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Entanglement spectra in the NRG

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Outline

- Brief introduction to the Numerical Renormalization Group (NRG)
  - iterative diagonalization of quantum impurity models
  - energy flow diagram and finite size scaling
  - entanglement entropy and area law
- Natural emergence of reduced density matrices
- Entanglement flow diagram
  - low-energy fixed point spectra
  - Important “feed-back” from small to large energy scales
- Summary and outlook

NRG framework for quantum impurity models

Wilson (1975)

Review Bulla et al. (RMP 2008)

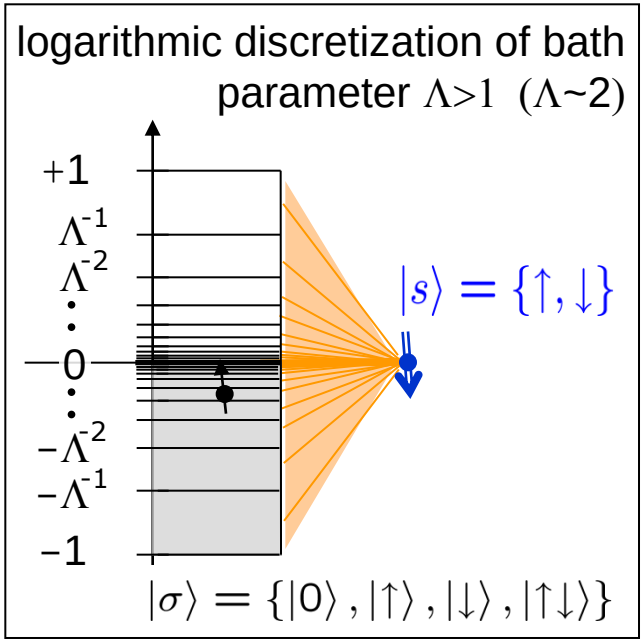
Kondo (1964)

Kondo Hamiltonian

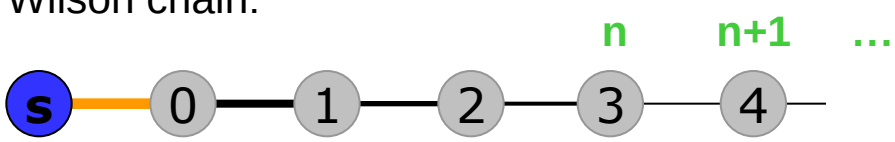
$$\hat{\mathcal{H}} = \mathbf{B}\cdot\hat{\mathbf{s}} + 2J\hat{\mathbf{s}}\cdot\hat{\mathbf{S}} + \int_{-D}^{D} d\epsilon\, \epsilon\, \hat{c}^\dagger_{\epsilon\mu}\hat{c}_{\epsilon\mu}$$

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

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



logarithmic discretization + tridiagonalization
→ Wilson chain:



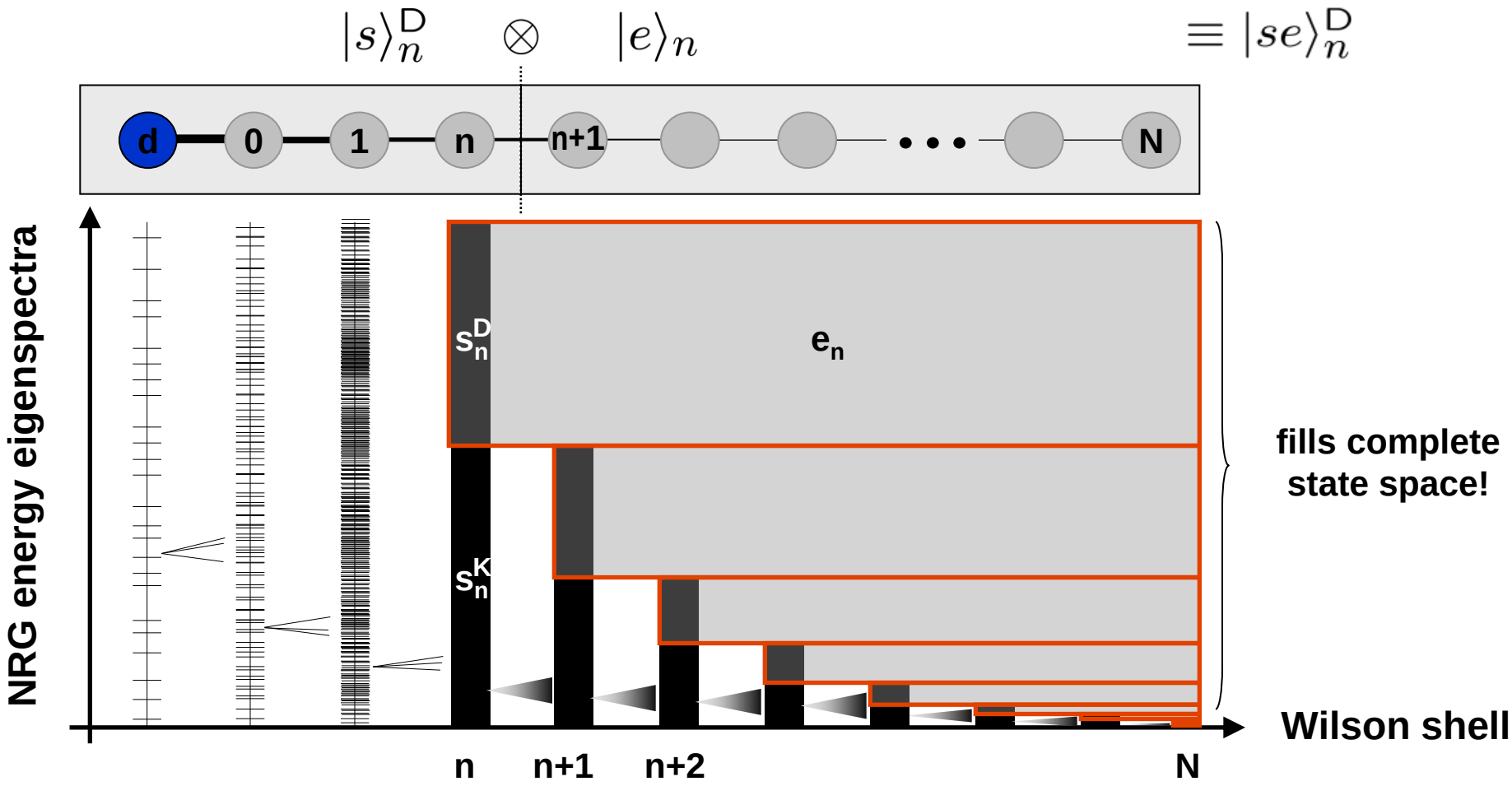
energy scale separation

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

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

Complete basis set on Wilson chain

Anders and Schiller (2005)

