Really (!) Useful Quantum Information Theory: Matrix Product States for Quantum Impurity Models

NRG meets DMRG

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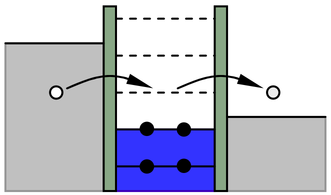
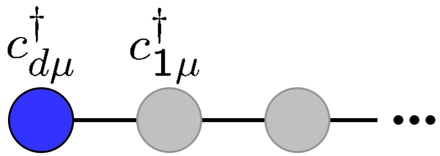
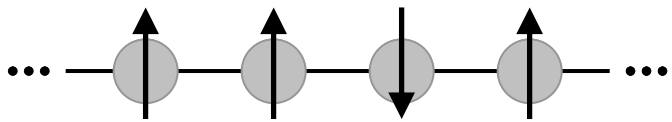
Quantum impurity models



Numerical Renormalization Group (NRG), Wilson 1975



Density Matrix Renormalization Group (DMRG), White 1992
quantum chains (spin, Hubbard, …)



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Outline

Acronyms:

NRG = Numerical Renormalization Group (Wilson, 1975)

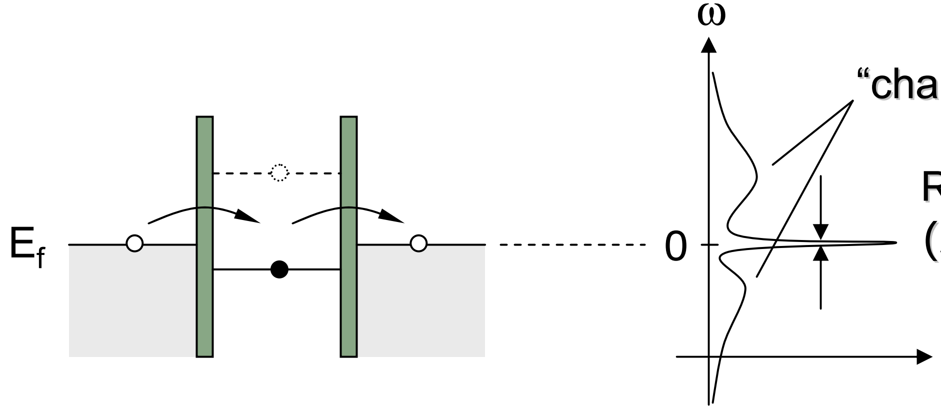
DMRG = Density Matrix Renormalization Group (White, 1992)

- Motivation, Goals
- Brief NRG review
- Central Idea: NRG produces Matrix Product State (MPS)
- Relation to DMRG
- Advantages of Matrix Product Formulation of NRG: Greater Flexibility
- Outlook: real-time evolution within DMRG framework

What one wants

- Spectral Function

$$G^c_\sigma(t) \equiv \langle\langle c_{d\sigma} | c^\dagger_{d\sigma} \rangle\rangle_t \equiv \vartheta(t) \langle 0 | \left\{ c_{d\sigma}(t), c^\dagger_{d\sigma} \right\} | 0 \rangle$$



$$A(\omega) \equiv \frac{1}{\pi} \mathrm{Im} \left[\langle\langle c_{d\sigma} | c^\dagger_{d\sigma} \rangle\rangle_\omega \right]$$

- Correlation functions
- Dynamic properties
  - through spectral function (Greens function for $\omega \neq 0$)
  - real-time simulation of strongly correlated systems using DMRG methods (Kollath, Schollwöck, White, Vidal 2004)

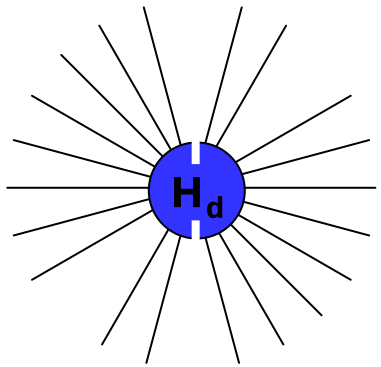
real-time evolution within NRG framework (F. Anders, 2005)

Quantum Impurity Systems (AM)

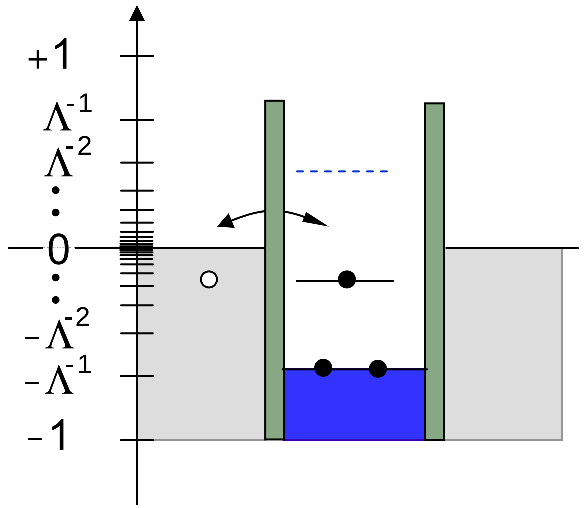
The Hamiltonian

$$\mathcal{H}_A = \underbrace{\sum_\mu \epsilon_d \, c^\dagger_{d\mu} c_{d\mu} + \frac{U}{2}\hat{n}_d(\hat{n}_d - 1)}_{\equiv H_{\text{dot}}} + \int d\epsilon \; \epsilon \, a^\dagger_{\epsilon\mu} a_{\epsilon\mu} + \underbrace{\left(\frac{\Gamma}{\pi}\right)^{1/2}}_{\Gamma \equiv \pi\rho V_d^2} \int d\epsilon \; \left(a^\dagger_{\epsilon\mu} c_{d\mu} + c^\dagger_{d\mu} a_{\epsilon\mu}\right)$$

