Numerical methods for low-dimensional quantum spin systems

$$\begin{pmatrix} h_{1,1} & h_{1,2} & \cdots & h_{1,n-1} & h_{n,n} \\ h_{2,1} & h_{2,2} & \cdots & h_{2,n-1} & h_{2,n} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ h_{n-1,1} & h_{n-1,2} & \cdots & h_{n-1,n-1} & h_{n-1,n} \\ h_{n,1} & h_{n,2} & \cdots & h_{n,n-1} & h_{n,n} \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_{n-1} \\ v_n \end{pmatrix}_\mu = E_\mu \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_{n-1} \\ v_n \end{pmatrix}_\mu$$

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Numerical methods: Overview

A) Wave-function based approaches:

$$H|\psi_n\rangle = E_n|\psi_n\rangle$$

→ Exact diagonalization: L~42

Sandvik, AIP Conf. Proc. 1297, 135 (2010), Prelovšek, Bonča, arXiv:1111.5931

→ Density matrix renormalization group (DMRG) method: L~100

Schollwöck Rev. Mod. Phys. 77, 259 (2005) & Ann. Phys. (NY) 326, 96 (2011)

B) Partition function-based techniques:

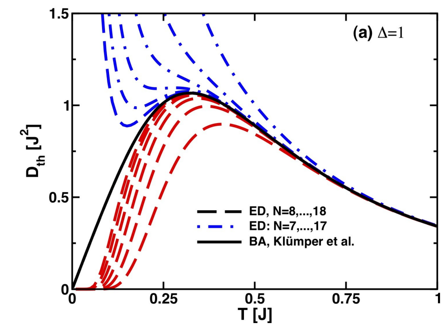
$$Z(\beta) = \exp(-\beta H)$$

→ Quantum Monte Carlo – Stochastic Series Expansion
→ Series Expansion

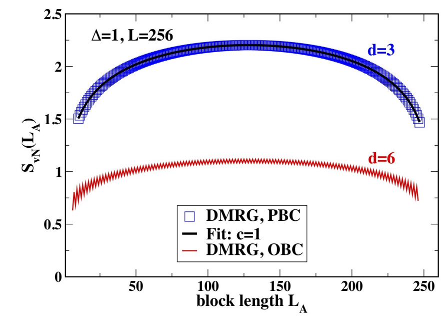
see, e.g., Oitmaa, Hamer, Zheng:
Series Expansion Methods for Strongly Interacting Lattice Models

Outline

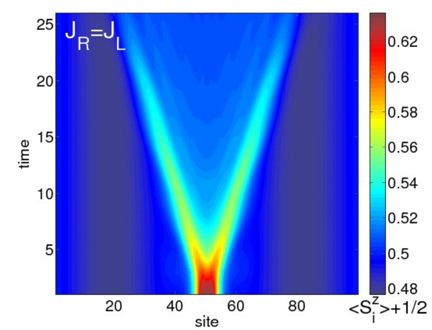
Part 1: Exact diagonalization
- Lanczos and complete ED
- Thermodynamics
- Transport coefficients



Part 2: DMRG
- Matrix Product States
- Ground-state energies
- Entanglement
- Correlation functions



Part 3: Time-dependent DMRG
- Non-equilibrium dynamics
- Spectral functions
- Finite temperatures
- Current auto-correlations



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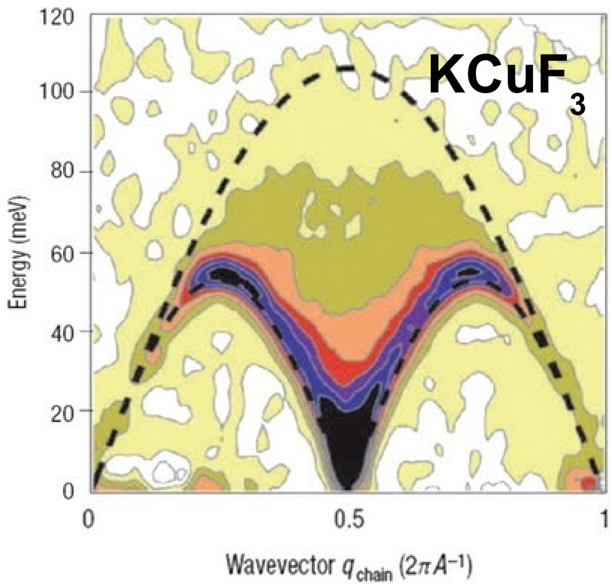
Heisenberg model

$$H = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_{i+1}$$



Tennant, Perring, Cowley, Nagler PRL 1993

1D, spin-½ XXZ chain:

$$H = J \sum_{i=1}^{L} \left[\frac{1}{2} \left(S_i^+ S_{i+1}^- + h.c. \right) + \Delta S_i^z S_{i+1}^z \right]$$

Quantum phases:

Excitations: Spinons

easy-plane, critical | AFM, gapped

$\Delta = 0$ — $\Delta = 1$ — Δ

free fermions

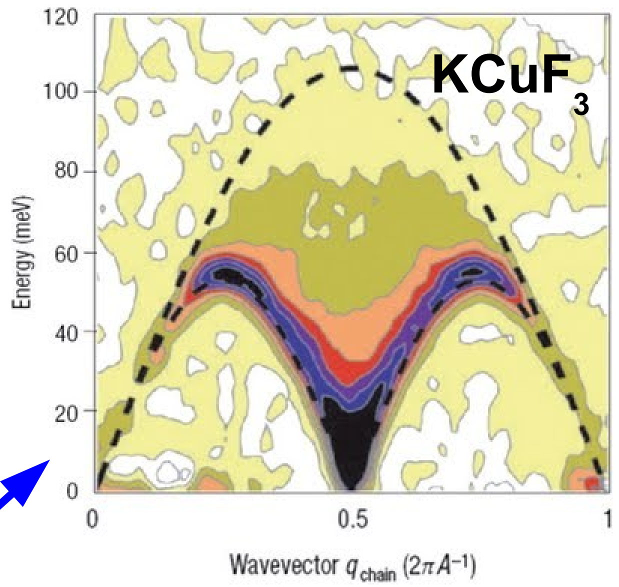
$\Delta = \infty$: Ising

Heisenberg model

$$H = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_{i+1}$$

1D, spin-½ XXZ chain:

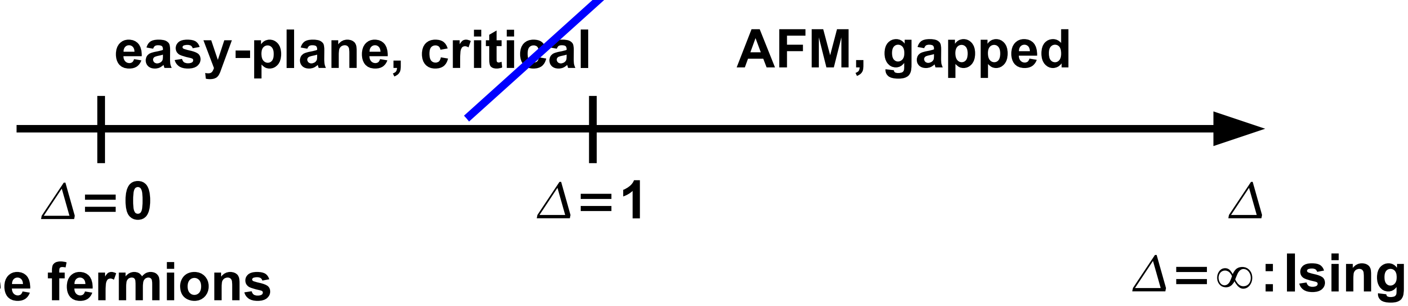
$$H = J \sum_{i=1}^{L} \left[\frac{1}{2} \left(S_i^+ S_{i+1}^- + h.c. \right) + \Delta S_i^z S_{i+1}^z \right]$$



Tennant, Perring, Cowley, Nagler PRL 1993

Quantum phases:

Excitations: Spinons



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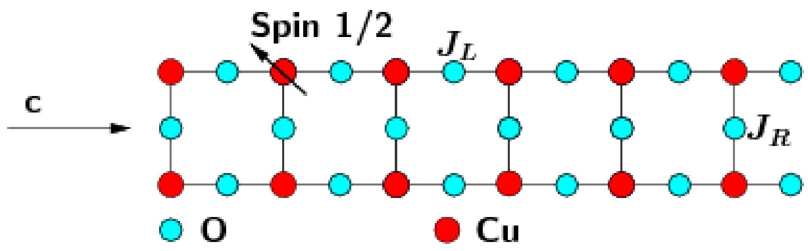
Lattice geometries

Lattice: any quasi-1D system:

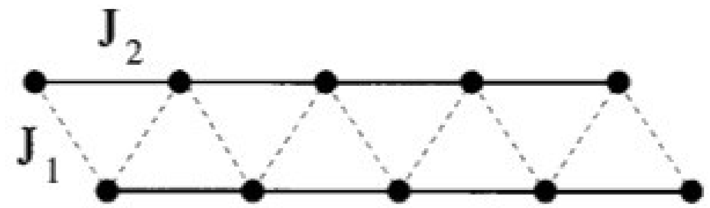


Ladders Noack, White, Dagotto, ...

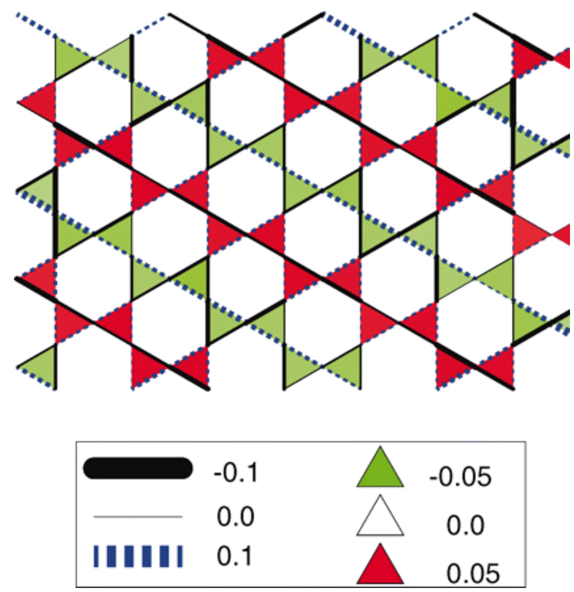
Zylinders (2D), e.g. Kagome
Square lattice

White, Chernyshev PRL 2008
Yan, Huse, White Science 2011

Frustrated systems



White, Affleck PRB 1996



Part 1:
Exact diagonalization

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Lanczos algorithm

Original Hamiltonian | **Tridiagonal matrix** | **diagonal**

$$\begin{pmatrix} h_{1,1} & h_{1,2} & \cdots & h_{1,n-1} & h_{n,n} \\ h_{2,1} & h_{2,2} & \cdots & h_{2,n-1} & h_{2,n} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ h_{n-1,1} & h_{n-1,2} & \cdots & h_{n-1,n-1} & h_{n-1,n} \\ h_{n,1} & h_{n,2} & \cdots & h_{n,n-1} & h_{n,n} \end{pmatrix} \longrightarrow \begin{pmatrix} \alpha_0 & \beta_0 & 0 & \ddots & \ddots & \ddots \\ \beta_0 & \alpha_1 & \beta_1 & 0 & \ddots & \ddots \\ 0 & \beta_1 & \ddots & \ddots & \ddots & \ddots \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ \ddots & \ddots & \ddots & \beta_{d-2} & \alpha_{d-1} & \beta_{d-1} \\ \ddots & \ddots & \ddots & 0 & \beta_{d-1} & \alpha_d \end{pmatrix} \longrightarrow \begin{pmatrix} E_0 & 0 & \ddots & \ddots & \ddots \\ 0 & E_2 & 0 & \ddots & \ddots \\ \ddots & \ddots & \ddots & \ddots & \ddots \\ \ddots & \ddots & \ddots & E_{d-1} & 0 \\ \ddots & \ddots & \ddots & 0 & d_d \end{pmatrix}$$

