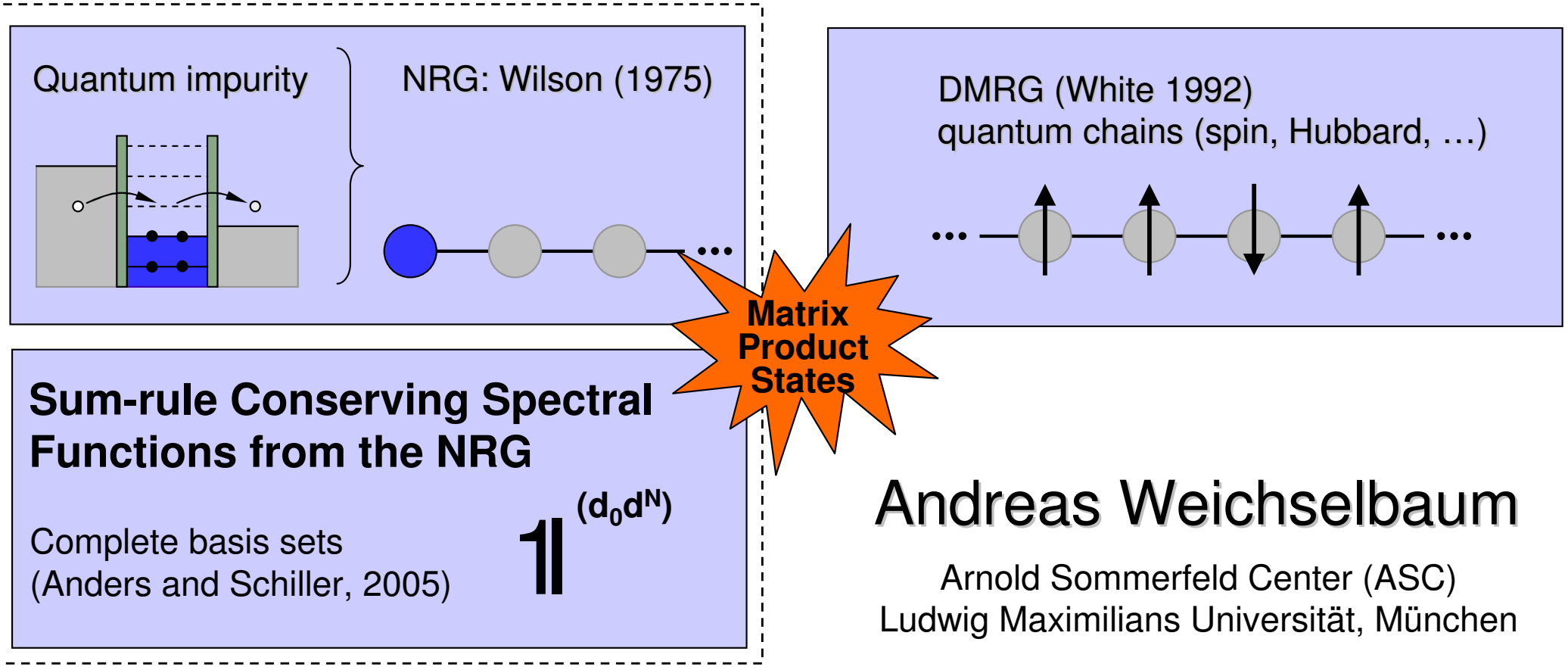
NRG = Numerical Renormalization Group
DMRG = Density matrix Renormalization Group



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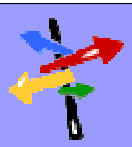
Outline

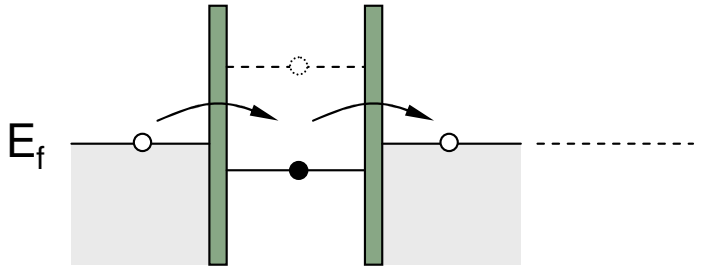


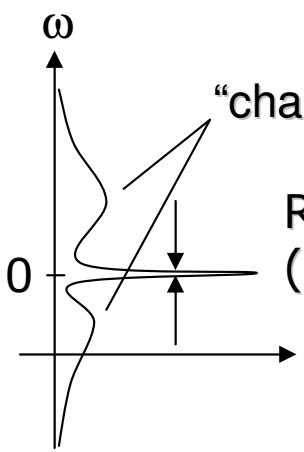
- NRG point of view to quantum impurity systems
  - Short review on Wilson's NRG
  - NRG generates Matrix Product State (and so does DMRG)
- Sum-rule conserving Correlation functions
  - Short review on complete basis set within NRG framework (Anders and Schiller, 2005)
  - Similarity to dm-NRG (Hofstetter 2000)
  - Connection to time-dependence
- Results
- Outlook