spin ↑



spin ↓



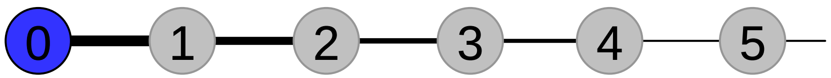
discretization parameter Λ

$\Lambda > 1 \quad (\Lambda \sim 2)$

logarithmic discretization + tridiagonalization
→ Wilson chain:

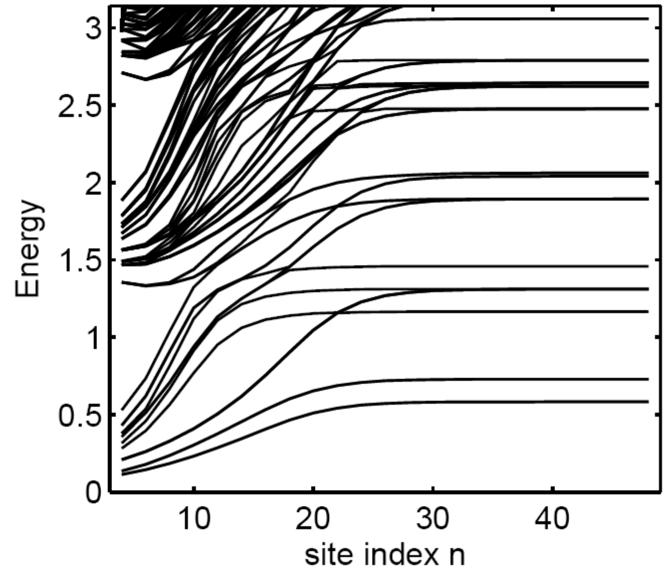
$$\lim_{n\to\infty} \xi_n = 1$$

$$\mathcal{H}_A = H_{\text{dot}} + \sqrt{\frac{2\Gamma}{\pi}}\left(f^\dagger_{0\mu} c_{d\mu} + c^\dagger_{d\mu} f_{0\mu}\right) + \frac{1}{2}\left(1 + \frac{1}{\Lambda}\right) \sum_{n=0}^{\infty} \frac{\xi_n}{\Lambda^{n/2}} \left(f^\dagger_{n\mu} f_{n+1,\mu} + f^\dagger_{n+1,\mu} f_{n\mu}\right)$$

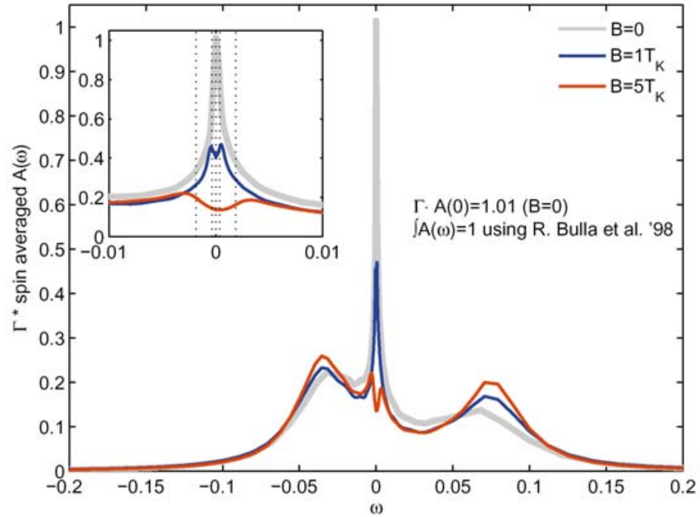


Typical Results

Flow diagram for finite size spectrum:
Useful for characterizing fixed points,
Extracting critical exponents,
Phase shifts (for T=0 transport)

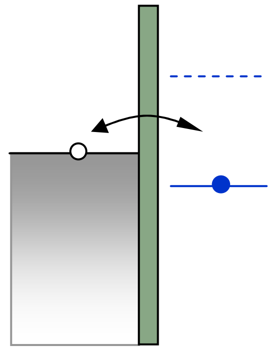


Impurity spectral function
(at zero or finite temperature):
Characterizes impurity dynamics,
(needed for T≠0 transport)