$\mathbf{dim = 2^L}$ $\mathbf{dim \sim 10^2 \cdots 10^3}$

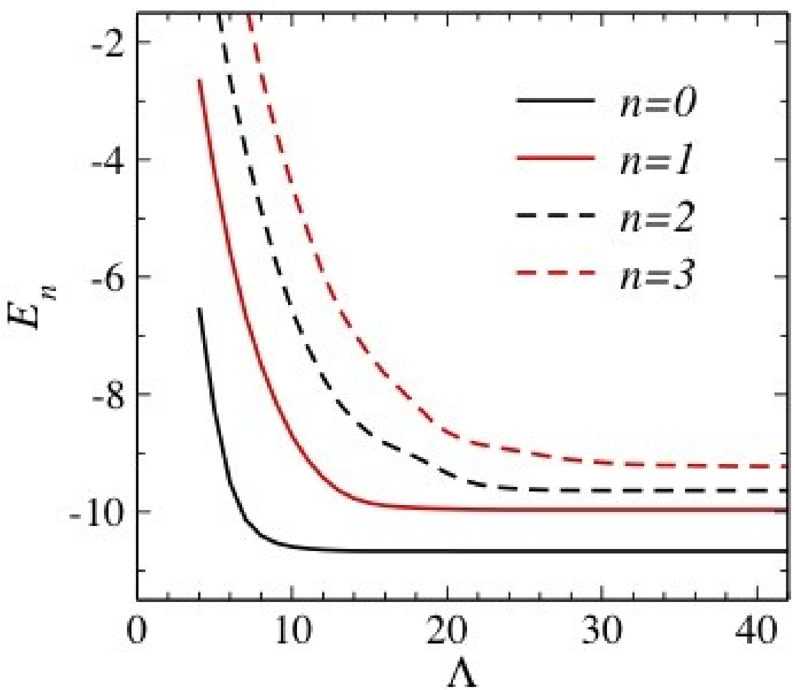
$|\psi_n\rangle = |\uparrow\downarrow\uparrow\uparrow\downarrow\cdots\rangle$ ⟶ **Krylov basis** $|f_i\rangle$ ⟶ $E_0, |\psi_0\rangle$

$$|f_{i+1}\rangle = H|f_i\rangle - \alpha_i|f_i\rangle - \beta_{i-1}^2|f_{i-1}\rangle$$

(random $|f_0\rangle$)

Lanczos algorithm

Convergence



(dim of tri-diag matrix)

24 sites, Sandvik, AIP Conf. Proc. 2011

This works because

$$H|\psi_n\rangle = E_n|\psi_n\rangle$$

$$H^{\Lambda}|\psi\rangle = \sum_{n=0}^{\dim-1} c_n E_n^{\Lambda}|\psi_n\rangle$$

$$\rightarrow c_{max} E_{max}\left[|\psi_{max}\rangle + \sum_{n\neq max} \frac{c_n}{c_{max}}\left(\frac{E_n}{E_{max}}\right)^{\Lambda}|\psi_n\rangle\right]$$

→ Method projects out states with small eigenvalues $|E_n|<|E_{max}|$

Works well for sparse matrices
Problem: orthogonality of states

Exploiting symmetries

$$[H,Q]=0$$

$$\begin{pmatrix} h_{1,1} & h_{1,2} & \cdots & h_{1,n-1} & h_{n,n} \\ h_{2,1} & h_{2,2} & \cdots & h_{2,n-1} & h_{2,n} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ h_{n-1,1} & h_{n-1,2} & \cdots & h_{n-1,n-1} & h_{n-1,n} \\ h_{n,1} & h_{n,2} & \cdots & h_{n,n-1} & h_{n,n} \end{pmatrix} \longrightarrow \begin{pmatrix} \begin{bmatrix} Q_1 \end{bmatrix} & \begin{bmatrix} 0 \end{bmatrix} & \begin{bmatrix} 0 \end{bmatrix} & \begin{bmatrix} 0 \end{bmatrix} & \begin{bmatrix} 0 \end{bmatrix} \\ \begin{bmatrix} 0 \end{bmatrix} & \begin{bmatrix} Q_2 \end{bmatrix} & \begin{bmatrix} 0 \end{bmatrix} & \begin{bmatrix} 0 \end{bmatrix} & \begin{bmatrix} 0 \end{bmatrix} \\ \ddots & \ddots & \ddots & \ddots & \ddots \\ \begin{bmatrix} 0 \end{bmatrix} & \begin{bmatrix} 0 \end{bmatrix} & \begin{bmatrix} 0 \end{bmatrix} & \begin{bmatrix} Q_{l-1} \end{bmatrix} & \begin{bmatrix} 0 \end{bmatrix} \\ \begin{bmatrix} 0 \end{bmatrix} & \begin{bmatrix} 0 \end{bmatrix} & \begin{bmatrix} 0 \end{bmatrix} & \begin{bmatrix} 0 \end{bmatrix} & \begin{bmatrix} Q_l \end{bmatrix} \end{pmatrix}$$

Block-diagonal matrix:
Diagonalize blocks separately

Typically:

- Total S^z
- Translational invariance
- Spin-inversion
- SU(2)
- …

State-of-the-art:

L~42 sites

Richter, Schulenburg, Honecker, Schmalfuß
Phys. Rev. B 70, 174454 (2004)
Laeuchli, unpublished

For applications, see Prelovšek, Bonča, arXiv:1111.5931, Dagotto RMP 1994

Complete diagonalization

$$\begin{pmatrix} h_{1,1} & h_{1,2} & \cdots & h_{1,n-1} & h_{n,n} \\ h_{2,1} & h_{2,2} & \cdots & h_{2,n-1} & h_{2,n} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ h_{n-1,1} & h_{n-1,2} & \cdots & h_{n-1,n-1} & h_{n-1,n} \\ h_{n,1} & h_{n,2} & \cdots & h_{n,n-1} & h_{n,n} \end{pmatrix} \longrightarrow \quad \textbf{all } n \ \{E_i, |\psi_i\rangle\}$$

→ **Problem is – again – to set-up H in block-diagonal form lapack does the rest**

→ **Finite temperatures**

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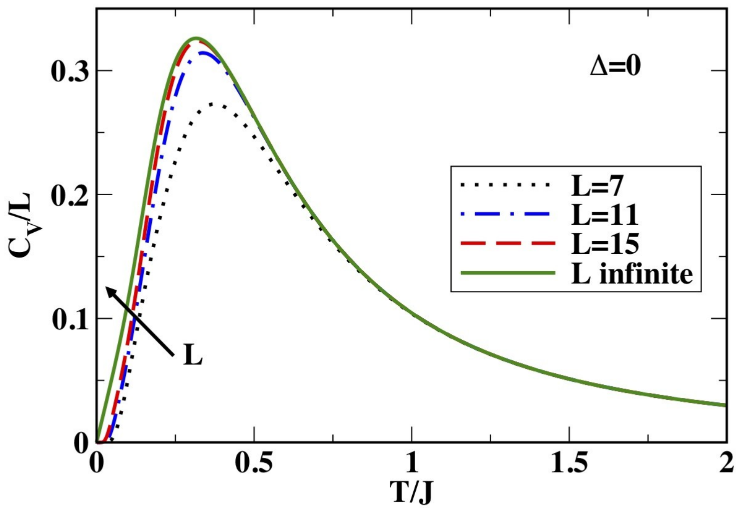
Examples: Thermodynamics

XXZ chain at $\Delta=0$

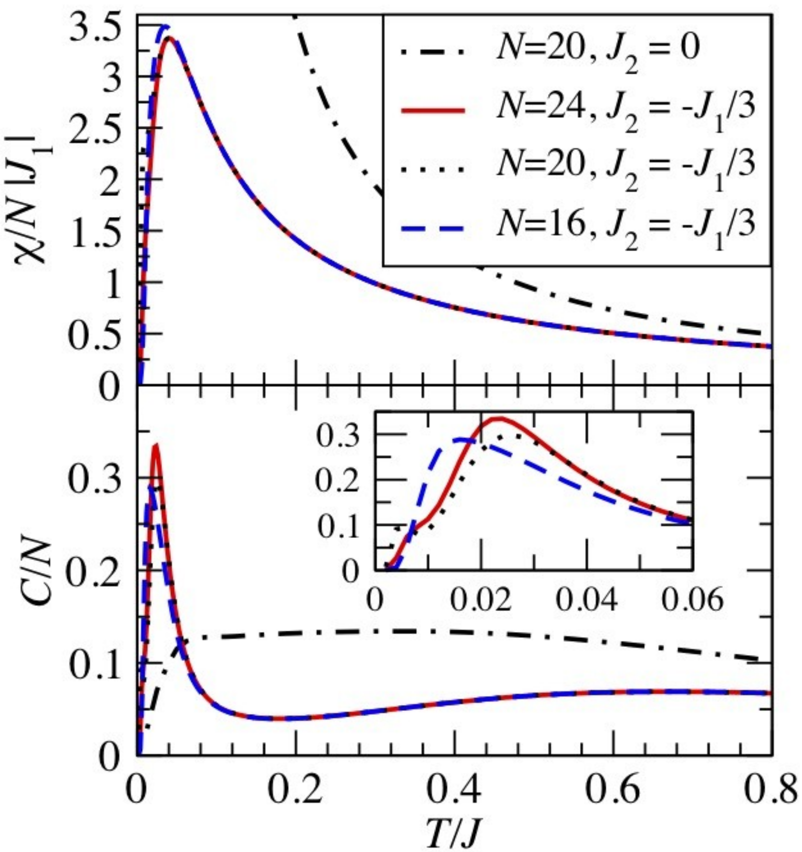
$$C_V = \frac{\langle H^2\rangle - \langle H\rangle^2}{(k_B T)^2};\ \langle H\rangle = \sum_n E_n \frac{e^{-\beta E_n}}{Z(\beta)}$$



Hauschild, Bachelor thesis, LMU 2012

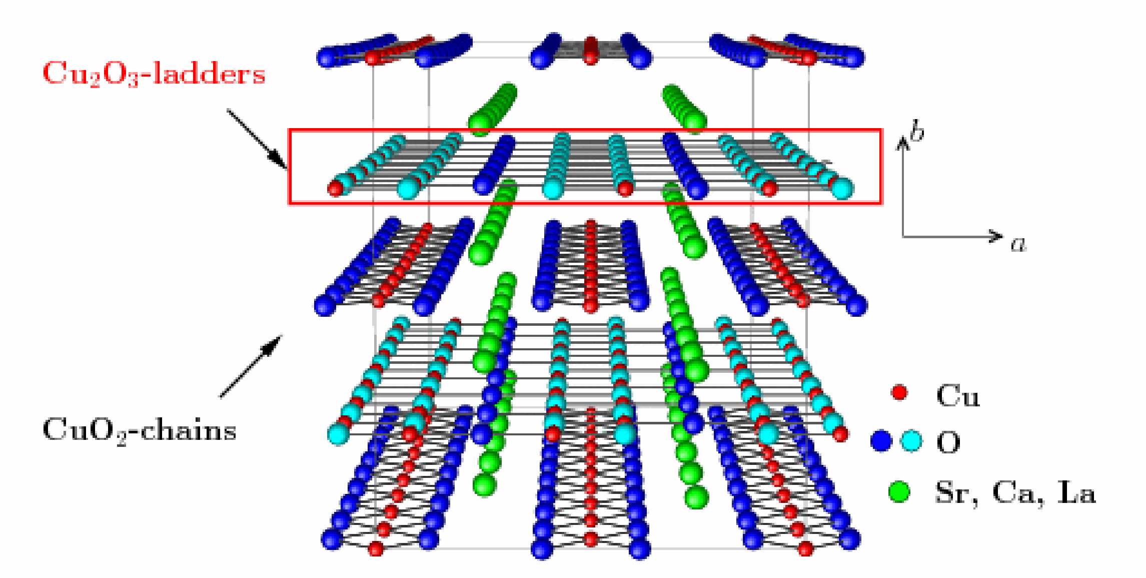
Frustrated FM chain

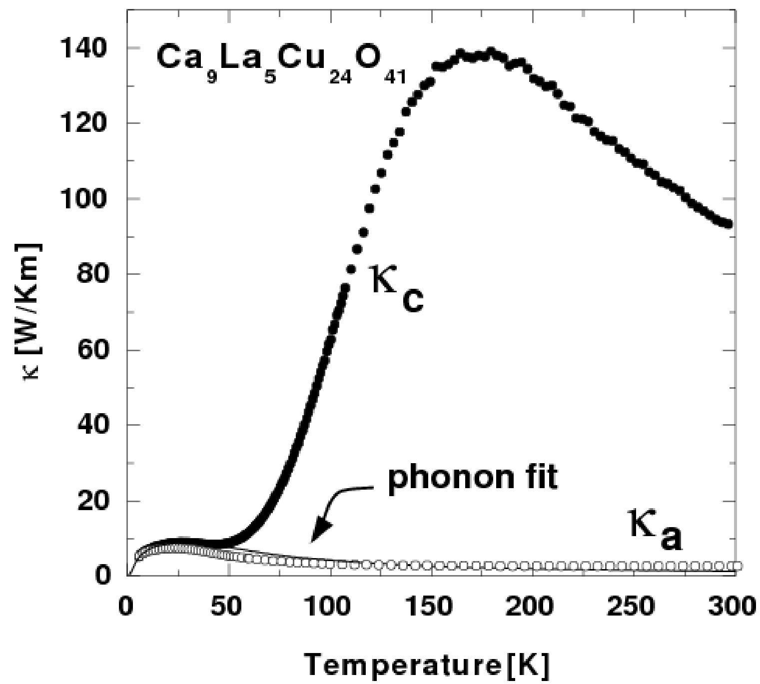
$L \leq 24$



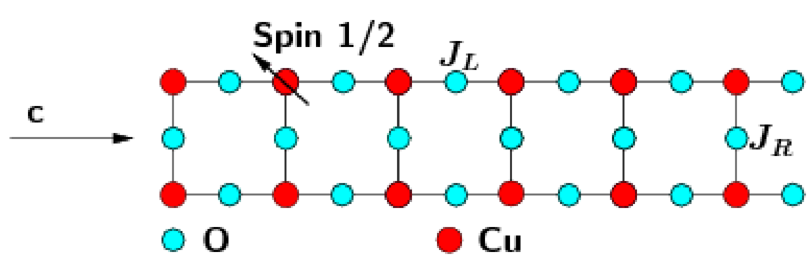
HM, Honecker, Vekua PRB 74, 020403 (2006)