Sum-rule Conserving Spectral Functions from the Numerical Renormalization Group
Andreas Weichselbaum and Jan von Delft (cond-mat/0607497)

What one wants

- Understanding of quantum systems embedded in their full many-body environment (bosonic, fermionic) i.e. “quantum impurity model”





“charge fluctuation peaks”

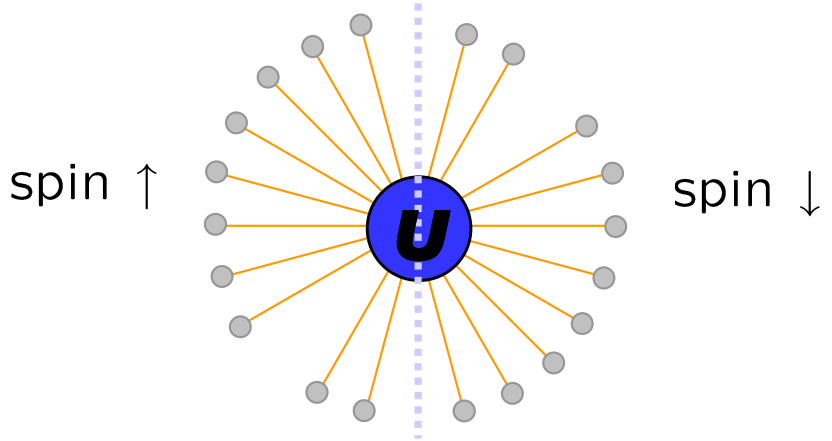
Resonance pinned at the Fermi energy
(Abrikosov–Suhl -, Kondo resonance)

- Dynamical properties
  - Correlation functions at finite ω (e.g. spectral functions, …)
  - real-time simulation of strongly correlated systems using
    - DMRG methods (Kollath, Schollwöck, White, Vidal 2004) } general for 1D short time scales
    - within NRG framework (Anders and Schiller 2005) } single “sudden switch” and large time scales
    - Flow-equation approach (Lobaskin and Kehrein, 2005) } single “sudden switch” and large time scales

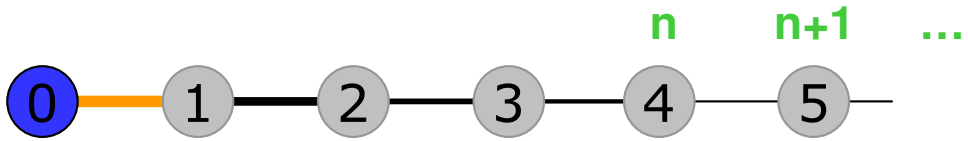
Quantum Impurity Models (NRG point of view)

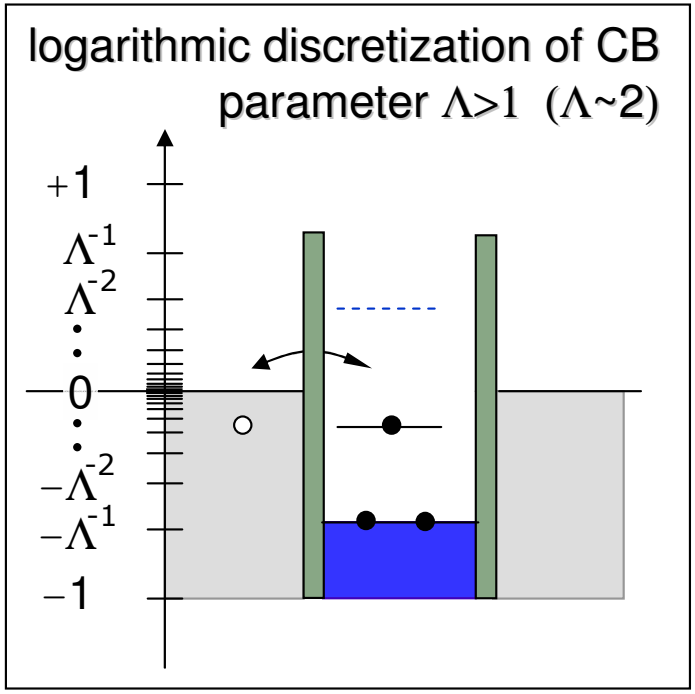
Single Impurity Anderson Hamiltonian (SIAM)