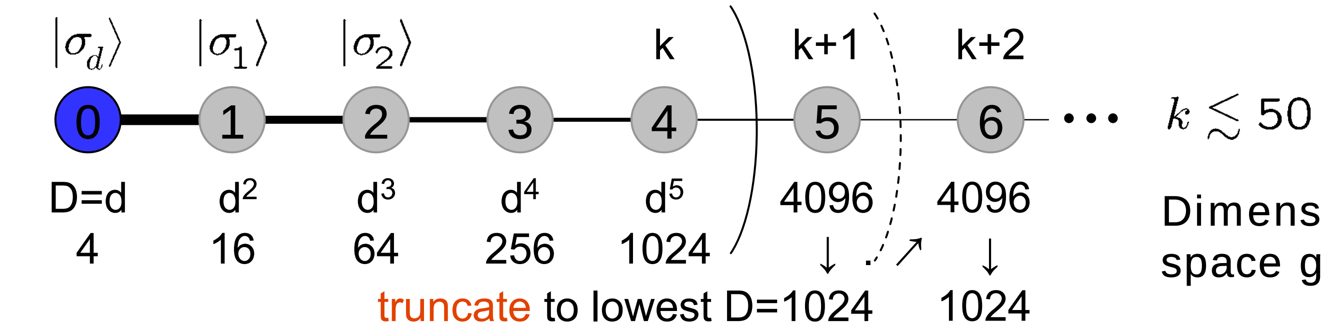
NRG obtains the low energy states iteratively

„decoupling of different energy scales“



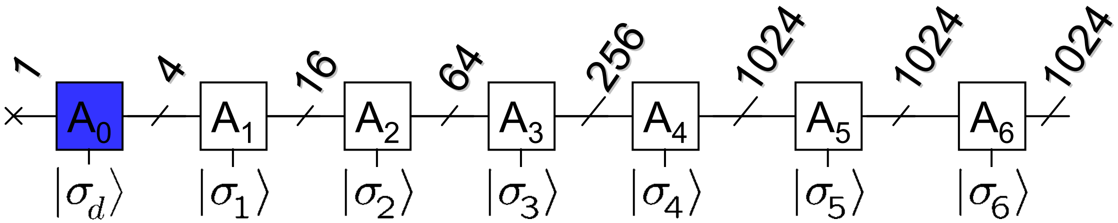
Example: Anderson model (nearest neighbor coupling only)

Local state space (d=4): $|\sigma\rangle = \{|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\}$



$k \lesssim 50$

Dimension of full Hilbert space grows like 4^k!



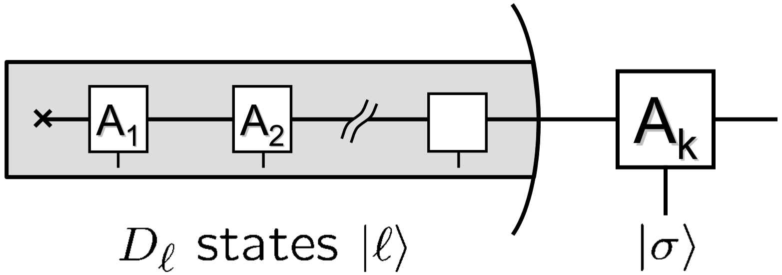
NRG generates a

Matrix Product State
(d matrizes for every site k)

$$|n\rangle_5 \equiv a^{\sigma_d}_{1i}|\sigma_d\rangle\, a^{\sigma_1}_{ij}|\sigma_1\rangle\, a^{\sigma_2}_{jk}|\sigma_2\rangle\, a^{\sigma_3}_{kl}|\sigma_3\rangle\, a^{\sigma_4}_{lm}|\sigma_4\rangle\, a^{\sigma_5}_{mn}|\sigma_5\rangle \cdots \equiv \sum_{\{\sigma\}} \prod_k A_k[\sigma_k]\, |\sigma_d, \sigma_1, \ldots\rangle$$

Key Observation

- NRG generates a Matrix Product State (MPS)