Magnetic heat transport in ladder systems





spin-½ moments on Cu sites



Large "magnon" thermal conductivity

Hess et al. PRB 2001

Theory on ladders: HM et al. PRB 2003; Zotos PRL 2004; Boulat et al. PRB 2007

Examples: Transport coefficients

Thermal conductivity

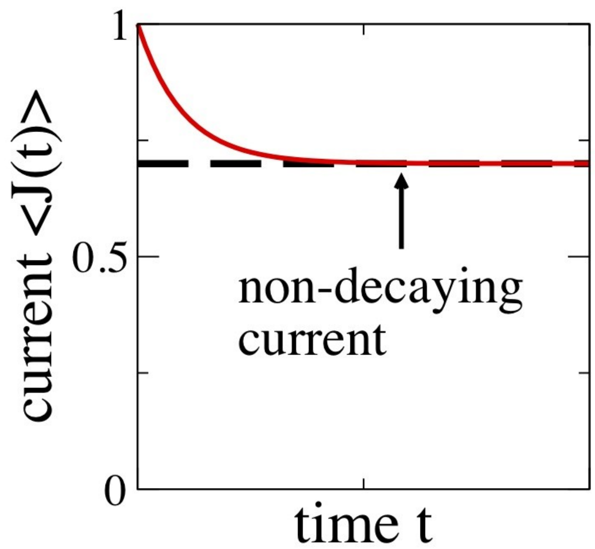
$$\kappa(\mathbf{T},\omega)=\mathbf{D_{th}}(\mathbf{T})\,\delta(\omega)$$

↑

divergent because

$$[\mathbf{H},\mathbf{J_E}]=\mathbf{0}$$

Zotos, Naef, Prelovšek
PRB 1997



Spin conductivity

$$\sigma(\mathbf{T},\omega)=\mathbf{D_s}(\mathbf{T})\,\delta(\omega)+\sigma_{\mathbf{reg}}(\omega)$$

↑

$\langle \mathbf{S^z}\rangle \neq \mathbf{0} \Rightarrow \mathbf{D_s} > \mathbf{0}$ **Zotos et al. PRB 1997**

$\langle \mathbf{S^z}\rangle = \mathbf{0}$

Drude weight
non-zero for |Δ|<1
Δ=1 still controversial

→ Ballistic transport at finite T

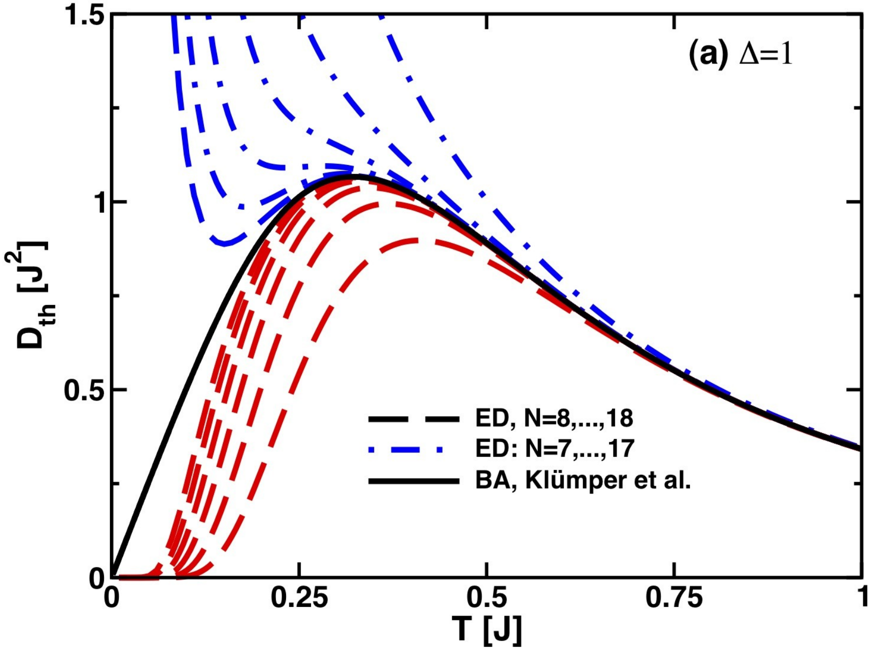
→ Prosen's talk!
PRL 2011

$$\sigma(\omega)\sim\int^{\infty}\mathbf{dt}\,\mathbf{e}^{-\mathbf{i}\omega\mathbf{t}}\int_{\mathbf{0}}^{\beta}\mathbf{d}\tau\,\langle \mathbf{J}\,\mathbf{J}(\mathbf{t}+\mathbf{i}\tau)\rangle$$

Examples: Transport coefficients

Thermal conductivity

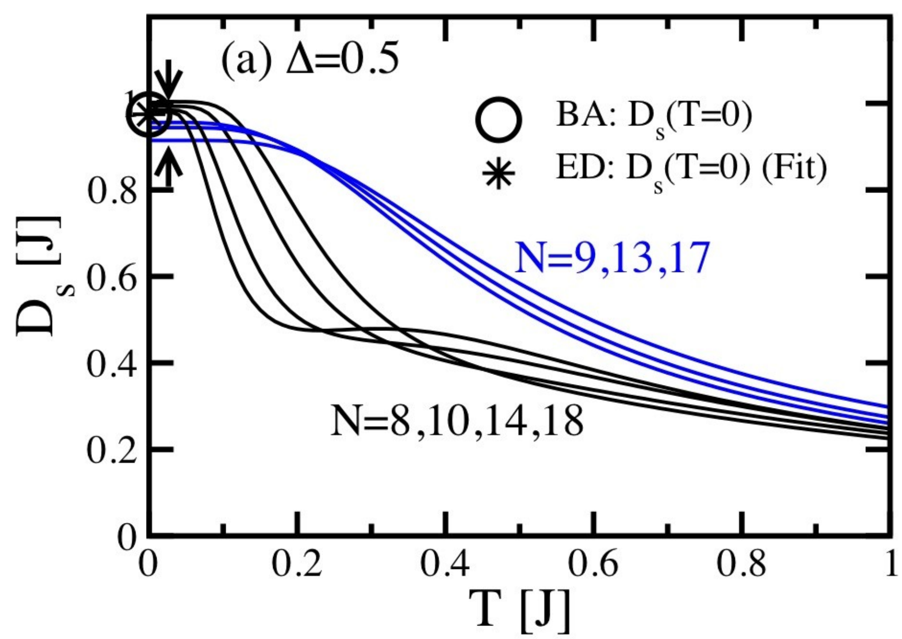
$$\kappa(T,\omega) = D_{th}(T)\,\delta(\omega)$$



HM, Honecker, Cabra, Brenig PRB 2002
Klümper, Sakai J Phys. A 2002

Spin conductivity

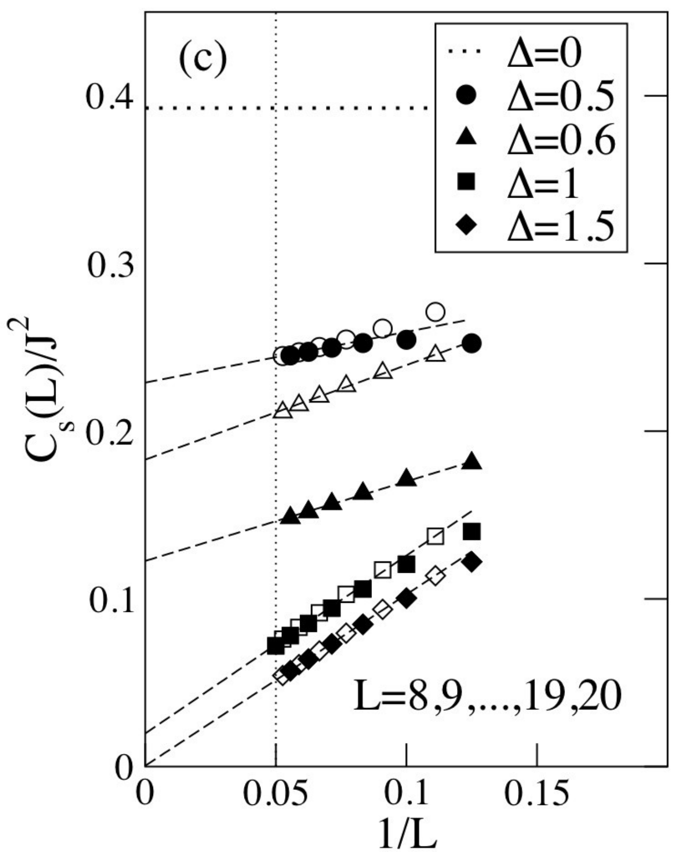
$$\sigma(T,\omega) = D_s(T)\,\delta(\omega) + \sigma_{reg}(\omega)$$



HM, Honecker, Cabra, Brenig PRB 2003

Examples: Spin Drude weight

$$D_s = \frac{\pi \beta}{L Z(\beta)} \sum_{S^z} \sum_{\substack{n,m \\ E_n = E_m}} e^{-\beta E_n} |\langle n | J | m \rangle|^2$$



Finite-size scaling at infinite T for $|\Delta| \leq 1$:

$$C_s = \lim_{T \to \infty} [T D_s(T)] > 0$$

HM, Honecker, Cabra, Brenig PRB 2003
HM, Honecker, Brenig EPJST 2007

At $\Delta = 1$, using canonical ensemble in $S^z = ½$:

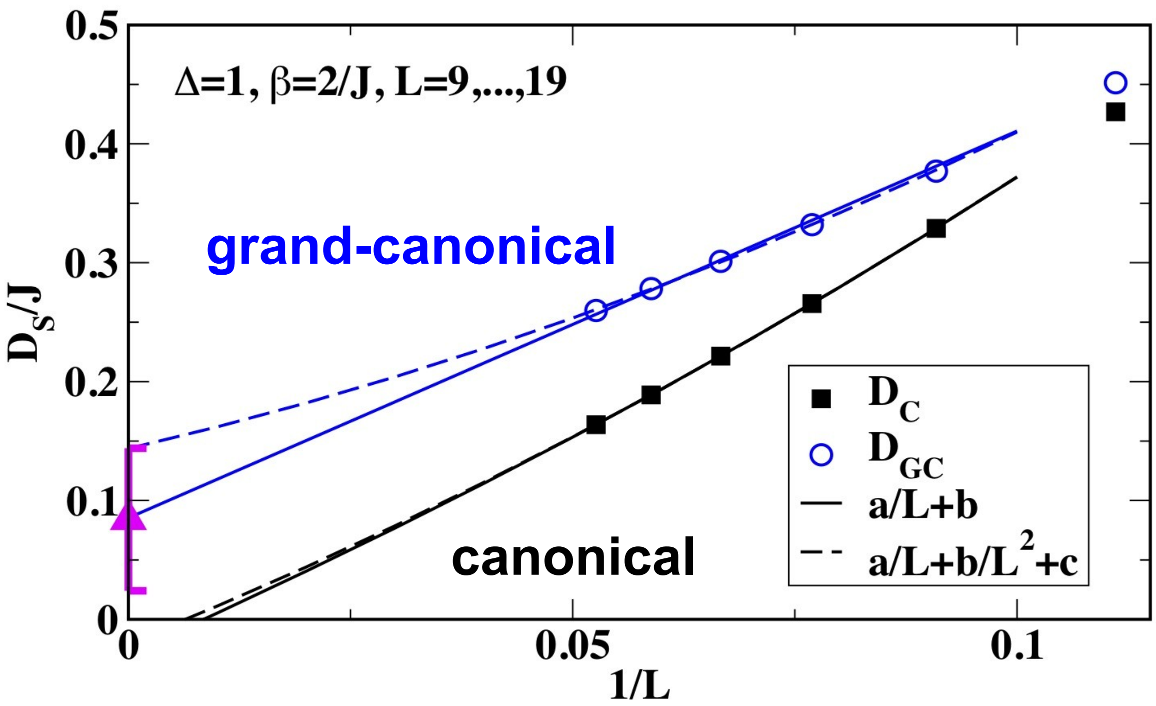
$$C_s \to_{L \to \infty} 0$$

Herbrych, Prelovšek, Zotos PRB 2011
Agrees with Zotos PRL 1999

See also Zotos, Prelovšek PRB 1996, Narozhny et al PRB 1998

Examples: Spin Drude weight

$$D_s = \frac{\pi\beta}{LZ(\beta)} \sum_{S^z} \sum_{\substack{n,m \\ E_n = E_m}} e^{-\beta E_n} |\langle n|J|m\rangle|^2$$



We need a theory for $D_s = D_s(L)$!