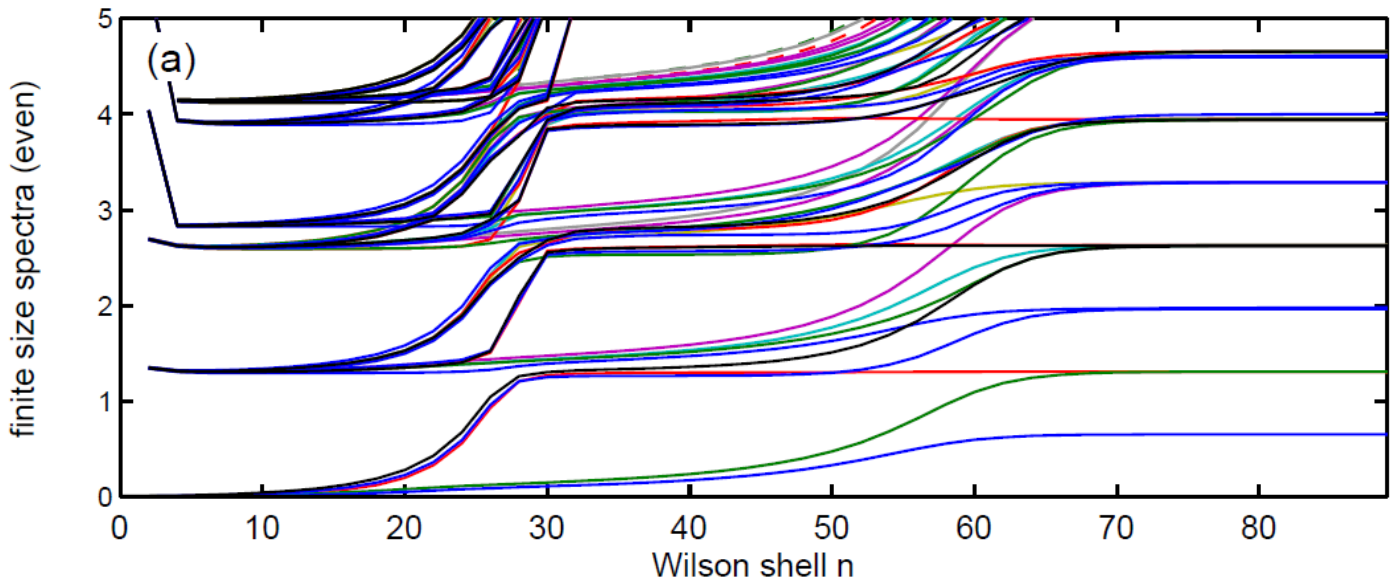


black-box algorithms for dynamical correlation functions (Lehmann representation)
AW and von Delft (2007), Peters et al. (2006), AW (condmat, 2012)

RG analysis: energy flow diagrams

- Single impurity Anderson model

$$\hat{\mathcal{H}} = \sum_{\sigma} \varepsilon_{d\sigma} \hat{n}_{\sigma} + U \hat{n}_{\uparrow} \hat{n}_{\uparrow} + \sqrt{\frac{2\Gamma}{\pi}} \sum_{k,\sigma} \left(\hat{c}^{\dagger}_{k\sigma} \hat{d}_{\sigma} + H.c. \right) + \sum_{k,\sigma} \varepsilon_{k\sigma} \hat{c}^{\dagger}_{k\sigma} \hat{c}_{k\sigma}$$



SIAM:
U=0.00024
ε_d=−U/2
Γ=U/24

free orbital (FO) | local moment (LM) | strong coupling (SC)

Correlation functions (Lehmann representation)