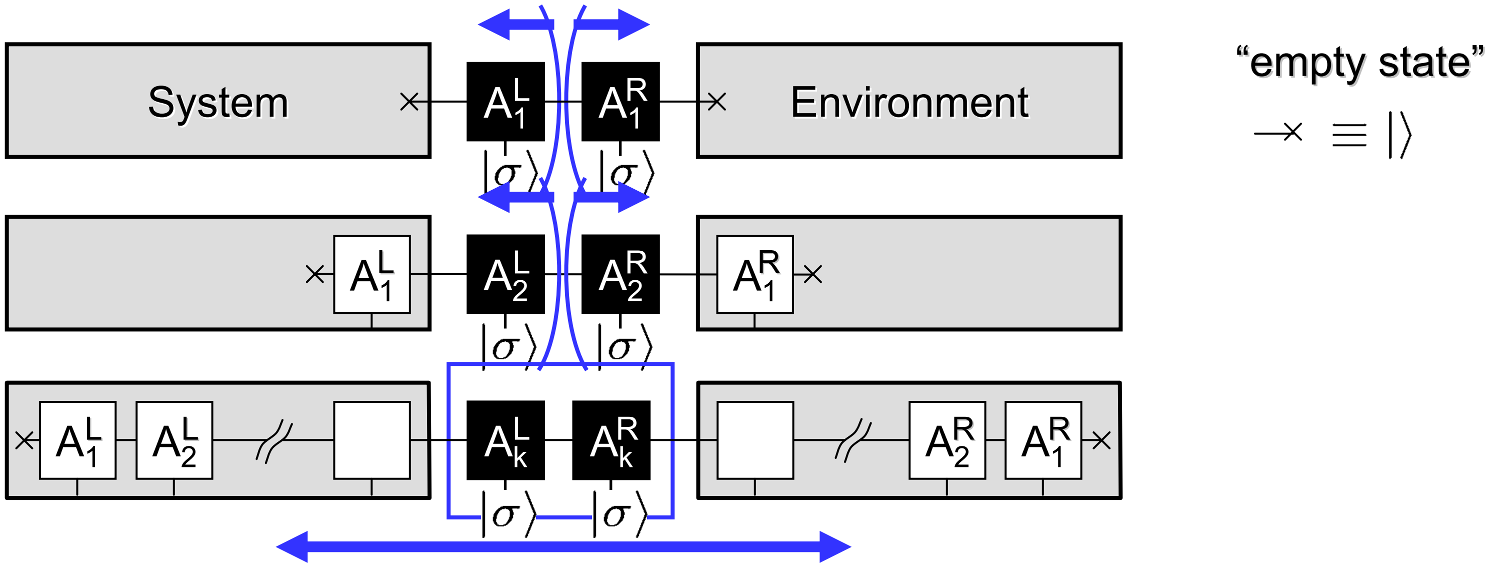


- Use this MPS structure for variational optimization
  - ↳ equivalent to one-site finite-size **DMRG** with open boundary conditions

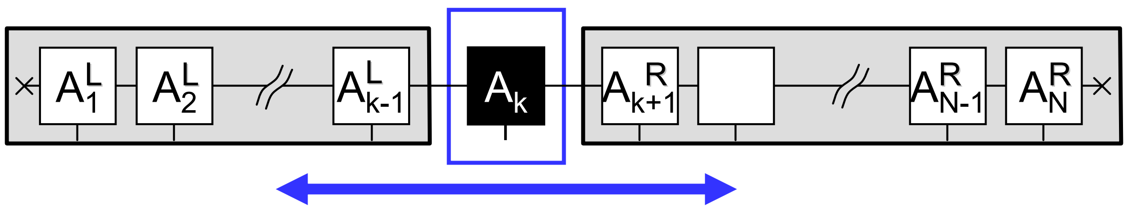
- Variational structure lifts strict NRG constraints
  - ✶ one can optimize initial NRG-MPS by subsequent variational sweeping
  - ✶ allows arbitrary discretization scheme of the conduction band
  - ✶ allows for more flexible MPS structure beyond 1D (star geometry)

DMRG (Primer)

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



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

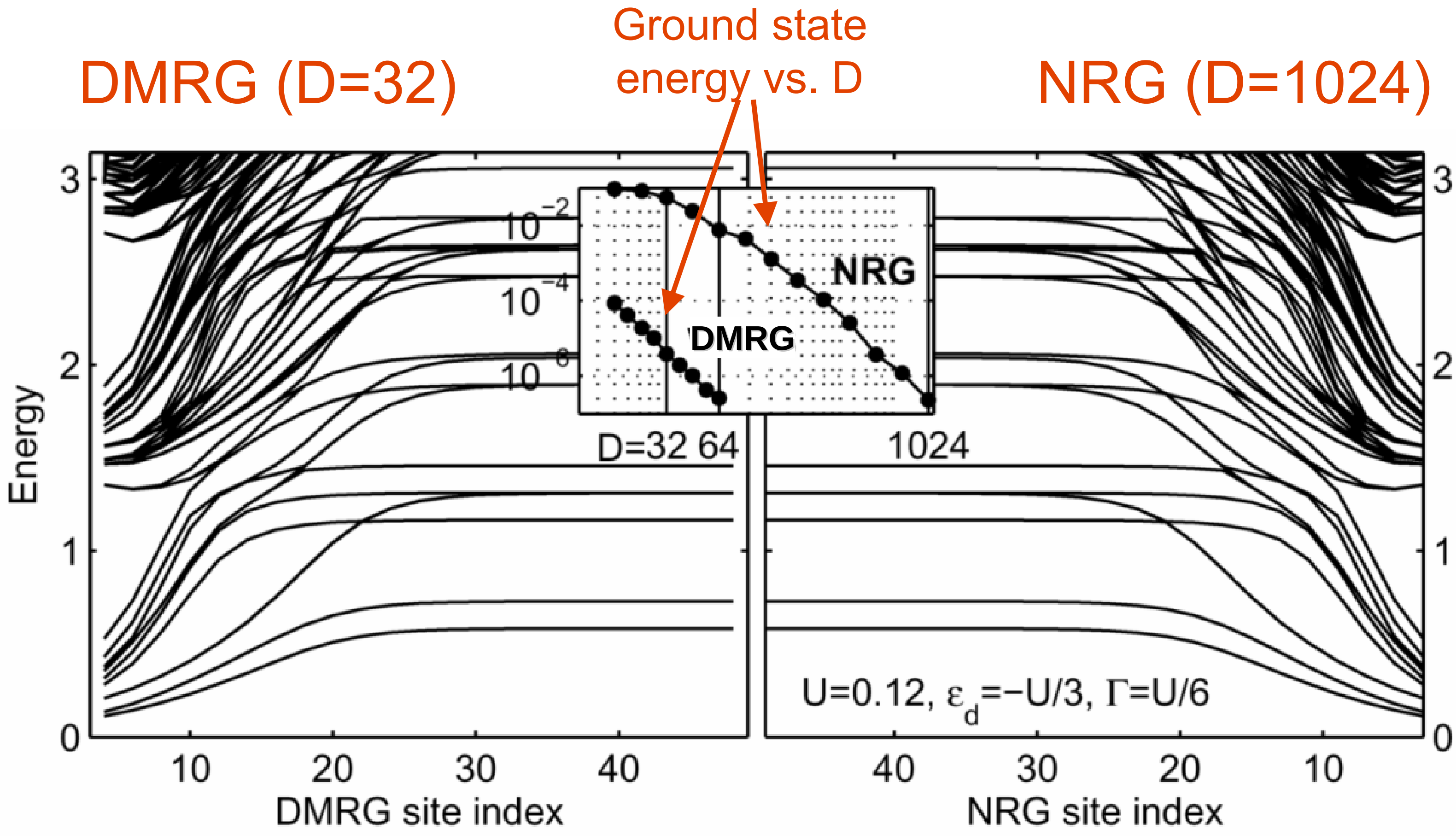


strictly variational within the space of MPS

Does it work in practice?