… so the Drude weight story continues …

Examples: Transverse current-autocorrelations

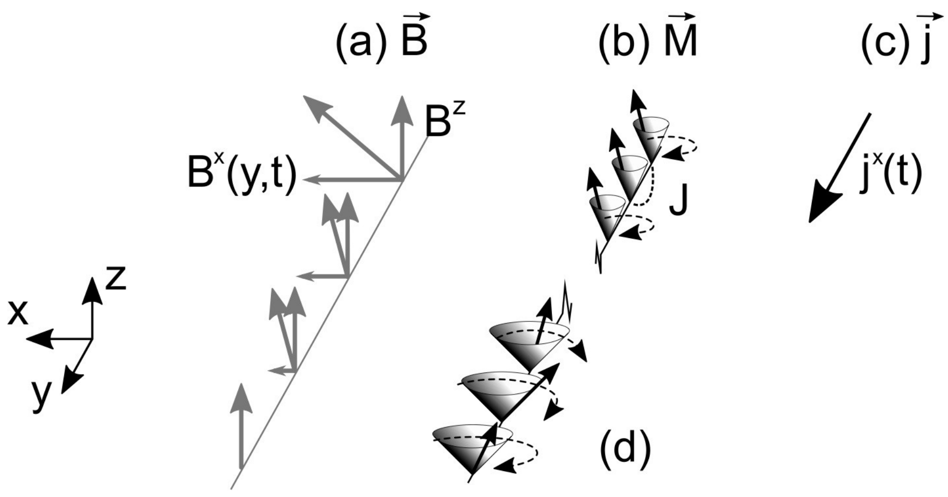
$$\vec{j} = i \sum_r \vec{S}_r \times \vec{S}_{r+1}$$

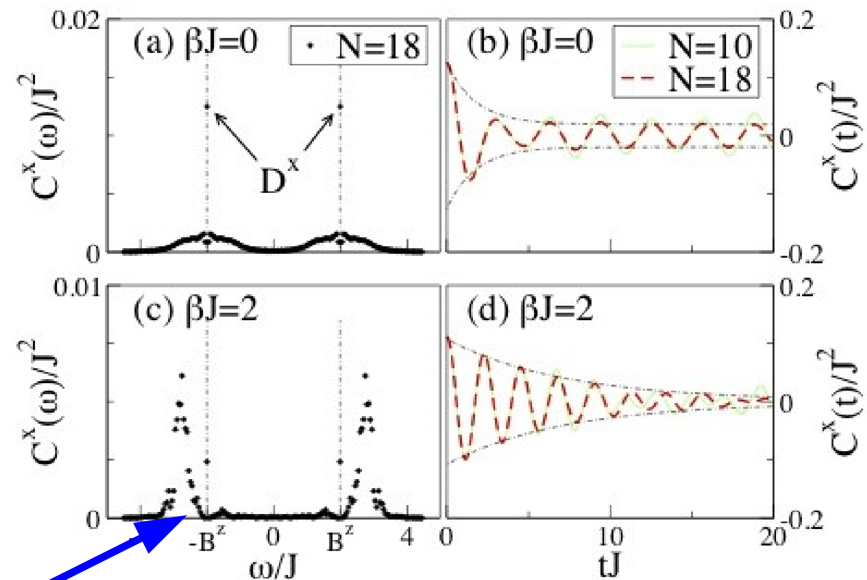
Usually:

$$C^z(t) = \langle j^z(t) j^z \rangle = C^x(t) = \langle j^x(t) j^x \rangle$$

$B^z \neq 0$

$$C^z(t) \neq C^x(t)$$



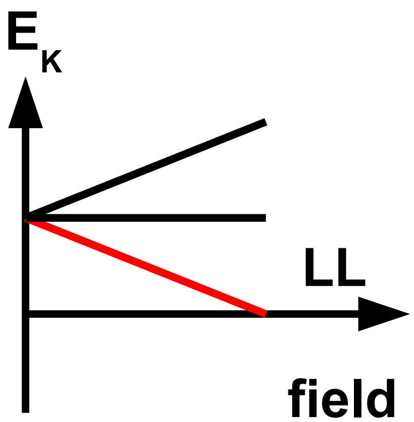


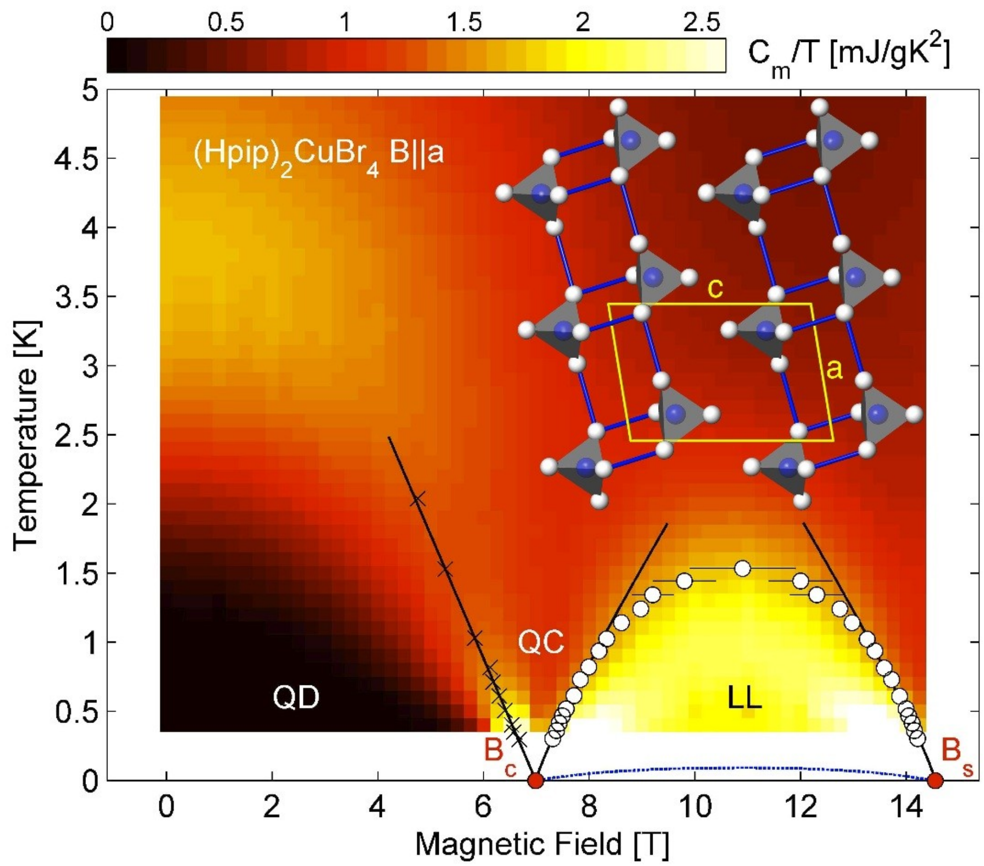
→ Non-trivial oscillation at frequency different from Larmor frequency

Steinigeweg, Langer, HM, McCulloch, Brenig PRL 2011

Transport in field-induced gapless phases

A spin ladder material with $J_{leg} < J_{rung}$: $(Hpip)_2CuBr_4$





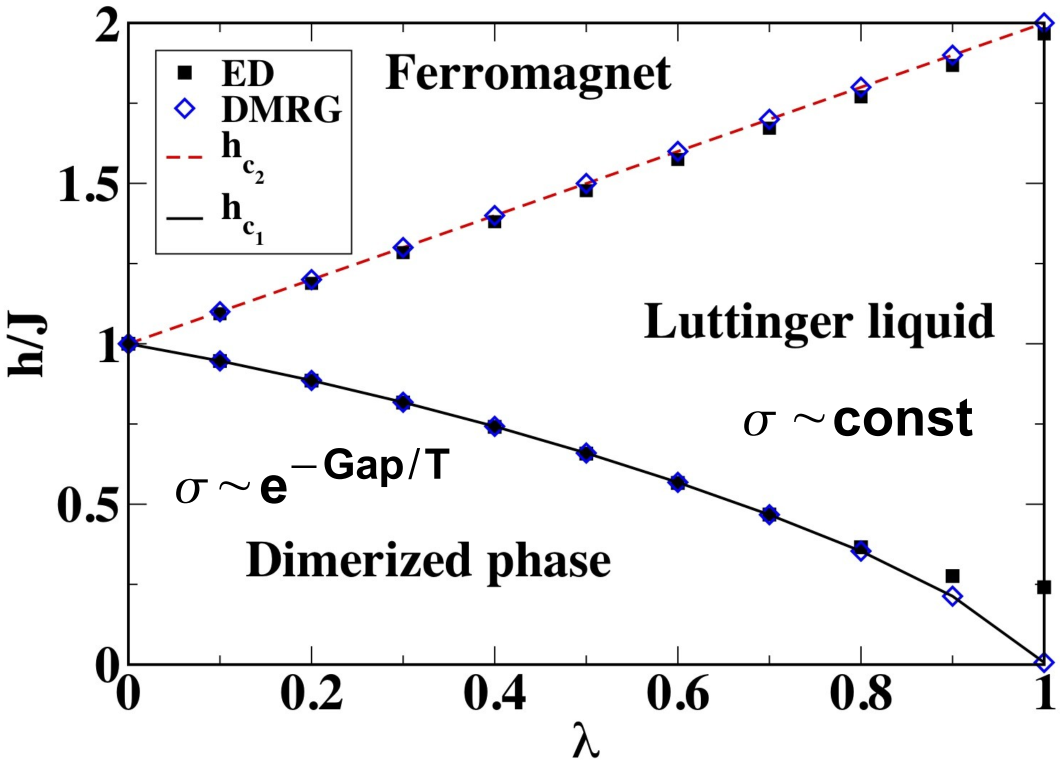
J_{rung} ~ 13K
"small"
- compared to telephone-# compounds J~1000K

→ no field-dependence of κ in the latter
Hess et al. PRB 2001

Rüegg et al. PRL 2008; Klanjsek et al. PRL 2008

Example: Dimerized spin-½ chain

$$H = J \sum_i (\vec{S}_{2i}\vec{S}_{2i+1} + \lambda \vec{S}_{2i+1}\vec{S}_{2i+2}) - h S^z_{total}$$



T=0 phase diagram:
Cabra & Grynberg PRB 1999, Honecker PRB 1999

With λ=0.5:
Spin gap 0.66J
h_{sat} = 1.48J

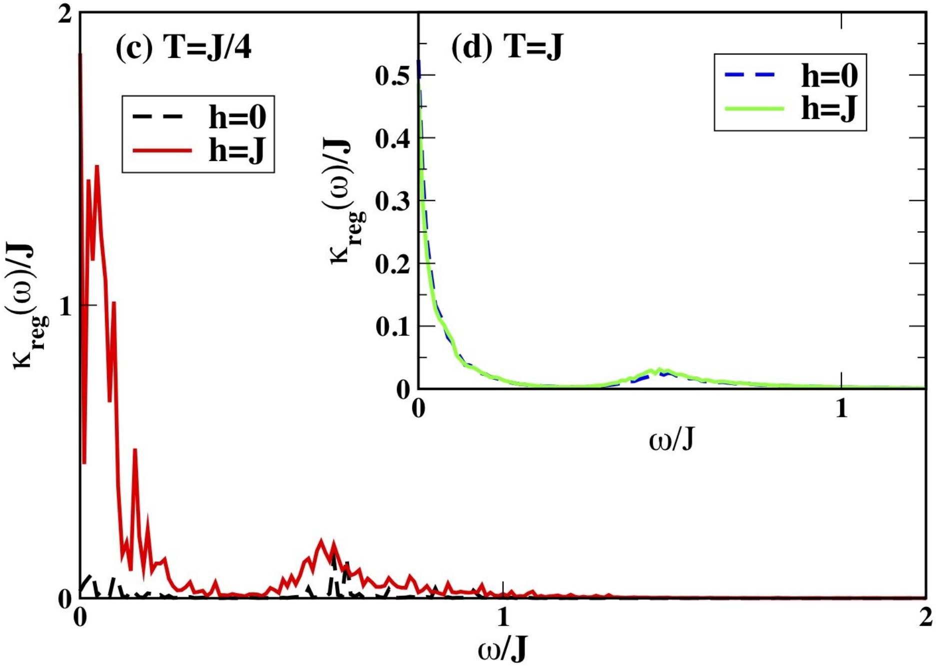
$$\sigma(\omega) = D_s \delta(\omega) + \sigma_{reg}(\omega)$$