$$\mathcal{H} = \sum_{\mu} \epsilon_d \, d^\dagger_\mu d_\mu + \frac{U}{2}\hat{n}_d\,(\hat{n}_d - 1) + \sqrt{\frac{\Gamma}{\pi}} \int_{-D}^{D} d\epsilon \left(a^\dagger_{\epsilon\mu} d_\mu + d^\dagger_\mu a_{\epsilon\mu}\right) + \int_{-D}^{D} d\epsilon \; \epsilon \; a^\dagger_{\epsilon\mu} a_{\epsilon\mu}$$



logarithmic discretization + tridiagonalization
→ Wilson chain:





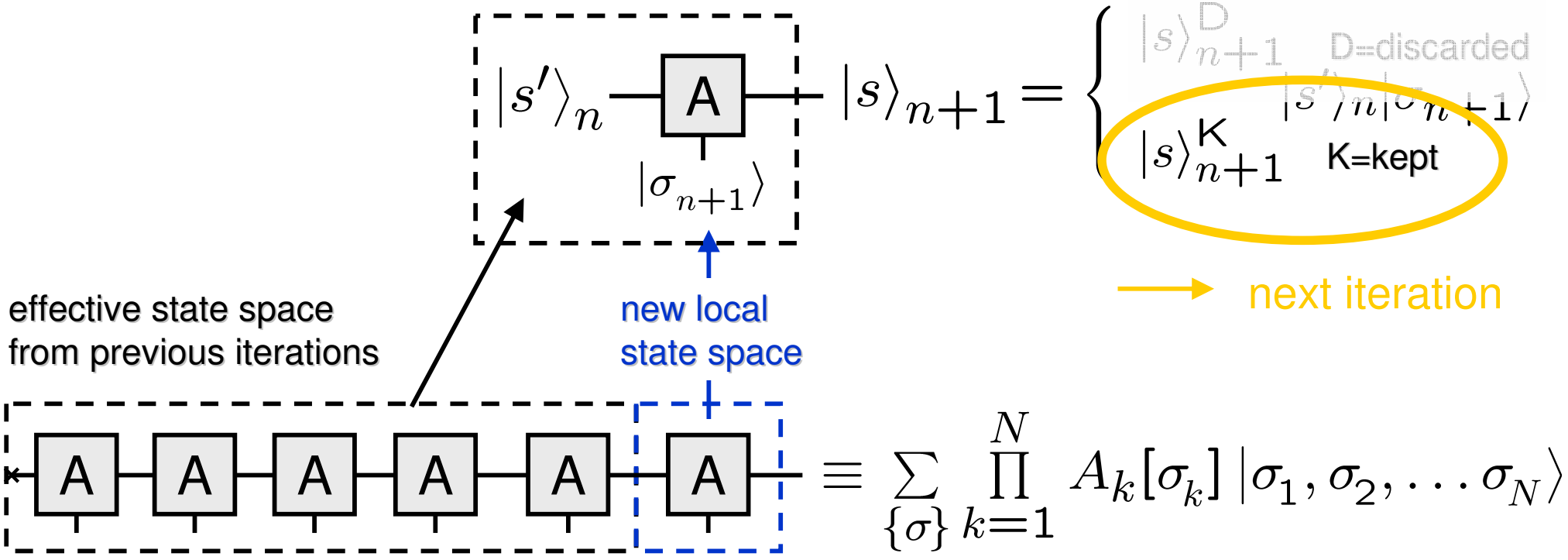
energy scale separation

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

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

NRG produces Matrix Product States

- Iterative procedures generate Matrix Product States (MPS)



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

Local correlation functions

- Local operators B and C

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

- Sum-rule

$$\int d\omega \mathcal{A}^{\mathcal{BC}}(\omega) = \sum_{a,b} \langle b|\hat{\mathcal{C}}|a\rangle \underbrace{\frac{e^{-\beta E_a}}{Z}}_{\equiv \rho} \langle a|\hat{\mathcal{B}}|b\rangle = \langle \hat{\mathcal{B}}\hat{\mathcal{C}} \rangle_T$$