Flow of Eigenenergies under Renormalization

Anderson Model



D = effective number of states kept per iteration

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Spectral Function

$$G_\sigma(\omega > 0)_{T=0} = \left\langle \psi_0^N \right| c_\sigma \cdot \frac{1}{\hat{H} - \left(E_0^N + \omega + i\eta\right)} \cdot c_\sigma^\dagger \left| \psi_0^N \right\rangle$$

$$A_\sigma(\omega) \equiv \frac{1}{\pi} \mathrm{Im} G_\sigma(\omega)$$

$$(H - z)\left|\chi\right\rangle = \left|c\right\rangle$$ "Ax=b"

→ solve iteratively, i.e. by sweeping

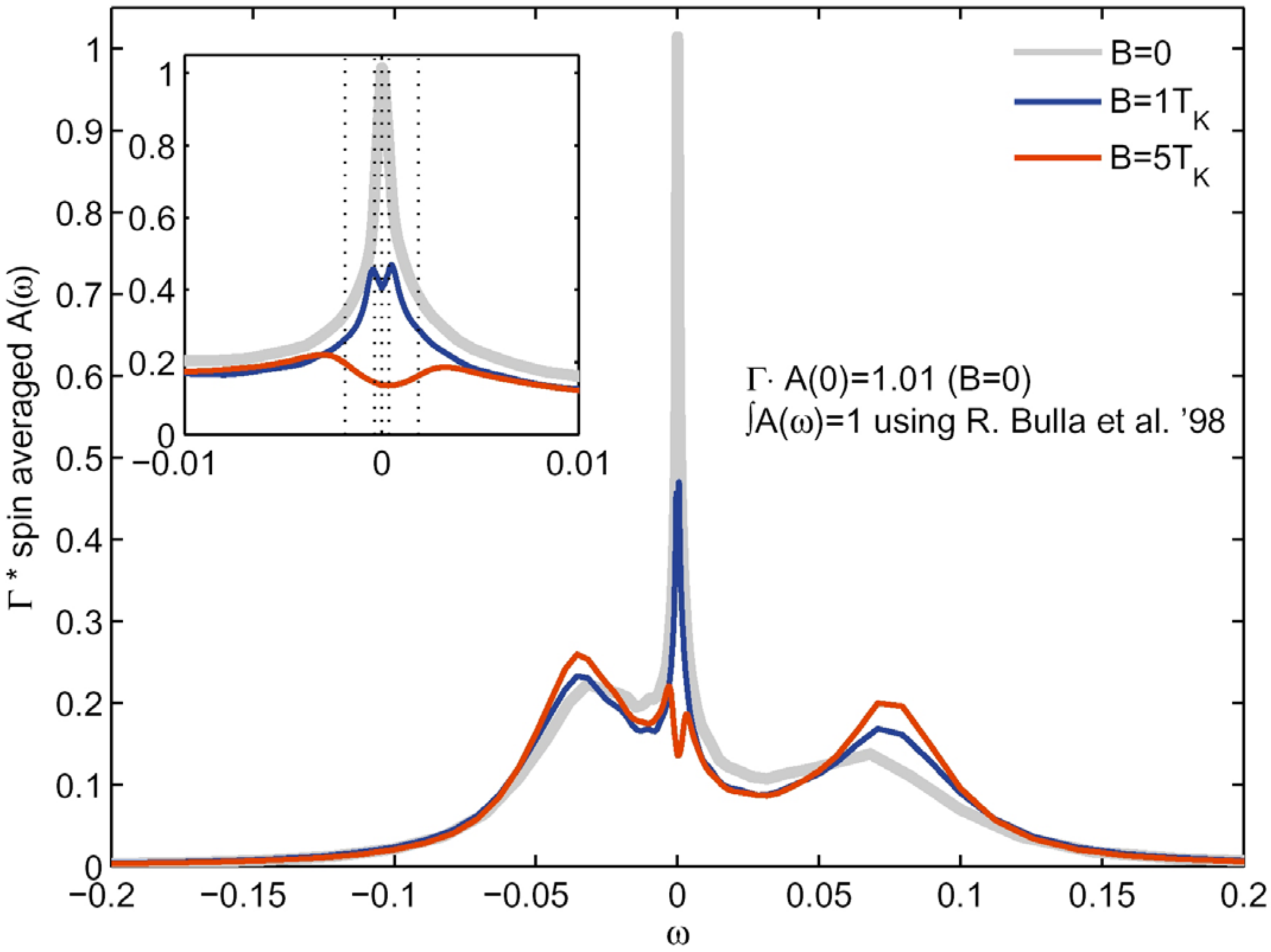
- Challenge
  - ★ need very small η to resolve sharp features (Kondo resonance)