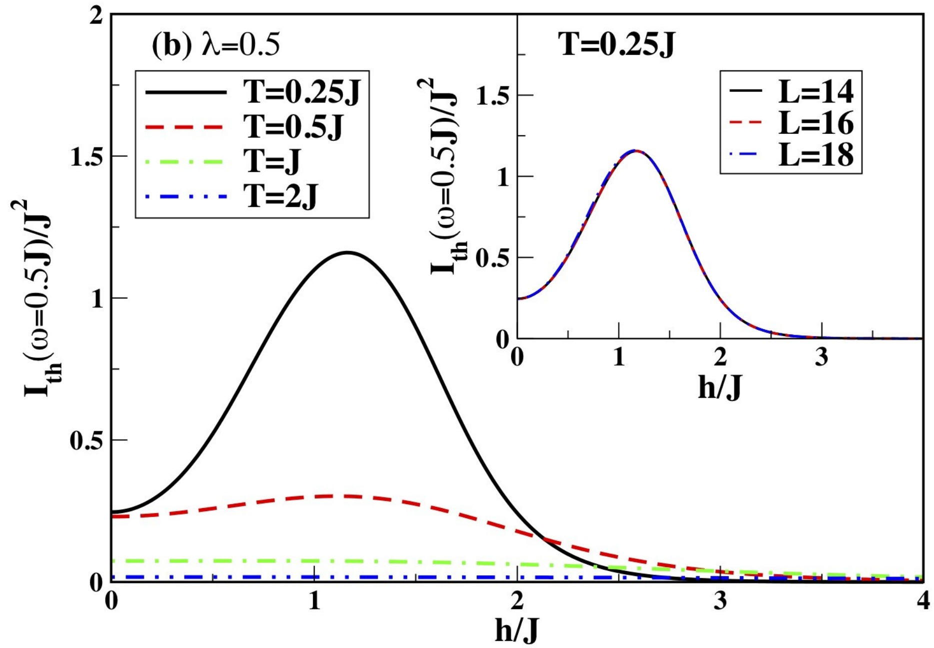
We'll look at:

Heat conductivity κ(ω)

Phonons not included here
Rozhkov, Chernyshev, PRL 2005
Boulat et al. PRB 2007

Heat conductivity: Spectrum

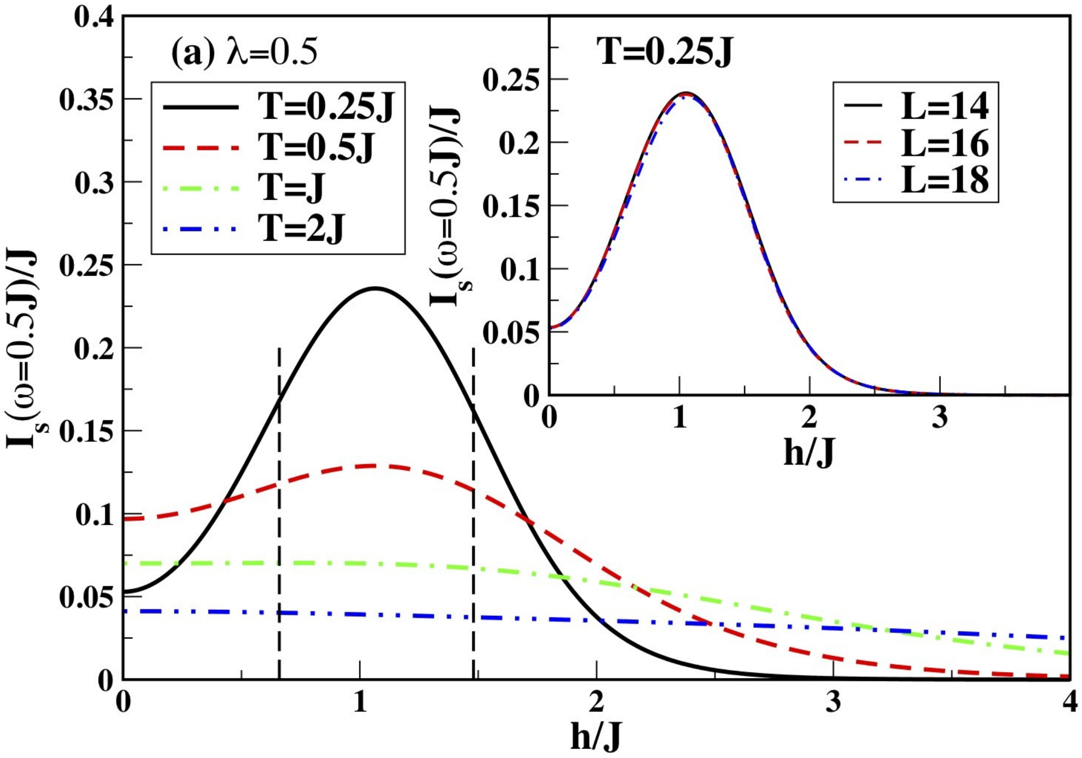




→ **Spectral weight increases at low-frequencies ω<gap=0.66J upon entering into LL phase**
So far, nothing seen in experiments
Sologubenko et al. PRB 2009

Langer, Darradi, HM, Brenig PRB 2010

Integrated spectral weight



→ **Increase above field-induced phase even at elevated T**

$$\mathbf{I_s}(\omega) = \int_{-\omega}^{\omega} \mathbf{d}\omega' \, \Re[\sigma(\omega')]$$

Langer, Darradi, HM, Brenig PRB 2010

Part 2:
Density matrix renormalization group

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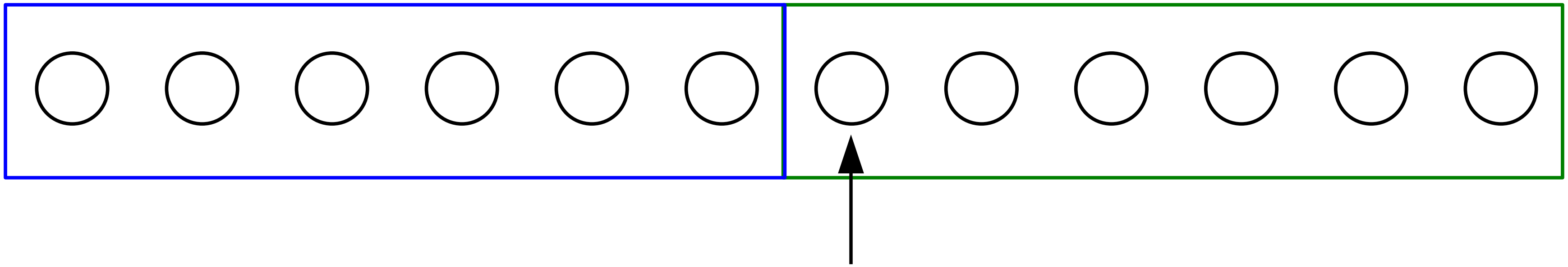
Ljubljana – June 4th, 2012

Fundamental problem

Length L →



Local Hilbert space: Dim = d

Hilbert space grows exponentially fast:

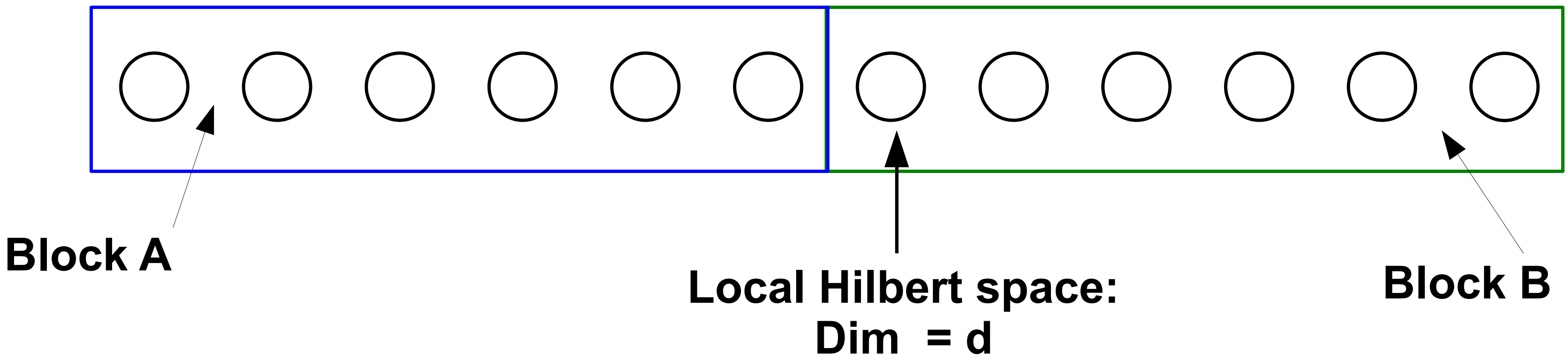
$$\mathrm{dim} = d^L$$

Typical Hamiltonian: spin-½ (d=2); Fermi-Hubbard (d=4); ...

$$H = J \sum_i \vec{S}_i \cdot \vec{S}_{i+1}$$

Basics of DMRG

Length L →



$$H_0|\psi\rangle_0 = E_0|\psi\rangle_0$$

White Phys. Rev. Lett. 1992
Schollwöck Rev. Mod. Phys. 2005

Matrix-Product-State dimension m

Rommer, Östlund PRL 1995, PRB 1997

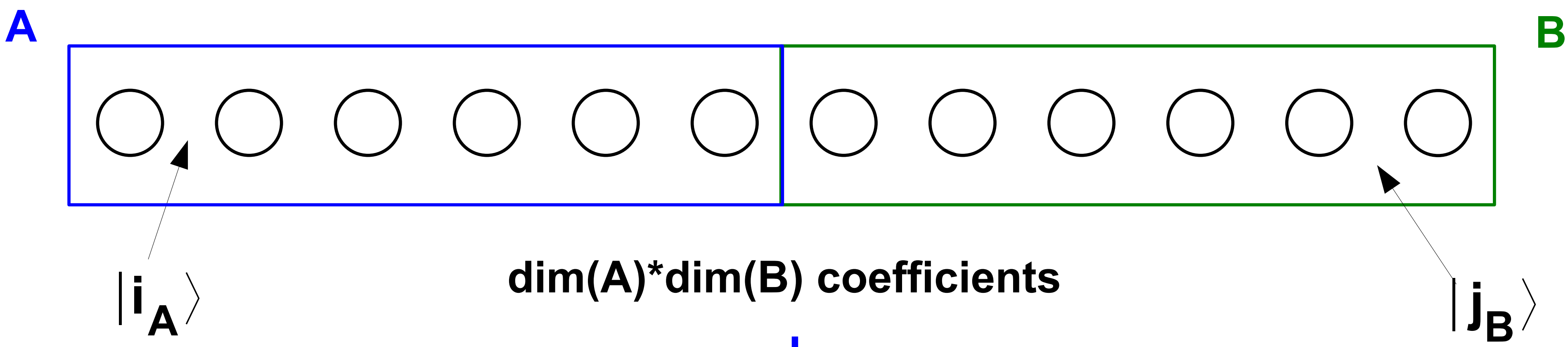
Reduced density matrix

$$\rho_A = \mathrm{tr}_B |\psi_0\rangle\langle\psi_0|$$

Entanglement

$$S_{vN} = -\mathrm{tr}[\rho_A \ln(\rho_A)]$$

Basics of DMRG



dim(A)*dim(B) coefficients

$$|\psi_0\rangle = \sum_{ij} c_{ij} |i\rangle_A \otimes |j\rangle_B$$

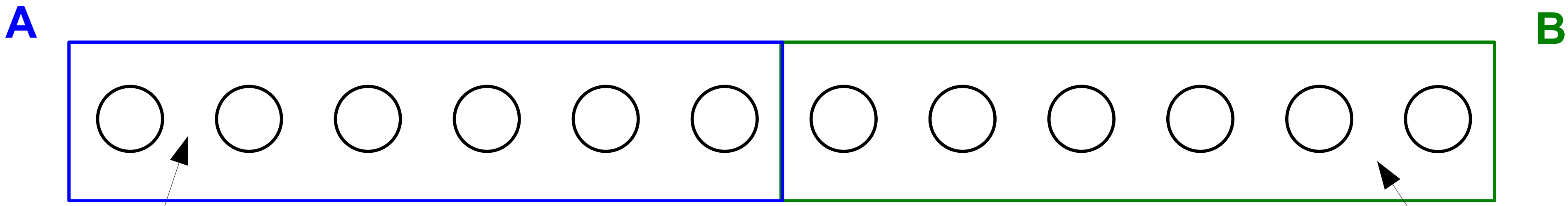
Singular value decomposition:

$$C = U \cdot S \cdot V^\dagger$$

In these new basis sets:

$$|\psi_0\rangle = \sum_{\alpha=1}^{s} \lambda_\alpha |\alpha\rangle_A \otimes |\alpha\rangle_B \qquad \lambda_1 > \lambda_2 > \cdots > \lambda_s > 0$$

Basics of DMRG



$|\alpha_A\rangle$

$|\alpha_B\rangle$

Approximation: discard states with smallest λ_α

$$|\psi_0\rangle \approx |\psi_m\rangle = \sum_{\alpha=1}^{m} \lambda_\alpha |\alpha_A\rangle \otimes |\alpha_B\rangle$$

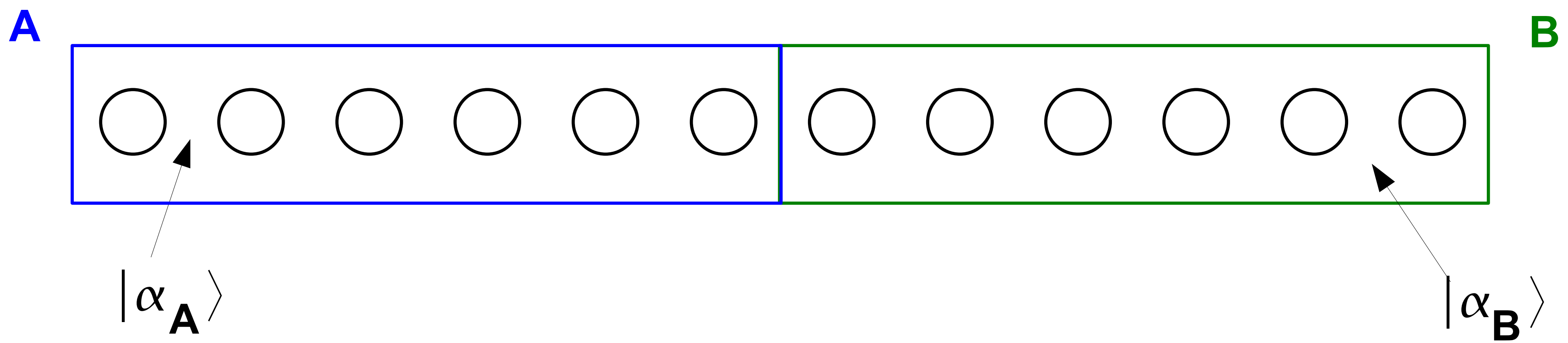
$$m \sim 10^3 \ll \min[\dim(A), \dim(B)]$$

Error ~ discarded weight

$$\langle \psi_m | \psi_m \rangle = 1 - \sum_{\alpha=m+1} \lambda_\alpha^2$$

$\delta\rho$

Where is the density matrix?