- Ex. Spectral function

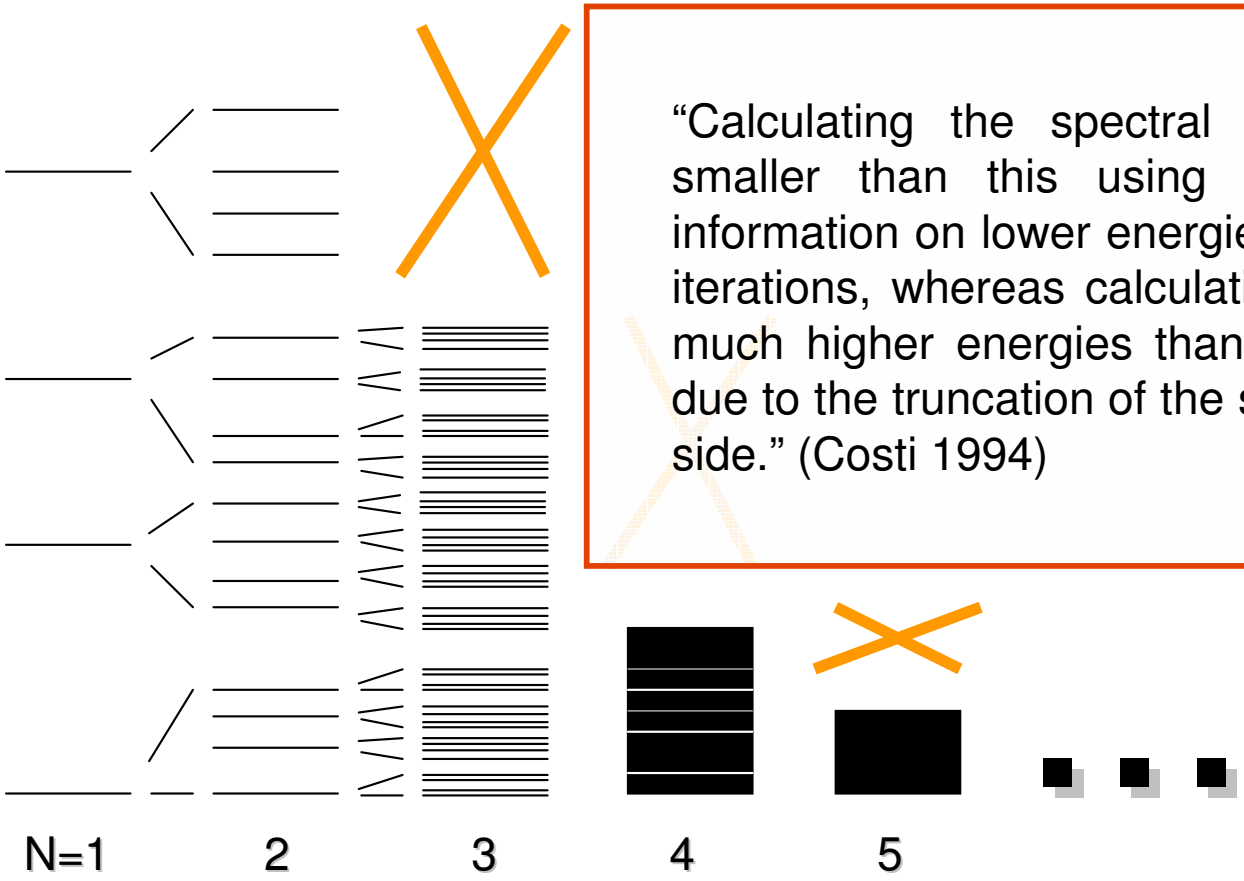
$$\begin{aligned} \mathcal{A}(\omega) &= \int \frac{dt}{2\pi} e^{i\omega t} \langle \left\{ \hat{d}_\mu(t), \hat{d}_\mu^\dagger \right\} \rangle_T \\ &= \left\langle \left\{ \hat{d}_\mu, \hat{d}_\mu^\dagger \right\} \right\rangle_T = 1 \end{aligned}$$

Sum-rules preserved only
if ***complete*** basis set is available
for the full many-body problem!