- Correlation functions

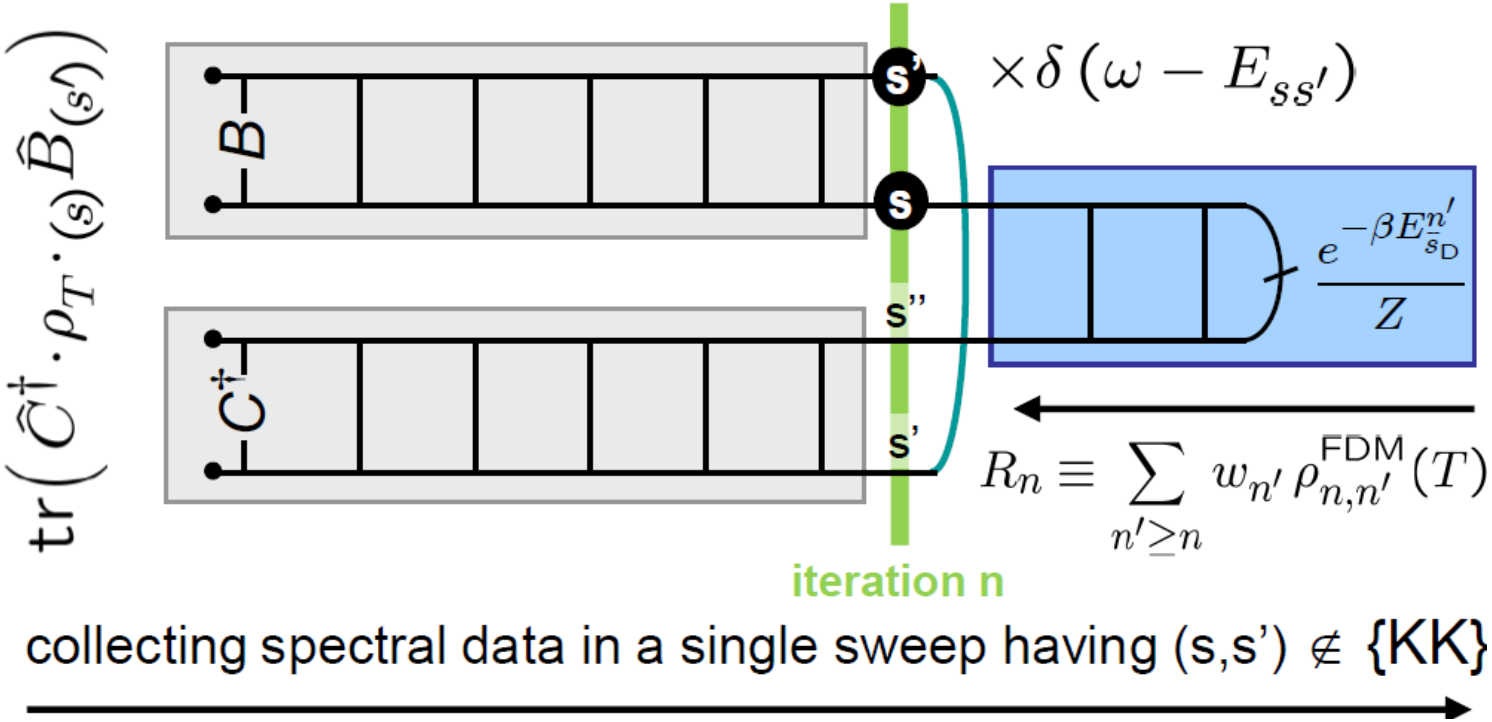
AW and von Delft (PRL 2007)

$$G_d(t) = \langle e^{i\hat{H}t}\hat{d}e^{-i\hat{H}t} \cdot \hat{d}^\dagger \rangle_T$$

$$\rightarrow \quad A_d(\omega) \equiv \int \frac{dt}{2\pi} e^{i\omega t} G_d(t) = \sum_n \sum_{ss' \notin \mathrm{KK},e} \rho^{[n]}_{ss'} \cdot \left| {}_n\langle se|\hat{d}|s'e\rangle_n \right|^2 \cdot \delta(\omega - E_{ss'})$$

$$\int A(\omega) d\omega = \left\langle \{d, d^\dagger\} \right\rangle_T = 1$$

fulfilled up to double precision noise! (10^{-16})

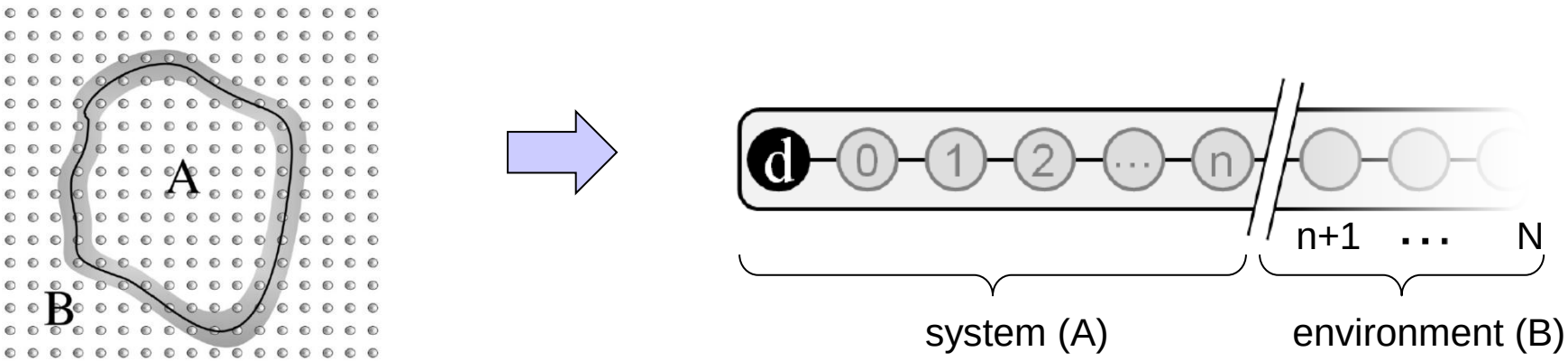


see also DM-NRG (Hofstetter, 2000)

NRG and area law

Verstraete et al. (2005), AW et al. 2007, 2009)