Reduced density matrix of block A:

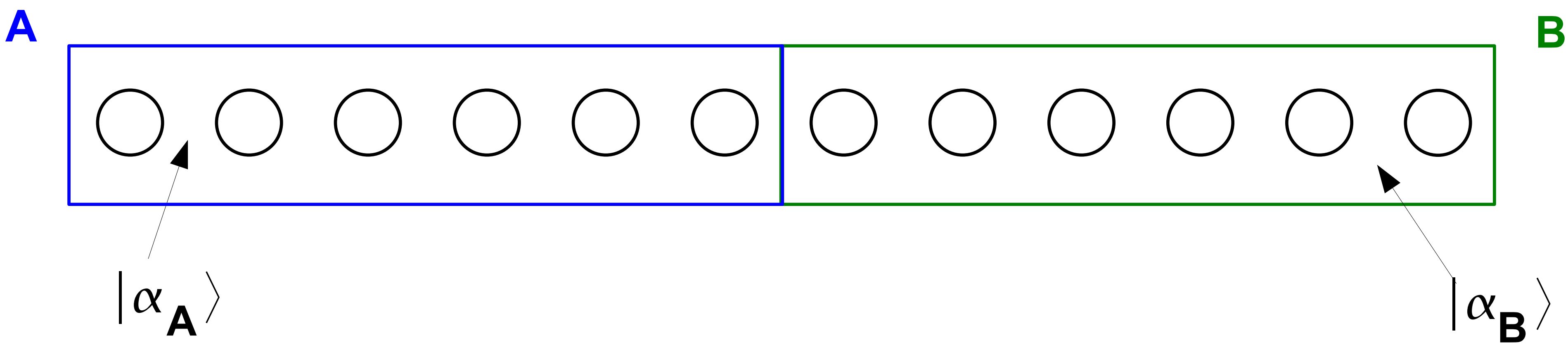
$$\rho = |\psi_m\rangle\langle\psi_m| \Rightarrow \rho_A = \mathrm{tr}_B(\rho) = \sum_\alpha \lambda_\alpha^2 |\alpha_A\rangle\langle\alpha_A|$$

→ **DMRG truncates in the eigenbasis of reduced DM!**

$$\langle O_A\rangle = \mathrm{tr}_A[\rho_A O_A] = \sum_\alpha \lambda_\alpha^2 \langle\alpha_A|O_A|\alpha_A\rangle$$

White PRL 1992, PRB 1993
Schollwöck Rev. Mod. Phys. 2005

Basics of DMRG



$$|\psi_0\rangle \approx |\psi_m\rangle = \sum_{\alpha=1}^{m} \lambda_\alpha |\alpha_A\rangle \otimes |\alpha_B\rangle$$

1) Mathematically: This is the best possible approximation (under the condition of keeping m states)

2) When is this a good – useful – approximation?

3) Can an efficient algorithm be designed? Yes, CPU~m^3

Schollwöck Rev. Mod. Phys. 2005

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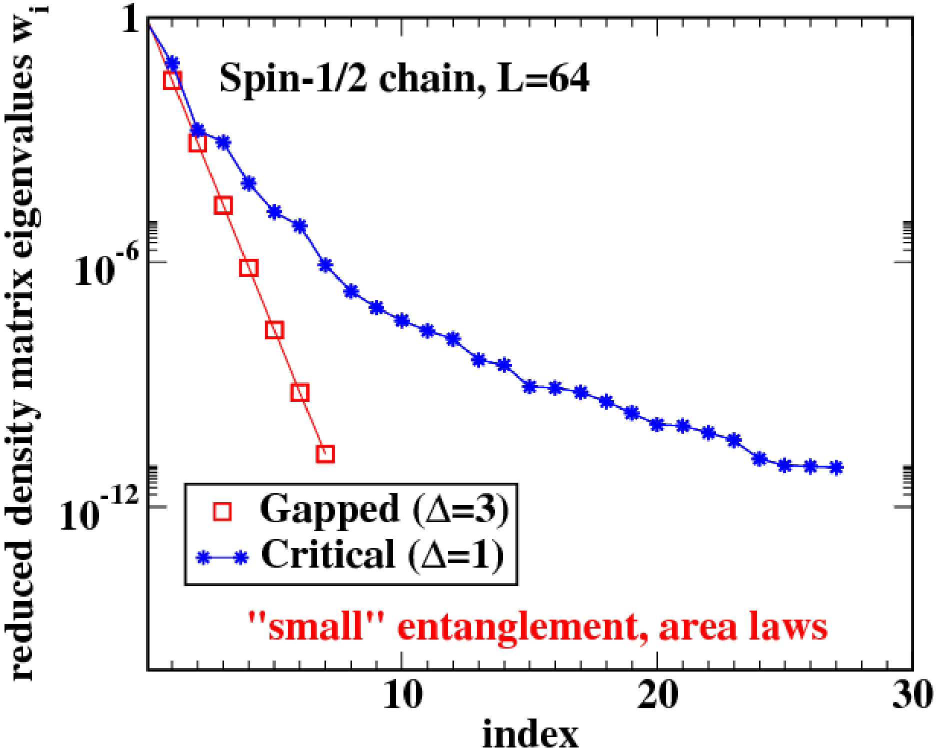
When does it work, and when not?

$$|\psi_0\rangle \approx |\psi_m\rangle = \sum_{\alpha=1}^{m} \lambda_\alpha |\alpha_A\rangle \otimes |\alpha_B\rangle$$

Singular values λ_α have to decay sufficiently fast!

Example: ground state of

$$H = J \sum_i \left[(S_i^+ S_{i+1}^- + h.c.)/2 + \Delta S_i^z S_{i+1}^z \right]$$



Kaulke, Peschel EPJB 1998,
Peschel, Kaulke, Legeza Ann. Phys. 1999

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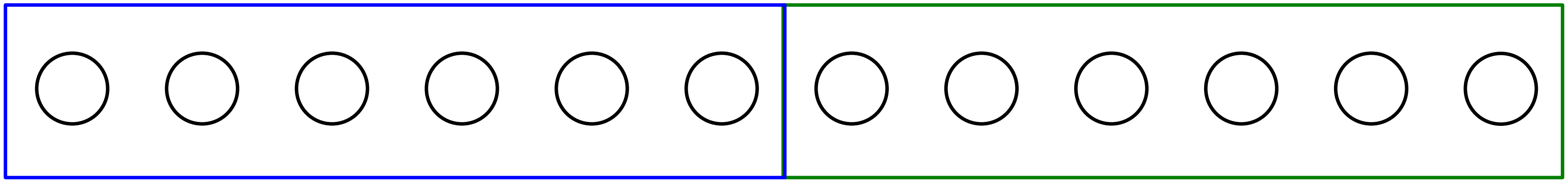
When does it work, and when not?



Von-Neumann entropy:

$$S_{vN} = -\mathrm{tr}[\rho_A \ln(\rho_A)] = -\sum_\alpha \lambda_\alpha^2 \ln(\lambda_\alpha^2)$$

Flat distribution:

$$\lambda_\alpha^2 \sim \frac{1}{m} \Rightarrow m \propto e^{S_{vN}(L)}$$

Ground states in 1D -
mildly entangled wave functions:

S_{vN} ~ const. ($L_A > \xi$)

S_{vN} ~ log L_A (critical systems)

More general: Area law

$$S_{vN} \sim L^{D-1}$$

$$S_{vN} \sim L\,(2D)$$

Review: Eisert, Cramer, Plenio RMP 2010

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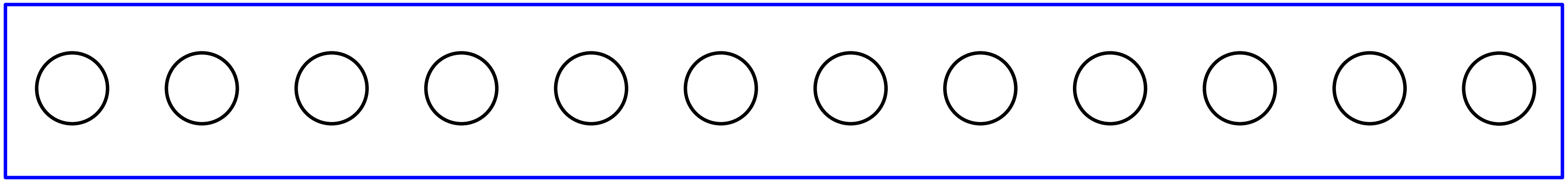
DMRG operates on Matrix Product States



$$c_{\sigma_1 \cdots \sigma_L} = \sum_{\alpha_1} \sum_{\alpha_2} \cdots \sum_{\alpha_{L-1}} \sum_{\alpha_{L-1}} A^{\sigma_1}_{\alpha_1} A^{\sigma_2}_{\alpha_1 \alpha_2} \cdots A^{\sigma_{L-1}}_{\alpha_{L-2} \alpha_{L-1}} A^{\sigma_L}_{\alpha_{L-1}}$$

$$|\psi\rangle = \sum_{\sigma_1 \sigma_2 \cdots \sigma_{L-1} \sigma_L} A^{\sigma_1} A^{\sigma_2} \cdots A^{\sigma_{L-1}} A^{\sigma_L} |\sigma_1 \sigma_2 \cdots \sigma_{L-1} \sigma_L\rangle$$

→ Matrix Product States

DMRG approximation:
Work with matrices with a maximum dimension m

Rommer, Östlund PRL 1995, PRB 1997
Schollwöck Ann. Phys. 2011

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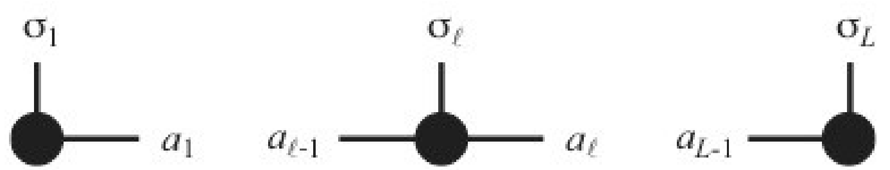
Matrix Product States: Graphical representation

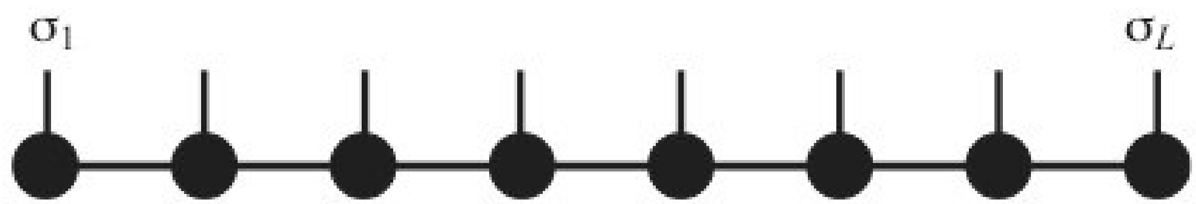
$$|\psi\rangle = \sum_{\sigma_1\sigma_2\cdots\sigma_{L-1}\sigma_L} A^{\sigma_1}A^{\sigma_2}\cdots A^{\sigma_{L-1}}A^{\sigma_L}|\sigma_1\sigma_2\cdots\sigma_{L-1}\sigma_L\rangle$$

→ Matrix Product States

A-matrices



MPS



Figures from Schollwöck Ann. Phys. 2011

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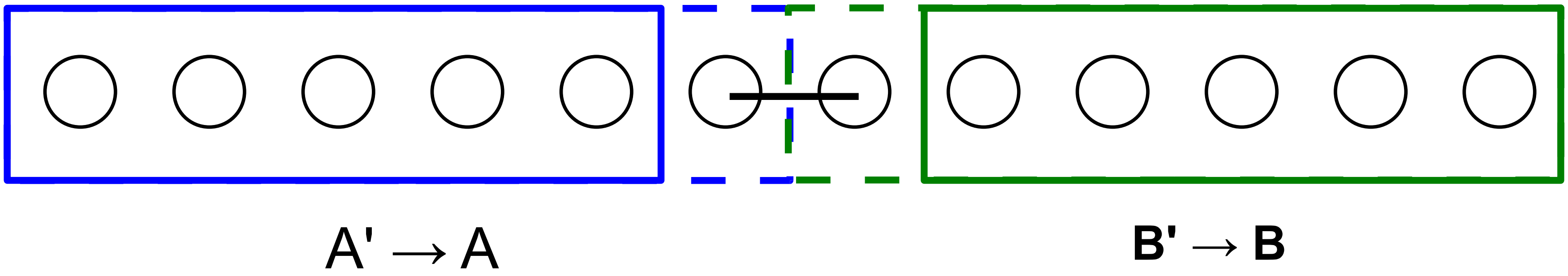
DMRG Algorithm



Initial guess: From small systems!