Traditional way of obtaining spectral data

Costi (1994)

- Collect data from every NRG iteration
- Overcounting within state space that is kept for next iteration!!
  → heuristic combination of data from different iterations



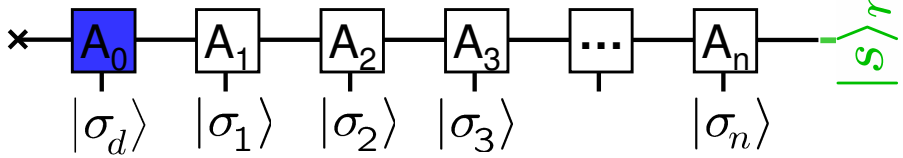
"Calculating the spectral density at energies much smaller than this using H_N is not justified, since information on lower energies is obtained in subsequent iterations, whereas calculating the spectral densities at much higher energies than this might introduce errors due to the truncation of the spectrum on the high-energy side." (Costi 1994)

DM-NRG – one "sweep"

Hofstetter (2000)

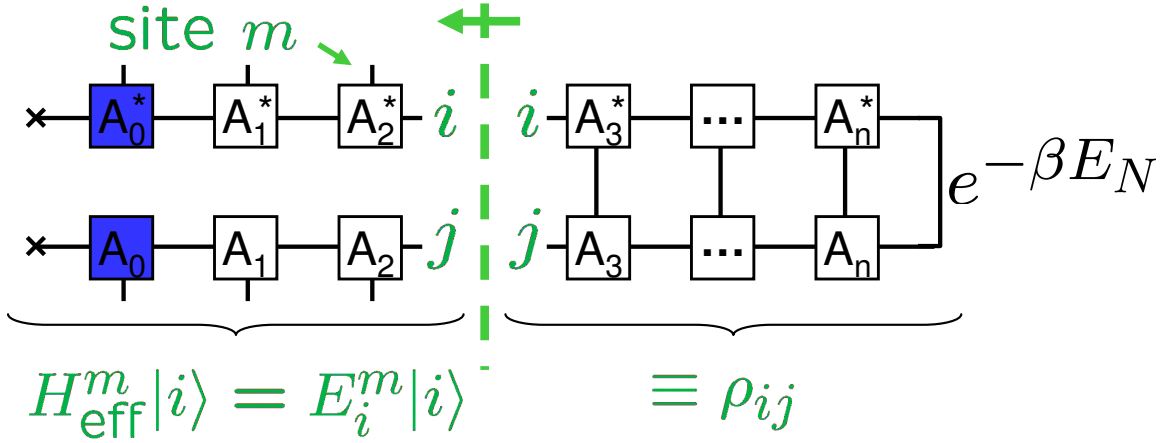
- Temperature dependent density matrix

  NRG: chain length determined by MAX(T,T_K)



$$\rho = \sum_s \frac{e^{-\beta E_s^n}}{Z} \; |s\rangle_n \; {}_n\langle s|$$

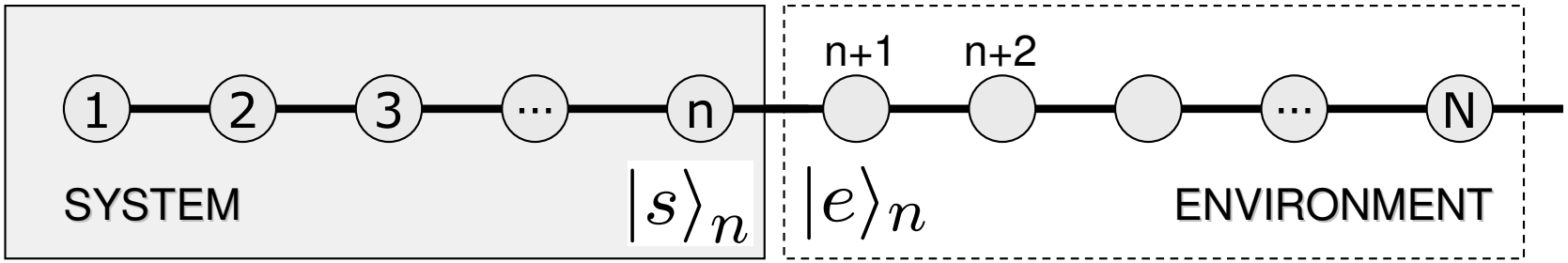
- Collect data from every iteration (last to first)



improves upon spectral data with finite ω and B≠0

Complete Basis Set on Wilson Chain

Anders and Schiller (2005)



- Complete orthonormal basis set for the **full** chain

still exponentially huge!
→ trace out!

$$\mathbb{1}^{(d^N)} = \sum_n \sum_{se} |se\rangle_n^{\mathrm{D}}\ {}_n^{\mathrm{D}}\langle se| \ , \quad |se\rangle_n^{\mathrm{D}} \equiv |s\rangle_n^{\mathrm{D}} \otimes |e\rangle_n$$

