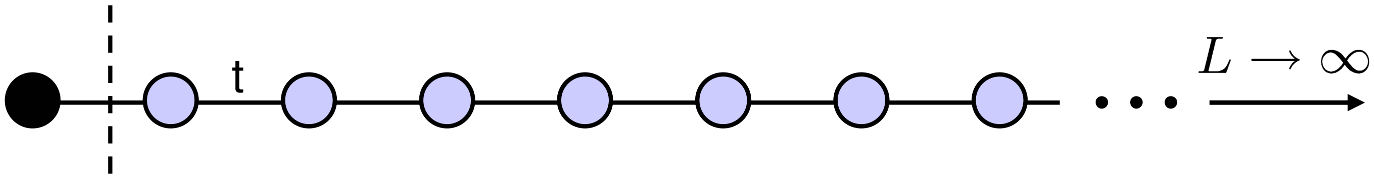
$$-N_F \mathrm{Im} T_\mu(\omega) = -J^2 \langle\langle \mathcal{O}_\mu^\dagger | \mathcal{O}_\mu \rangle\rangle_\omega, \quad where \;\; \mathcal{O}_\mu \equiv \mathbf{S} \cdot \sigma_{\alpha\alpha'} c_{\alpha'}^\dagger$$



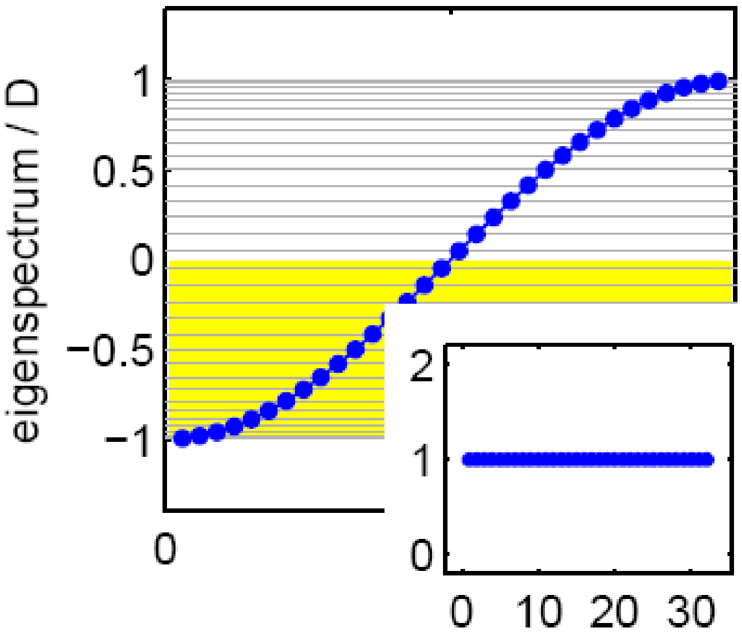
J=0.16; TK=7.7218 10^{-4}

State coupled to non-interacting Fermi sea

mapping onto semi-infinite chain with the impurity coupling to first site only

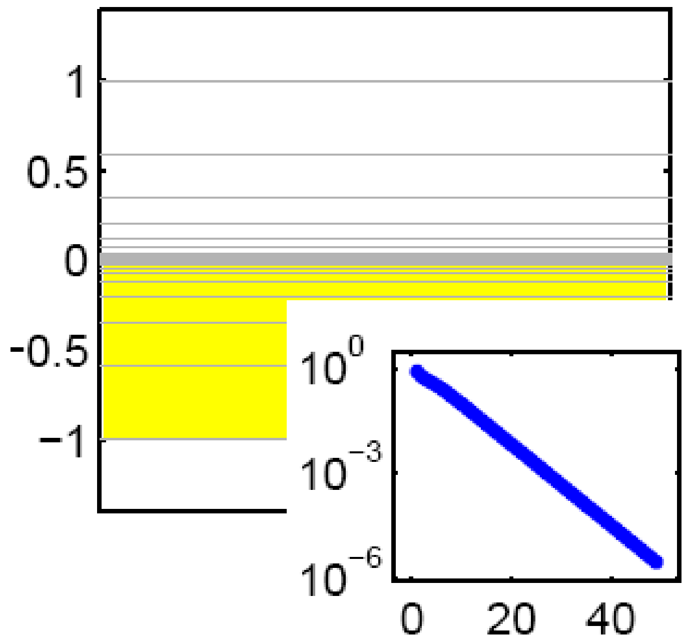


tight binding chain



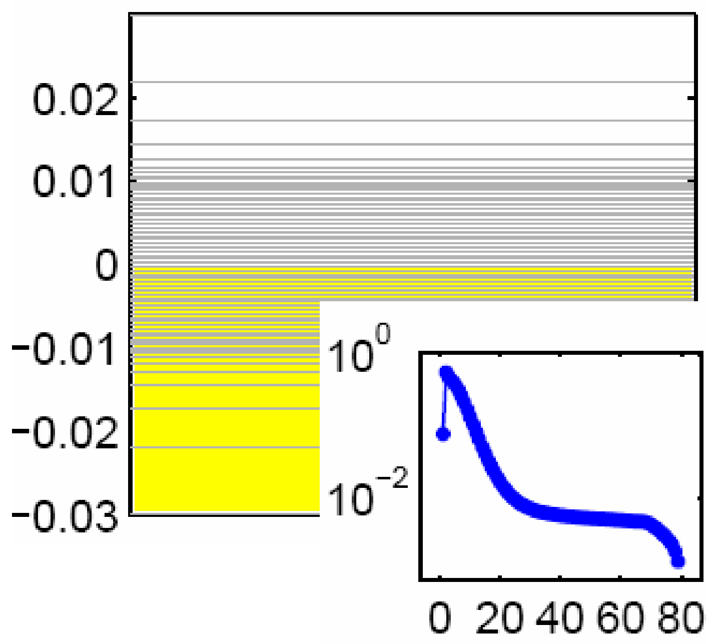
uniform hopping

Wilson discretization



exponentially decaying hopping

adaptive discretization

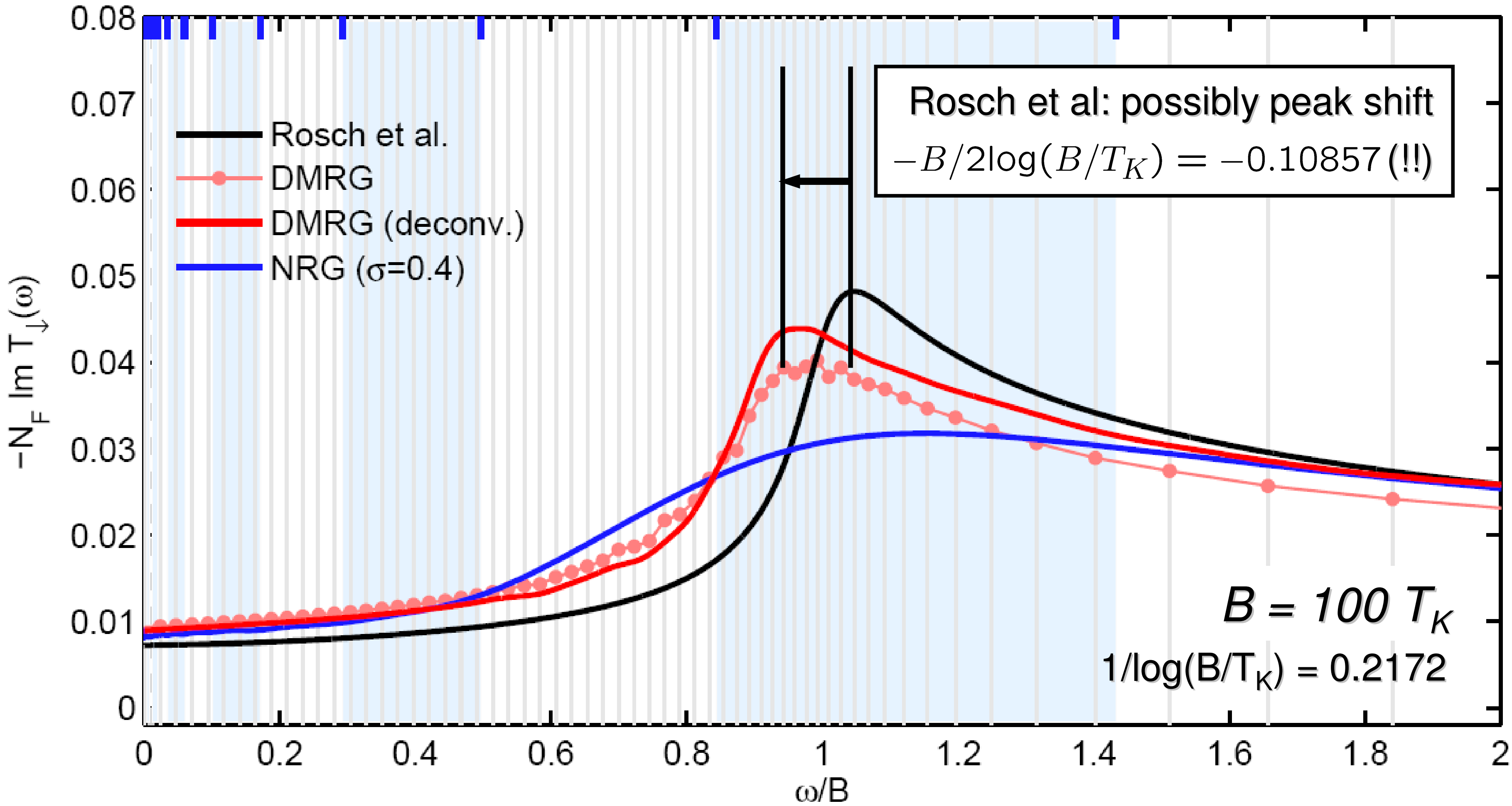


mixed behaviour

Kondo: T-matrix at large magnetic field

Rosch et al. (PRB, 2003)

$$-N_F \mathrm{Im} T_\mu(\omega) = -J^2 \langle\langle \mathcal{O}_\mu^\dagger | \mathcal{O}_\mu \rangle\rangle_\omega, \quad where \;\; \mathcal{O}_\mu \equiv \mathbf{S} \cdot \sigma_{\alpha\alpha'} c_{\alpha'}^\dagger$$



Moore et al. (PRL, 2000): peak (flank) position of spinon density of states

Summary

- ★ applied DMRG to calculate correlation functions for quantum impurity models
- ★ employed flexible discretization scheme
- ★ sharp features clearly not resolvable by NRG
- ★ good agreement with analytic results

AW et al (submitted)
A. Holzner et al. (cond/mat 0804.0550)
H. Saberi et al. (to appear in PRB)

Outlook

- ★ energy scale separation / complete basis sets for DMRG?
- ★ application to multi-channel models, dynamic meanfield, …
- ★ application to true out of equilibrium in transport

Acknowledgment

Ralf Bulla, Frithjof Anders, Achim Rosch, Markus Garst and Theresa Hecht for fruitful discussions.

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