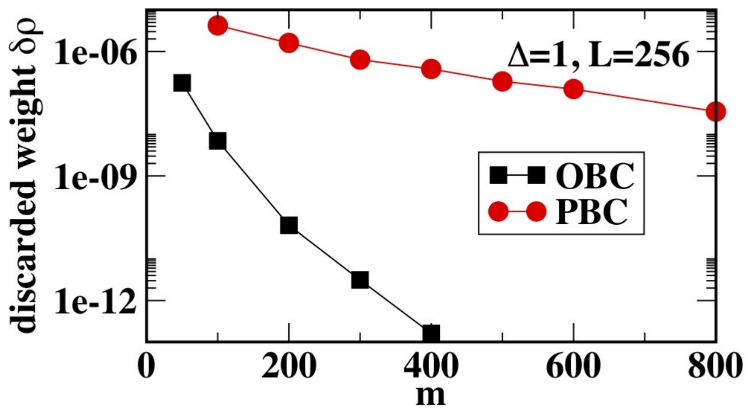
1) Get ground-state of super-block from Lanczos
2) Form reduced DM ρ_A from $|\psi_0>$
3) Diagonalize ρ_A
4) Rotate all operators into eigen-basis of ρ_A
5) Truncate in that basis
6) Rotate $|\psi_0>$ into basis of next bipartition

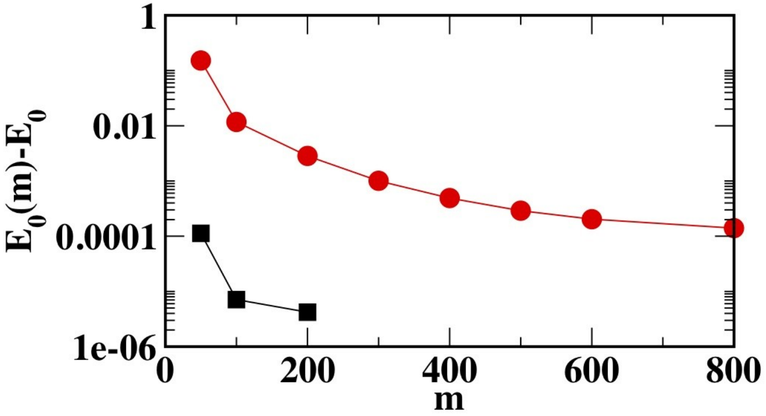
White PRL 1992, PRB 1993
In MPS language: McCulloch J. Stat. Mech. 2007

DMRG at work: Ground-state energy

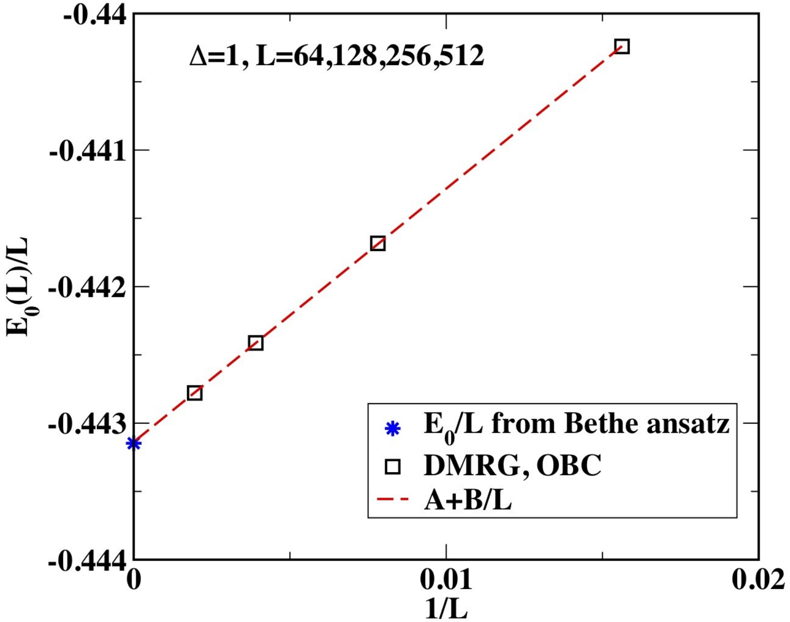
$$H = J\sum_{i=1}^{L}\left[\frac{1}{2}\left(S_i^+ S_{i+1}^- + h.c.\right) + \Delta S_i^z S_{i+1}^z\right] - h\sum_i S_i^z$$

Convergence with #states m





Ground-state energy infinite system



$$\frac{E_0}{LJ} = -\ln(2) + \frac{1}{4} \approx -0.4431(4)$$

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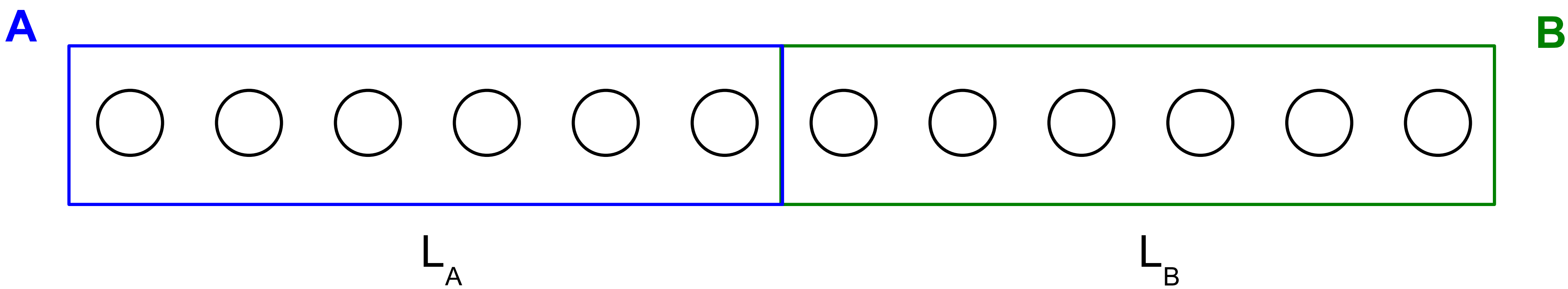
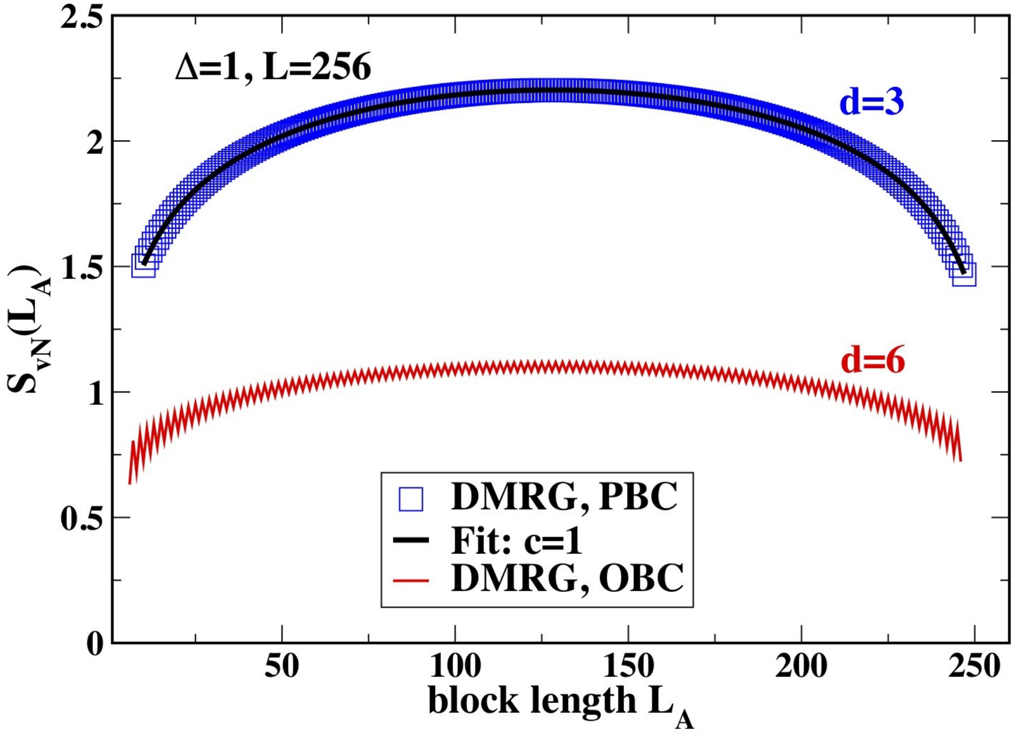
DMRG at work: Entanglement entropy





Scaling of von-Neumann entropy

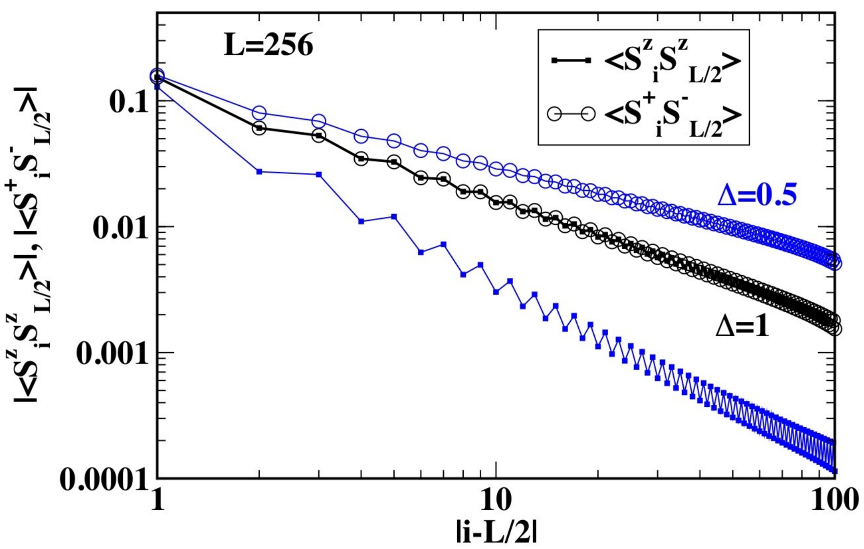
$$S_{vN}(L_A) = \frac{c}{d} \ln\left(\frac{\pi}{L}\sin(\pi L_A/L)\right) + g$$

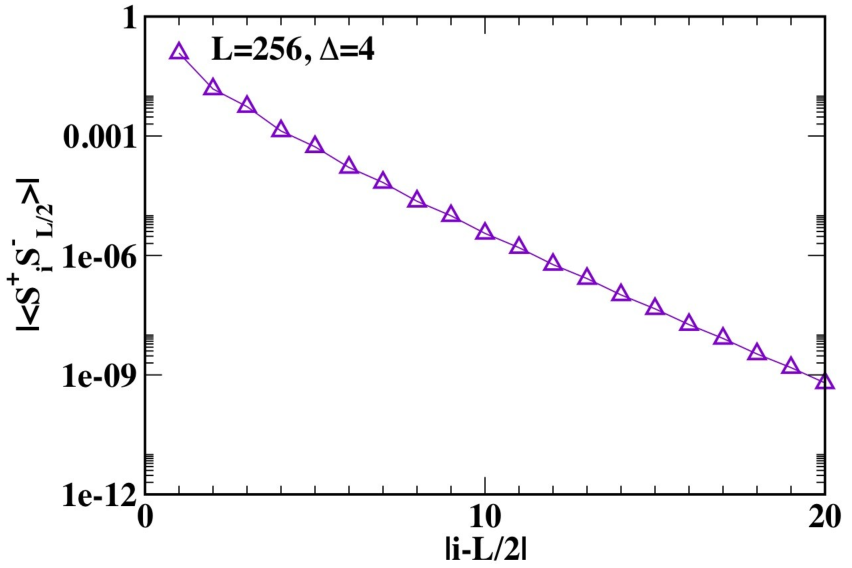
→ **central charge: c=1**

Calabrese, Cardy, J. Stat. Mech. (2004) P06002
Vidal, Latorre, Rico, Kitaev, PRL 2003