- **The** NRG Assumption = Energy scale separation

$$\hat{H}_N |se\rangle_n \simeq E_s^n |se\rangle_n$$

Generalization to Full Density Matrix

AW, cond-mat/0607497

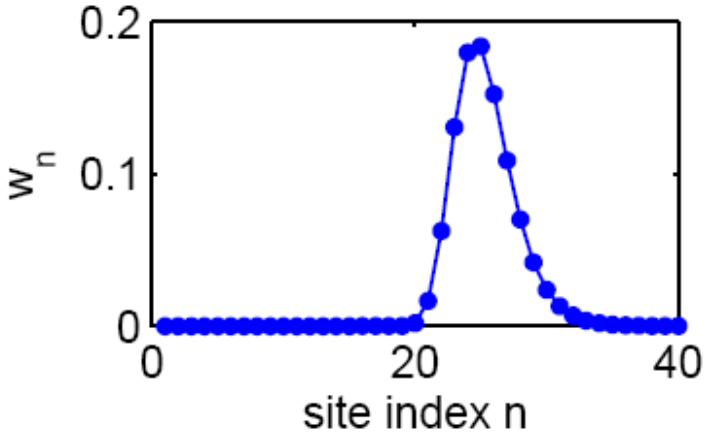
- Full density matrix in NRG state space

$$\rho_T^{(d^N)} \simeq \sum_n \sum_{se} \frac{e^{-\beta E_s^n}}{Z} |se\rangle_n^D \, {}_n^D\langle se|$$

with sum over *discarded* states of shell n with overall weight

$$w_n = \frac{d^{N-n}}{Z} \sum_s^D e^{-\beta E_s^n}$$

degeneracy of remainder of chain



Spectral Function at finite temperature

AW, cond-mat/0607497

$$\mathcal{A}_T(\omega) = \frac{1}{2\pi}\int dt\ \mathbf{tr}\left(\rho_T \bullet e^{iHt}\hat{d}e^{-iHt} \bullet \hat{d}^\dagger\right)e^{i\omega t}$$