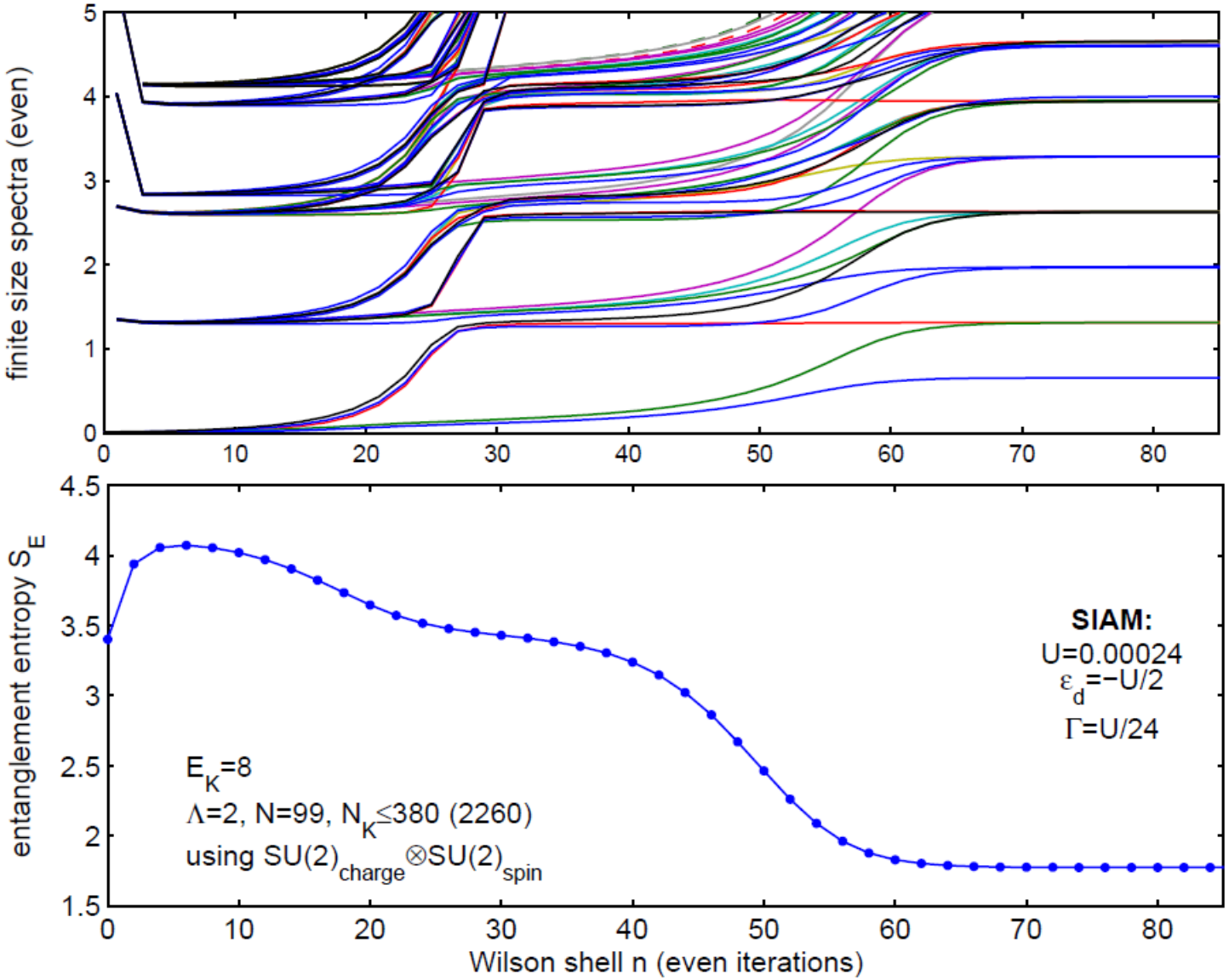
- NRG and DMRG are based on the same algebraic structure: matrix product states (MPS)
- MPS successful in 1D because of area law: entanglement entropy S



$$S = \mathrm{tr}\,(\rho_A \log \rho_A) = \mathrm{tr}\,(\rho_B \log \rho_B)$$
$$\propto \text{area between A and B}$$
$$\lesssim \log L \text{ (for ground states in 1D)}$$

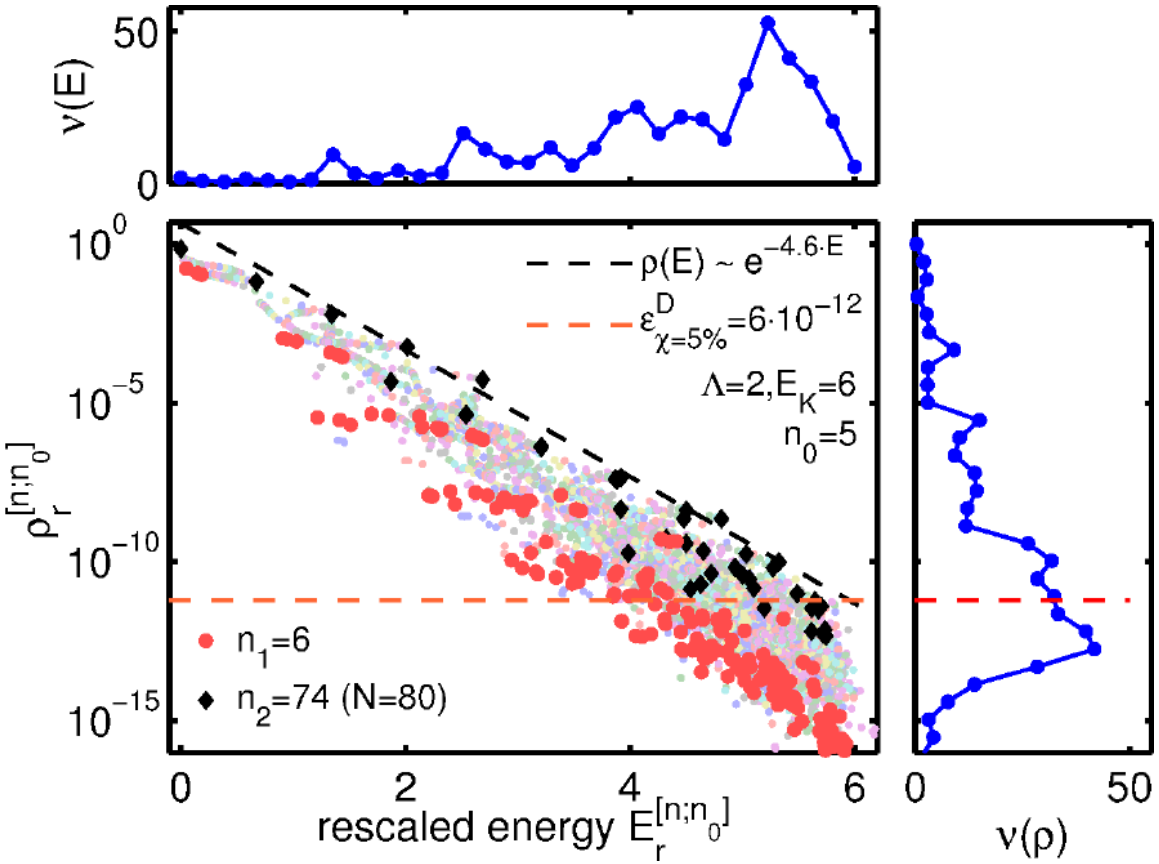
Wolf et al. (PRL 2008); Eisert et al. (RMP 2010)