    $\eta \lesssim T_K$ for $\omega \simeq 0$

    thus *1/(H-z)* can be become rather ill-conditioned
- In practice
  - ★ use variable broadening: η ~ 0.4 ω (in analogy to log-gauss broadening in NRG)
  - ★ get smoother spectral function by calculating self-energy using F(ω)

    Bulla (1998), Raas, Anders (2005) $F_\sigma(\omega > 0)_{T=0} = \langle c| \hat{n}_{\bar{\sigma}} |\chi_\sigma(\omega)\rangle$

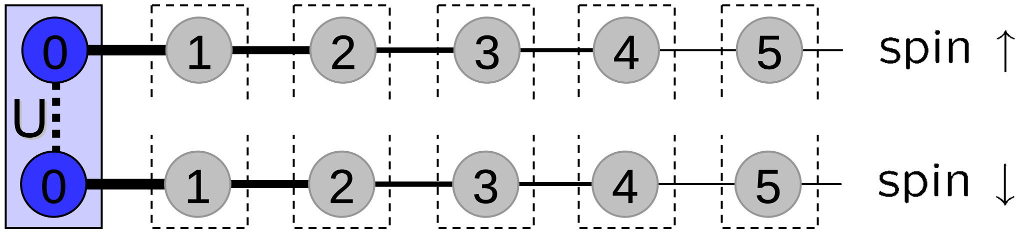
Spectral Function



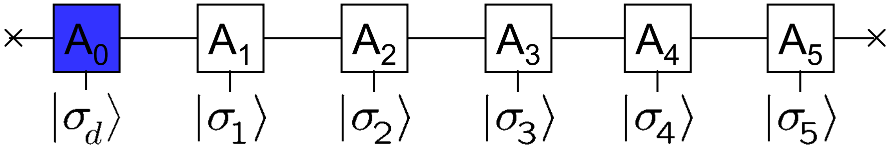
Advantage of MPS Formulation: Greater Flexibility!

Variational procedure loosens NRG constraints

- Unfolding the spins within NRG chain
  (completely violates basic NRG constraints!)



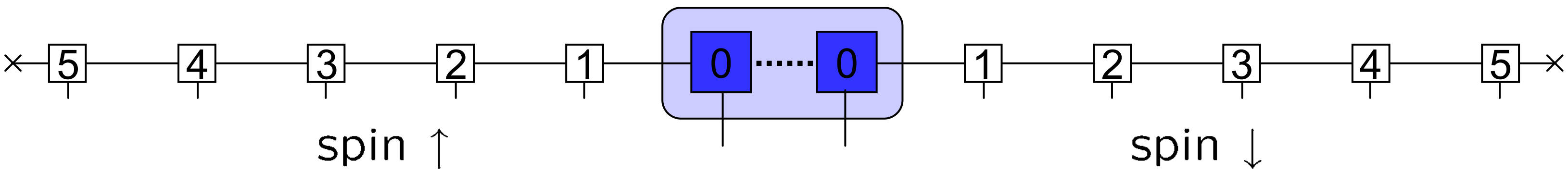
$$"|\sigma\rangle" = \{|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\}$$
$$\equiv \left\{|0_\uparrow\rangle, |1_\uparrow\rangle\right\} \otimes \left\{|0_\downarrow\rangle, |1_\downarrow\rangle\right\}$$



$$\square \simeq \square \otimes \square$$

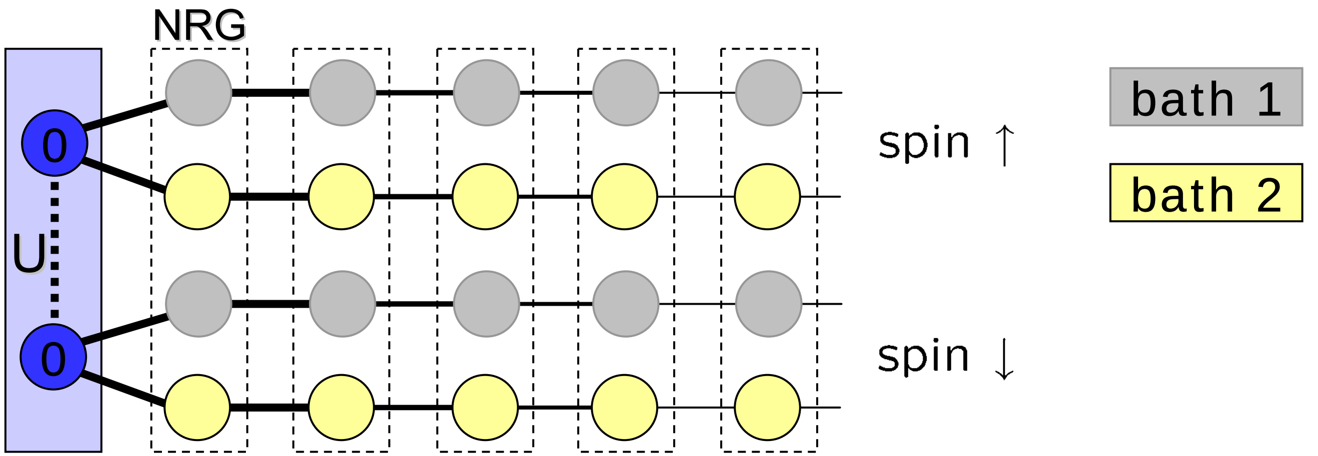
$$A_k[\uparrow,\downarrow] \simeq A_k[\uparrow] \otimes A_k[\downarrow]$$