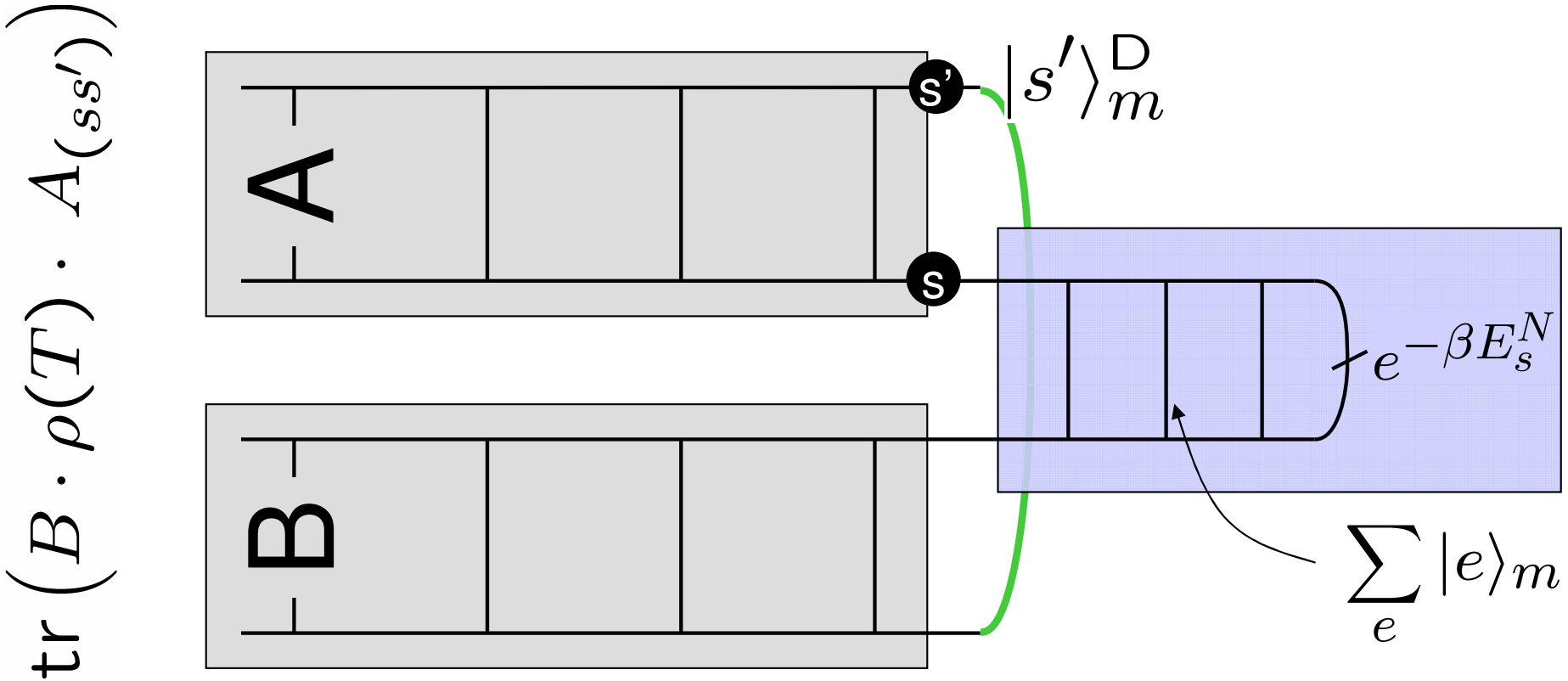
$\mathbb{1}_{(i)}$ $\mathbb{1}_{(j)}$

- ★ insertion of effectively two full identity operators for the **whole** chain
- ★ available in praxis in NRG through emphasis on truncated state space (!) (Anders and Schiller, 2005)

Spectral Function at finite temperature

AW, cond-mat/0607497

$$\mathrm{tr}\left(\rho_T A_{(ij)} B\right)\delta\left(\omega - E_{(ij)}\right) \equiv \mathrm{tr}\left(B\cdot\rho_T\cdot A_{(ss')}\right)\delta\left(\omega - E_{(ss')}\right)$$



collect data in a single sweep along Wilson chain (index m)
using effective density matrices for the remainder of the chain

Results for Correlation Functions
Single Impurity Anderson Model (SIAM)

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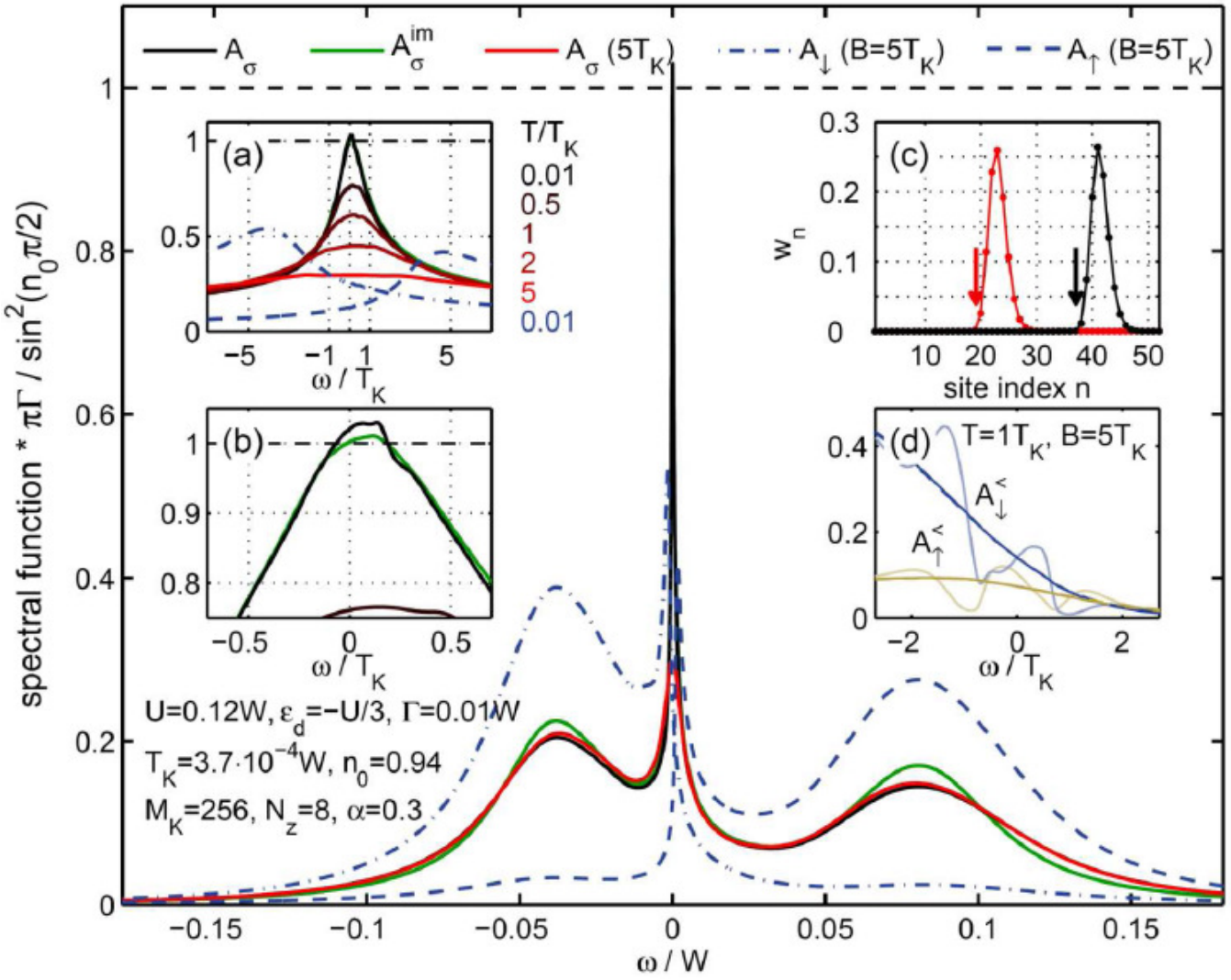