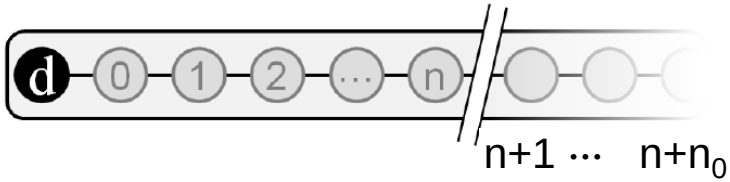
NRG and area laws



calculated w.r.t.
“overall ground state”

Exponentially reduced importance of states at higher energy





For each iteration n:

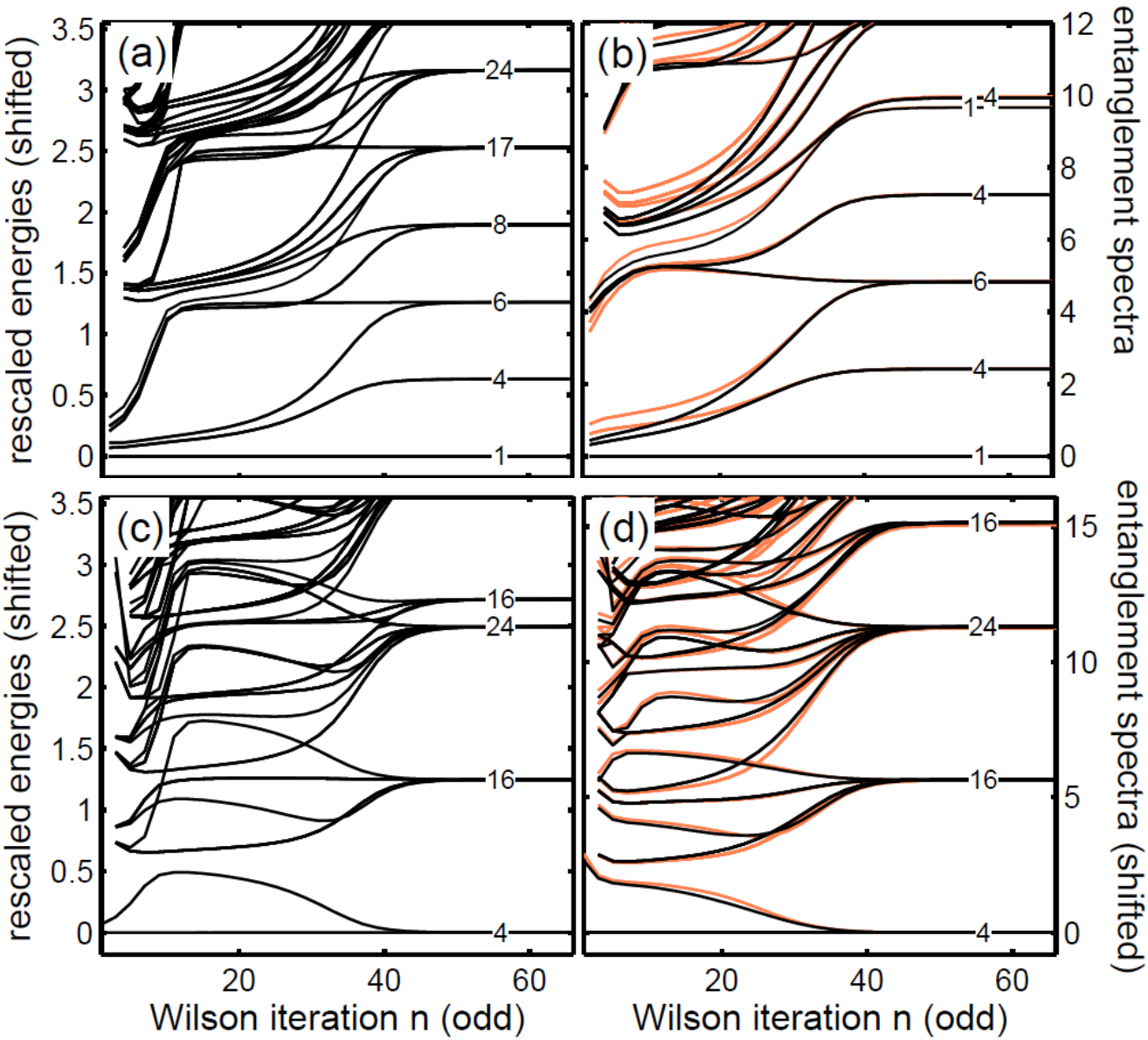
$$\hat{H}|s\rangle = E_s|s\rangle \;\Leftrightarrow\; \rho_s \equiv \langle s|\hat{\rho}|s\rangle$$

$$\boxed{\hat{\rho}|r\rangle = \rho_r|r\rangle \;\Leftrightarrow\; E_r \equiv \langle r|\hat{H}|r\rangle}$$

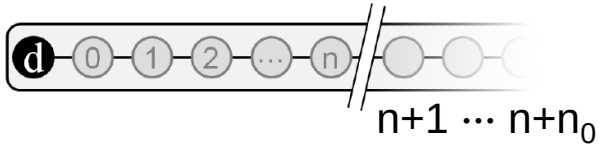
eig(ρ) decays exponentially with excitation energy (non-gapped system!)