★ well-known mapping onto XX spin Hamiltonian



Prospects

- Multi-channel impurity models



Computational complexity

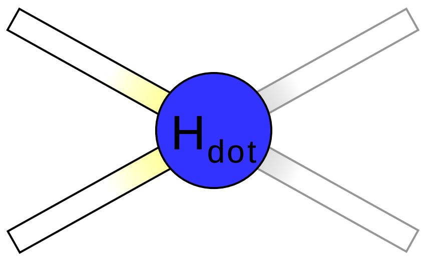
with K = number of channels
and d=2 for single fermionic state — *K=2*

$d_{\mathrm{NRG}} = d^{2K}$ — *16*

$d_{\mathrm{DMRG}} = d$ — *2*

$\Rightarrow \quad D_{\mathrm{DMRG}} \sim (D_{\mathrm{NRG}})^{\frac{1}{2K}}$ — *10 000 → 10 (!!)*

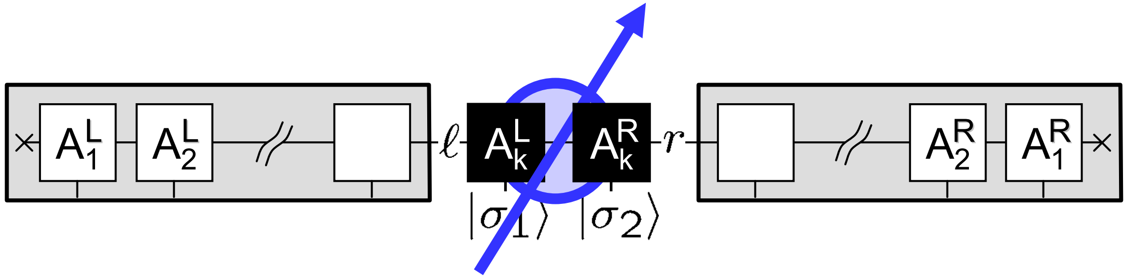
Star geometry (quasi 1D-MPS)



NB! computational cost scales like D^3 (!!) for both, NRG and DMRG

Benefit : Resource Efficiency

- control on DMRG truncation error allows optimization of D
  i.e. by looking at bipartite entanglement using reduced density matrix



MPS state decomposition around site (k,k+1)

$$|\Psi_k\rangle = \sum_{\ell r \sigma_1 \sigma_2} a^{(k)}_{\ell r \sigma_1 \sigma_2} |\ell r \sigma_1 \sigma_2\rangle_k$$

Reduced density matrix

$$\rho^{(k,L)}_{\text{red}} \equiv \text{tr}_{\{r,\sigma_2\}} (|\Psi_k\rangle \langle \Psi_k|) = \sum_{\ell\sigma_1,\ell'\sigma'_1} \rho^{(k,L)}_{\ell\sigma_1,\ell'\sigma'_1} |\ell\sigma_1\rangle \langle \ell'\sigma'_1|$$

Bipartite entanglement

$$S_k = \sum_\alpha \varrho^{(k)}_\alpha \log \varrho^{(k)}_\alpha$$

Estimate of optimal D

$$D^{(k)}_{opt} \approx \text{const} \cdot e^{S_k}$$

(const ~10 since spectrum typically falls off exponentially)