Results for Correlation Functions
Single Impurity Anderson Model (SIAM)

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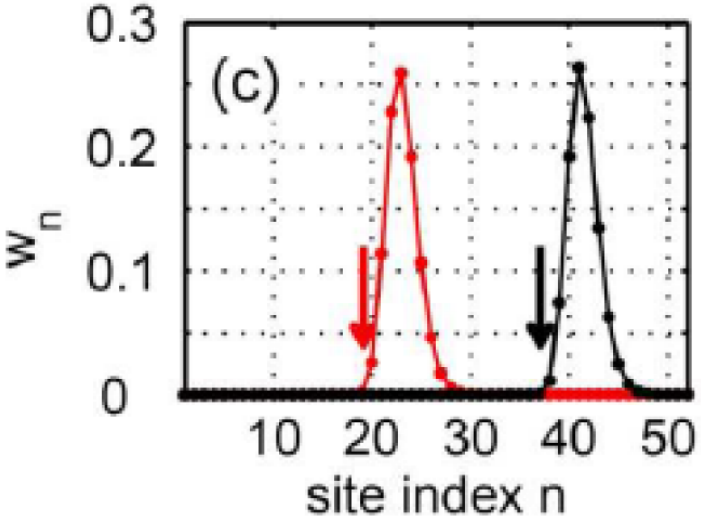
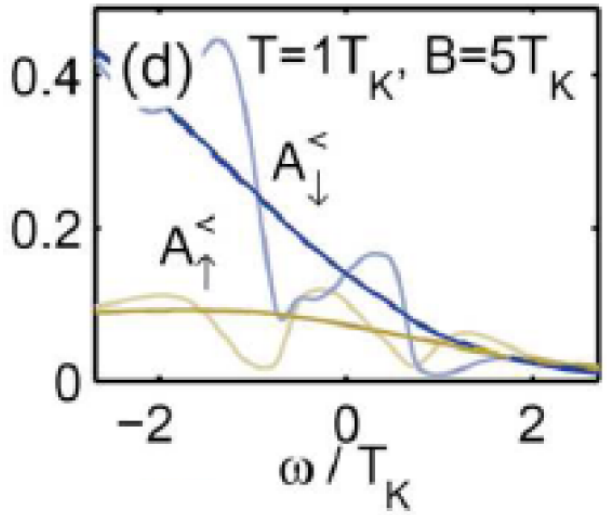


contributions from
window of energy shells (~10 iterations)



significantly improved resolution for $\omega<T$

sum rules are conserved up to
numerical precision (10^{-15})

Summary

- ★ complete basis set on the full Wilson chain numerically tractable!
- ★ Used to **derive** an algorithm to obtain correlation functions
  optimal within NRG framework
  greatly improves for $\omega < T$
- ★ elegant description in terms of Matrix Product States

Outlook

- ★ Time-dependent NRG implemented (Anders and Schiller, 2005) and generalized to full density matrix (vs. single shell approximation)
- ★ Generalization to more than a single time step
- ★ Out of equilibrium in transport

Acknowledgment

Ralf Bulla (Augsburg), Theresa Hecht and Frithjof Anders for fruitful discussions.

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