⇨ a consequence of energy scale separation

Entanglement flow diagram (SIAM, B=0)



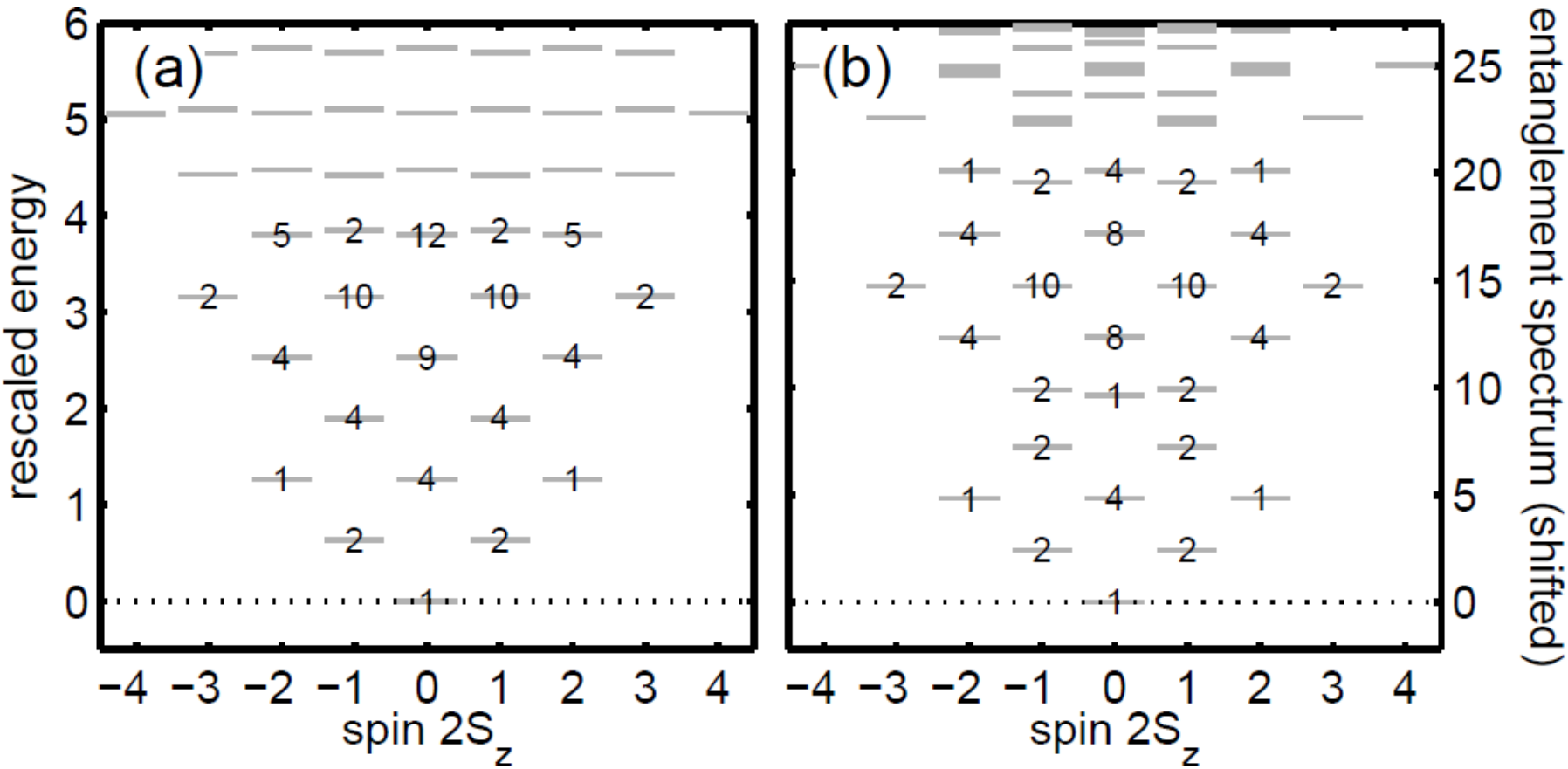
Entanglement spectra
Li, Haldane (2008)