Benefit : Resource Efficiency

- control on DMRG truncation error allows optimization of D
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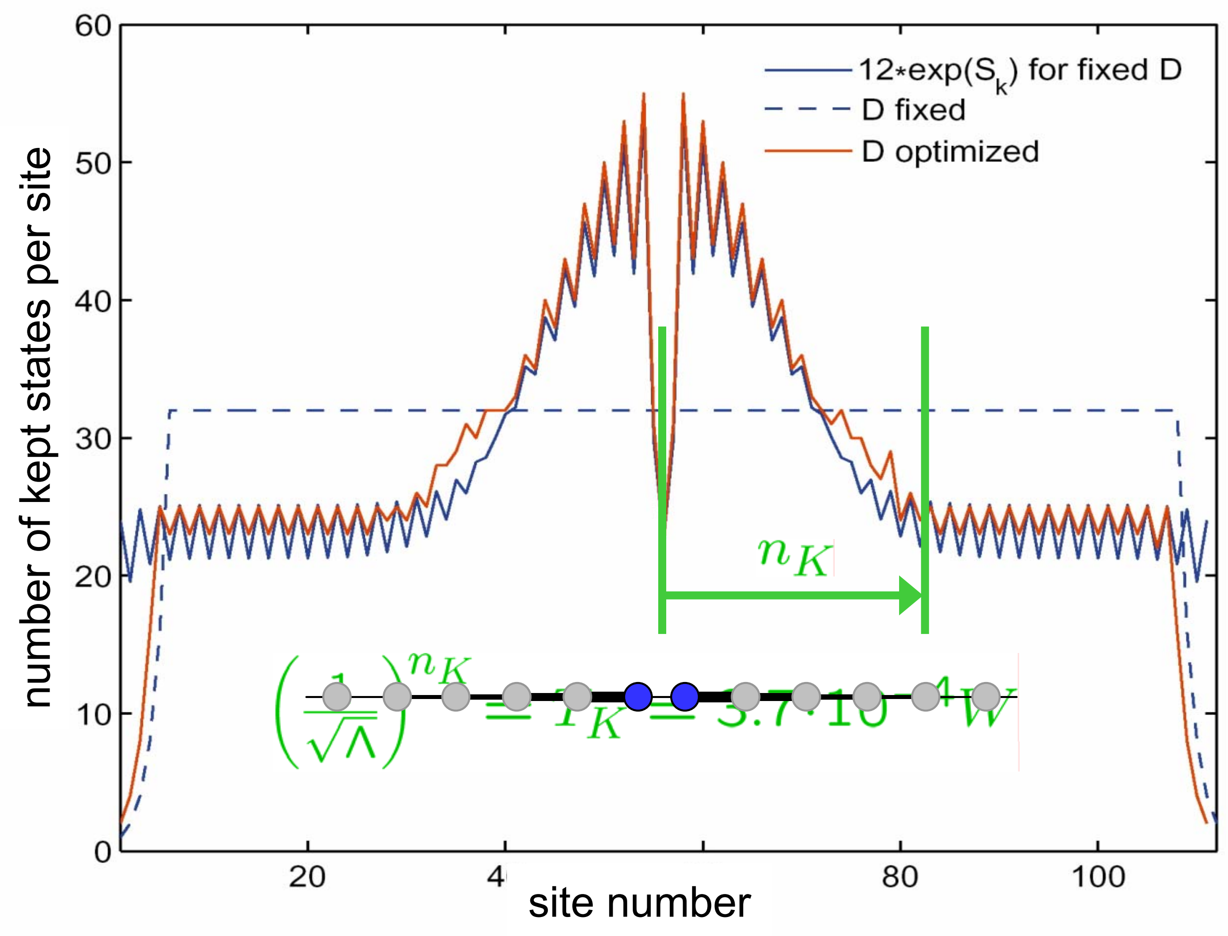
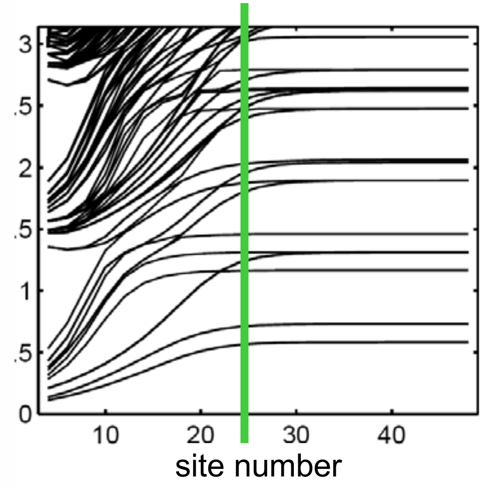


compare to
energy flow diagram



Prospects

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

- Time-dependence
- Out-of-equilibrium

Prospect: Time dependence using MPS

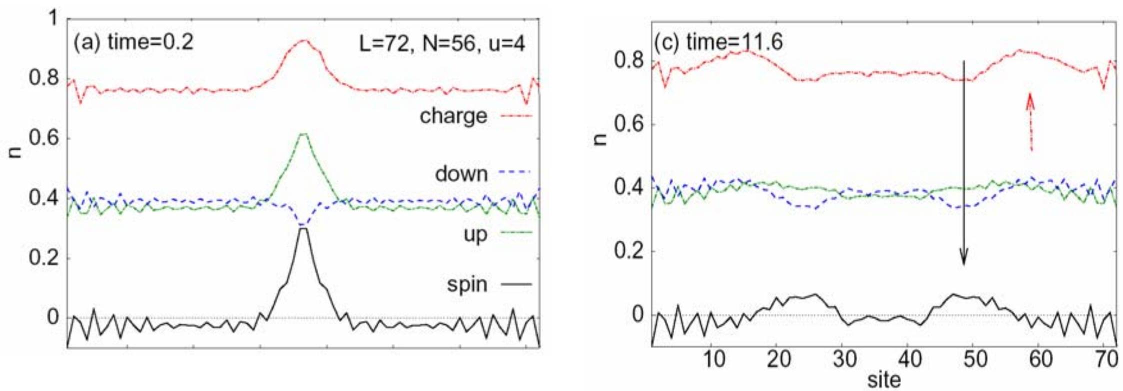
- Schrödinger equation (Crank-Nicholson)

$$i\frac{d}{dt}|\psi\rangle = H|\psi\rangle$$

- (higher-order) Suzuki-Trotter decomposition

$$|\psi(t+dt)\rangle = U|\psi\rangle \text{ with } U = e^{-iHdt}$$

- search in recent literature
  - ★ Collapse and Revival Starting from a Luttinger Liquid (Manmana, Noack 2006)
  - ★ Real-time dynamics in spin-1/2 chains with adaptive time-dependent DMRG (Gobert 2005)
  - ★ Spin-Charge Separation in Cold Fermi Gases: A Real Time Analysis (Kollath 2005)



Outlook

Matrix Product States Technology is a powerful tool for numerically describing quantum impurity models
Close connection to DMRG methodology means: all DMRG tricks can be fruitfully employed here, too!

★ very clear conceptual structure (MPS)
★ Optimization of numerical resources using quantum information concepts
★ simulating real-time evolution

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Variational matrix product state approach to quantum impurity models
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