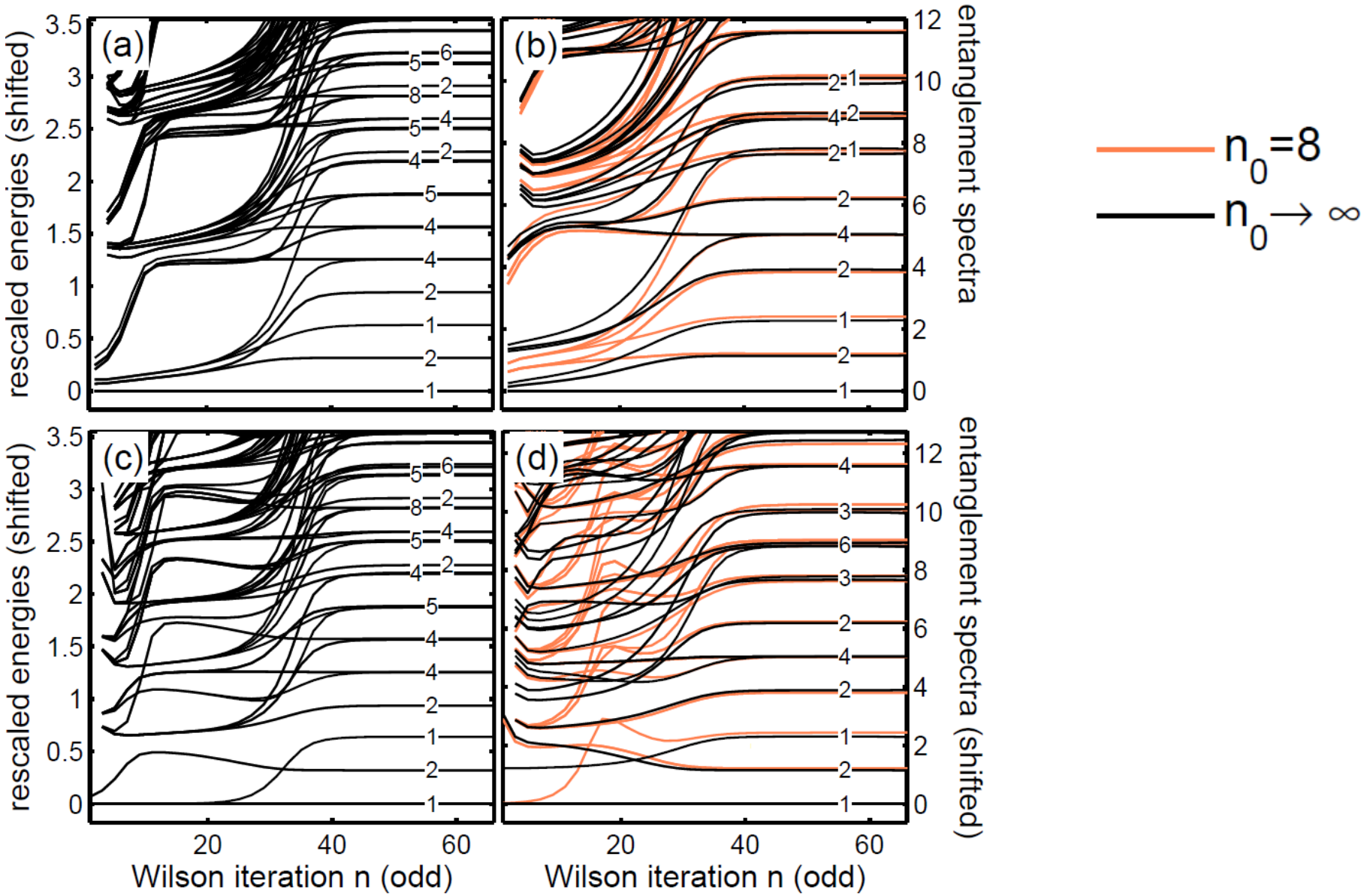
$n_0=8$

$n_0 \to \infty$

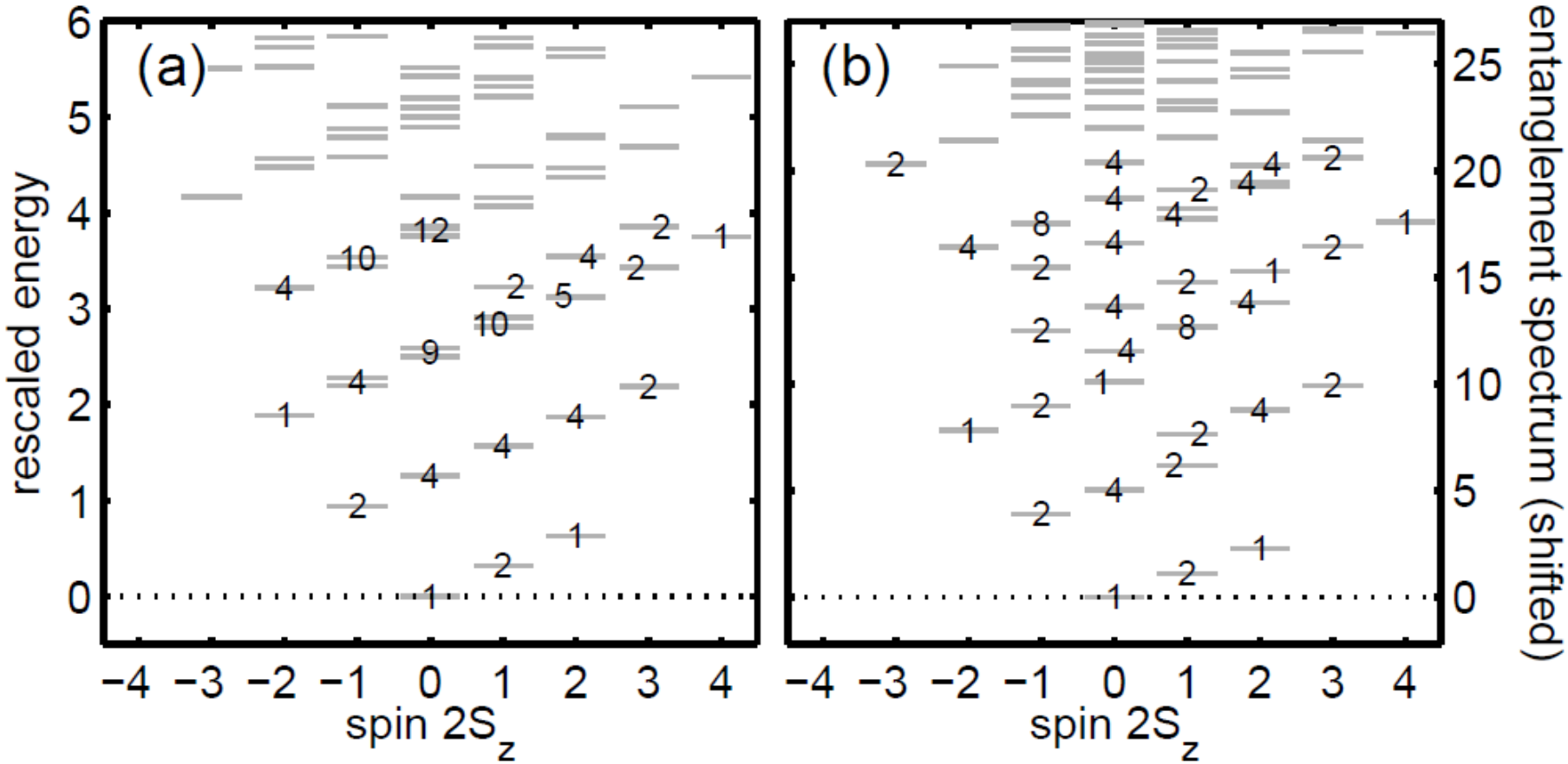
Strong coupling fixed point spectra (SIAM, B=0)



Entanglement flow diagram (SIAM, B>0)

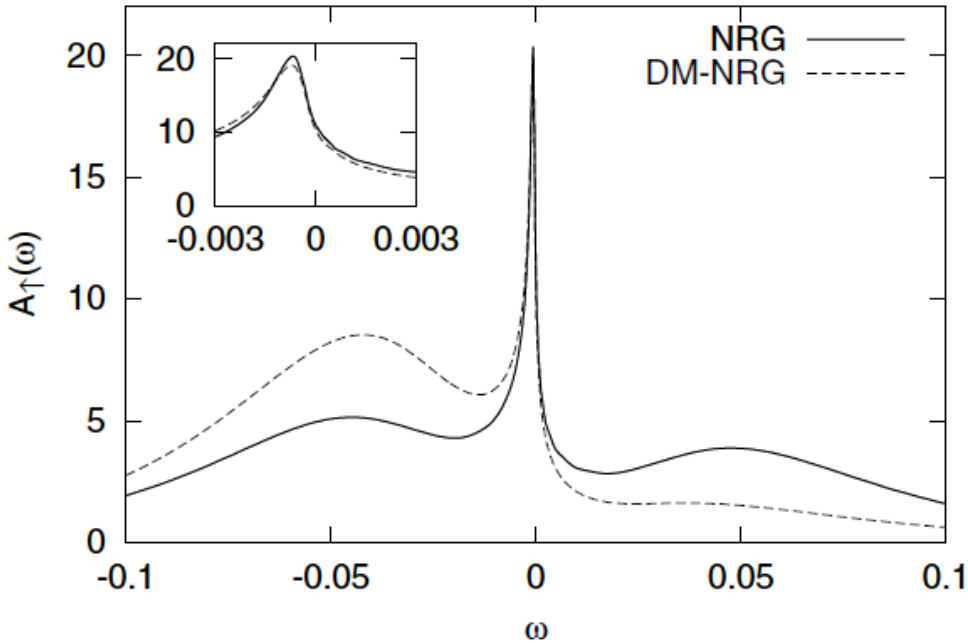


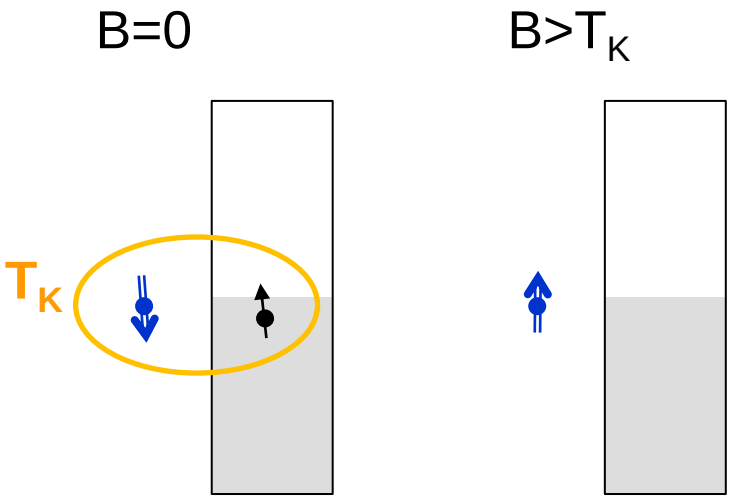
Entanglement spectra (SIAM, B>0)



Important "feed-back" from small to large energy scales

DM-NRG (Hofstetter 2000): $B \lesssim T_K$

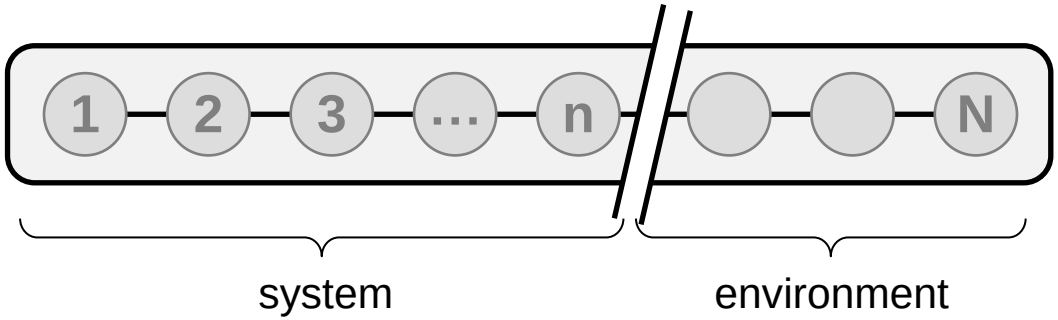




- requires reduced density matrices which *properly* encode the low-energy physics
- the resulting DM is *not necessarily* a thermal density matrix at intermediate iteration n!
- important for DMFT in the presence of (small) symmetry breaking perturbations

Implications

- Within NRG / DMRG / VMPS / PEPS typically got *both*: $\mathbf{H_{eff}(n)}$ and $\boldsymbol{\rho}\mathbf{(n)}$



- Q. How does $H_{eff}(n)$ compare with entanglement Hamiltonian of $\rho(n)$?

- Taking overall ground state: if $H_{eff}(n)$ differs strongly from the entanglement Hamiltonian of $\rho(n)$, this indicates
  - importance of physics at significantly smaller energy scale
  - not just finite size effect: also affects dynamics at large energies

Summary and Outlook

AW, PRB **84**, 125130 (2011)

- Analyzed entanglement spectra within the NRG
  - unique perspective: H_{eff} (n) built from *large* energies
  - ρ_{red}(n) represents the traced out *low-energy* physics
- Two regimes at higher energies
  - entanglement spectrum ES[ρ_{red}(n)] w.r.t. overall ground state does / does not agree with eigenspectrum of H_{eff}(n)
- Clear relevance for dynamical quantities at finite (high) energies
- Linked to "further relevant information" at the low-energy scale

Outlook

- "non-thermal" reduced density matrices
- better quantitative understanding of connection between H_{eff} (n) and ρ_{red}(n)

Acknowledgment

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