DMRG at work: Correlation functions

$$H = J\sum_{i=1}^{L}\left[\frac{1}{2}\left(S_i^+ S_{i+1}^- + h.c.\right) + \Delta S_i^z S_{i+1}^z\right] - h\sum_i S_i^z$$





→ **Power-law decay, for Δ<1, longitudinal correlations decay faster**

→ **Exponential decay of transverse correlations**

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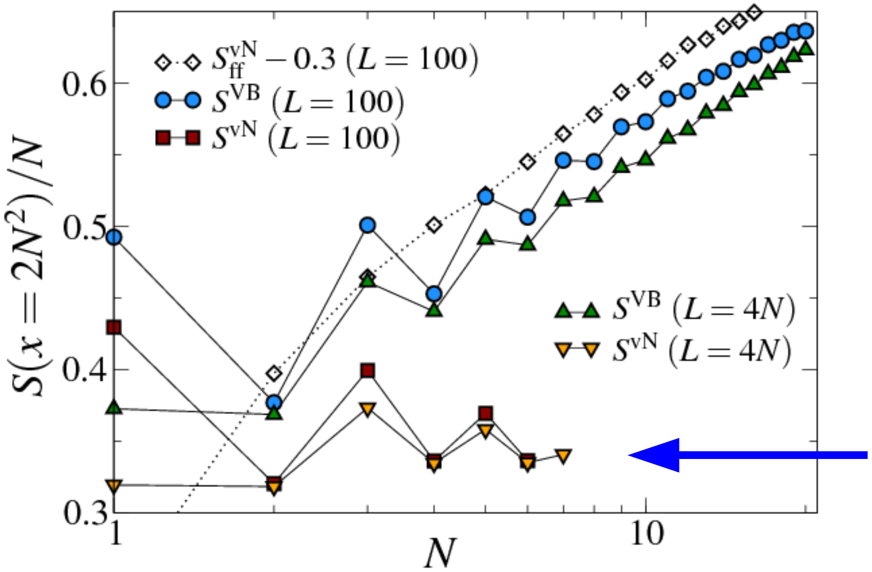
DMRG for two-dimensional systems

$$H = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j$$

2D square lattice: Néel state

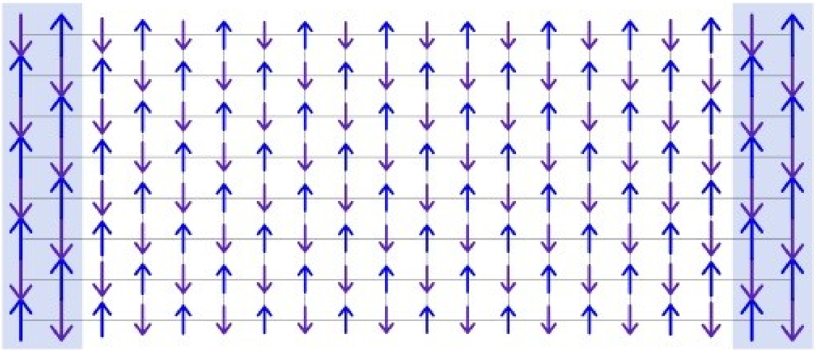
N-leg ladders



→ **Area law seems valid** $S_{vN,L} \sim L^{d-1}$

Kallin, Gonzalez, Hastings, Melko PRL 2009

DMRG on cylinders



Stoudenmire, White
Ann. Rev. Cond. Matt. Phys 2012

Magnetic moment:

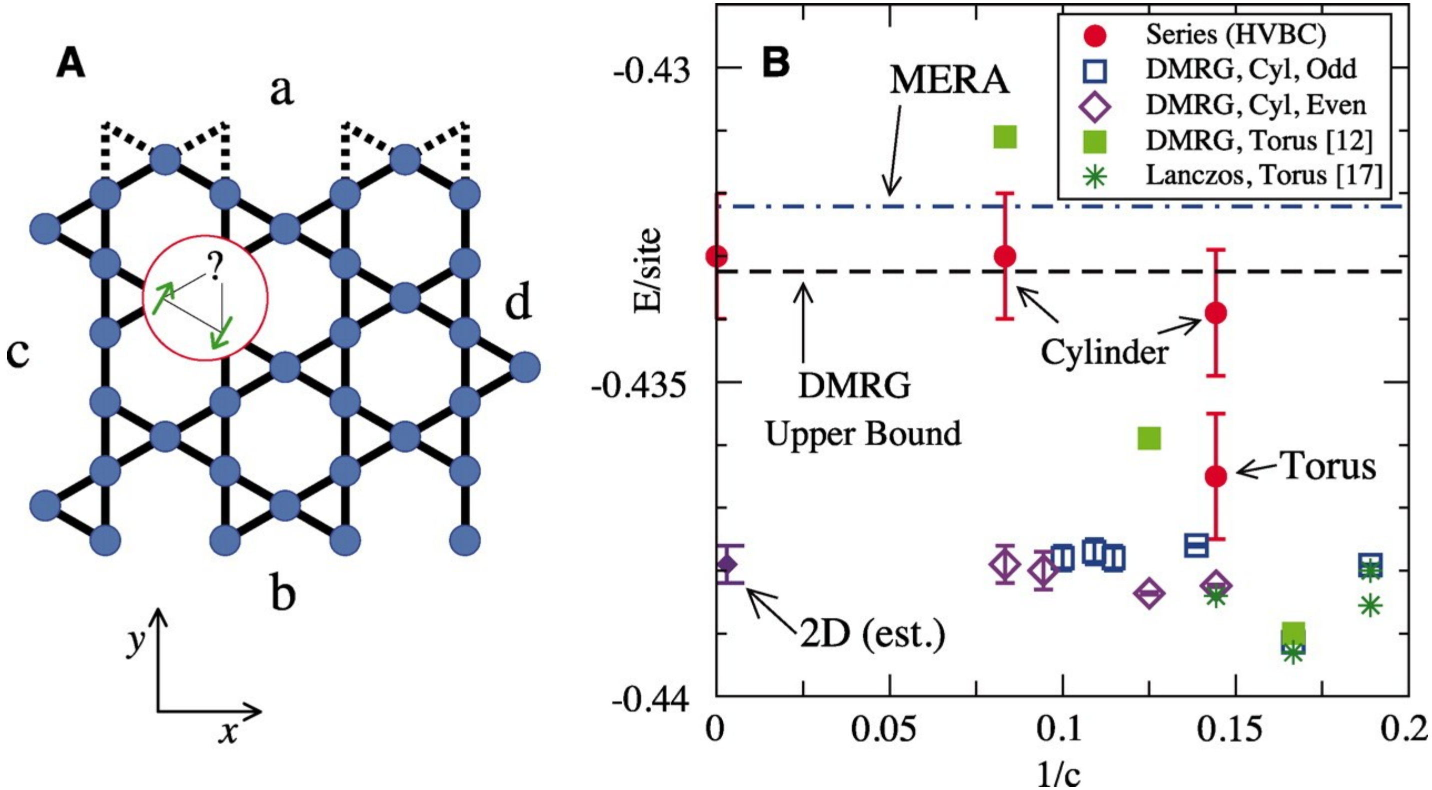
$M_0 = 0.3067 (DMRG)$

$M_0 = 0.3070(3) (SSE)$

White, Chernyshev PRL 2007
SSE: Sandvik PRB 1997

Kagome lattice

Frustrated lattice → sign problem, QMC not applicable



→ Interpretation: gapped topological spin liquid

Yan, Huse, White Science 2011
Depenbrock, McCulloch, Schollwöck arxiv:1205.4858

Part 3:
Time-dependent DMRG

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Ljubljana – June 4th, 2012

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Time evolution via Trotter-Suzuki

$$|\psi(t)\rangle = \boxed{\exp(-iHt)}|\psi(t=0)\rangle$$

$$H = \sum_{\text{bonds}} h_{i,i+1} = \sum_{\substack{\text{odd}\\\text{bonds}}} h_{i,i+1} + \sum_{\substack{\text{even}\\\text{bonds}}} h_{i,i+1}$$

1) M time slices (exact)

$$e^{-iHt} = (e^{-iH\delta t})^M$$

$$t = M * \delta t$$

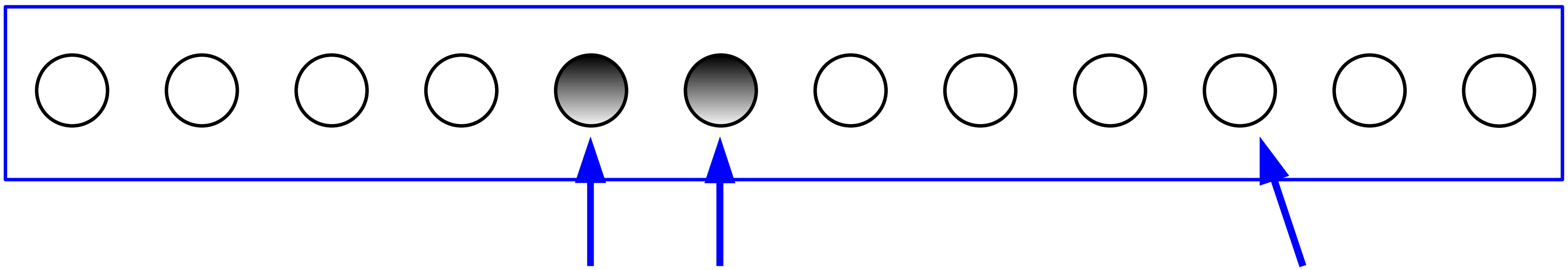
2) Trotter-Suzuki approximation

$$e^{-iH\delta t} \approx e^{-iH_{odd}\delta t} \bullet e^{-iH_{even}\delta t}$$

3) Factorize exponentials (exact)

$$e^{-iH_{odd}\delta t} = \prod_{\substack{\text{odd}\\\text{bonds}}} e^{-ih_{i,i+1}\delta t} = \prod U_{i,i+1}$$

Time-dependent DMRG



$|\sigma_i\rangle$ $|\sigma_{i+1}\rangle$

Local Hilbert space:
Dim = d

$$e^{-i h_{i,i+1} \delta t} = U_{(\sigma_1 \sigma_2)(\sigma'_1 \sigma'_2)}$$

$(d_i d_{i+1})^*(d_i d_{i+1})$ matrix

→ tDMRG amounts to applying a set of unitaries (two-site gates) to a MPS + truncation (dim(MPS) grows by applying U)

U can be cast into the form of an Matrix-Product-Operator

Time-dependent DMRG: Graphical representation

1) All U_{odd} applied to MPS

2) Regain MPS form:

dim=d^2m

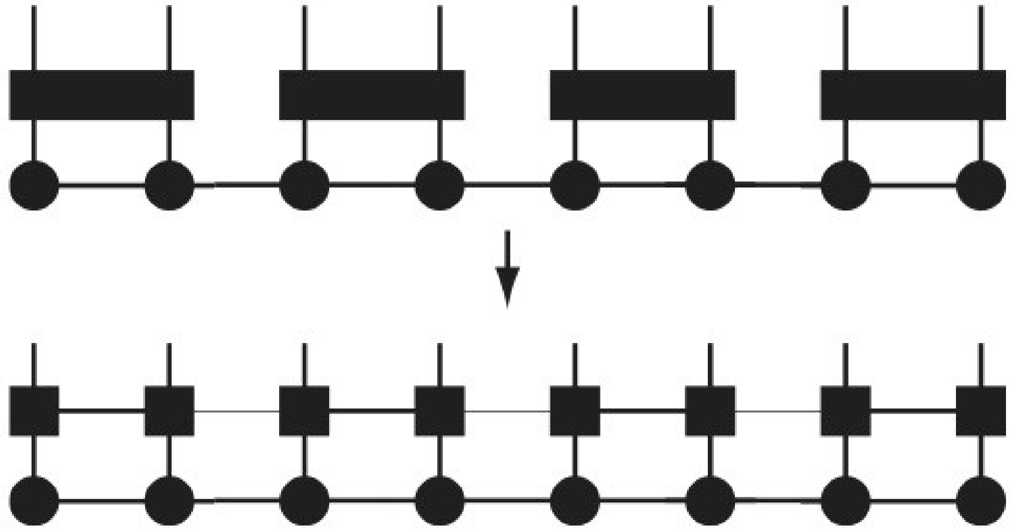


Figure from Schollwöck Ann. Phys. 2011

3) Truncate back to max. dimension m using SVDs

4) Apply all U_{even}

TEBD: Vidal PRL 91, 147902 (2003); PRL 93, 040502 (2004)
tDMRG: Daley, Kollath, Schollwöck, Vidal J. Stat. Mech (2004) P04005
White, Feiguin Phys. Rev. Lett. 93, 076401 (2004)
tMPS: Verstraete, Garcia-Ripoll, Cirac PRL 93, 207204 (2004)

Time-dependent DMRG: Simulability, errors

Initial state:

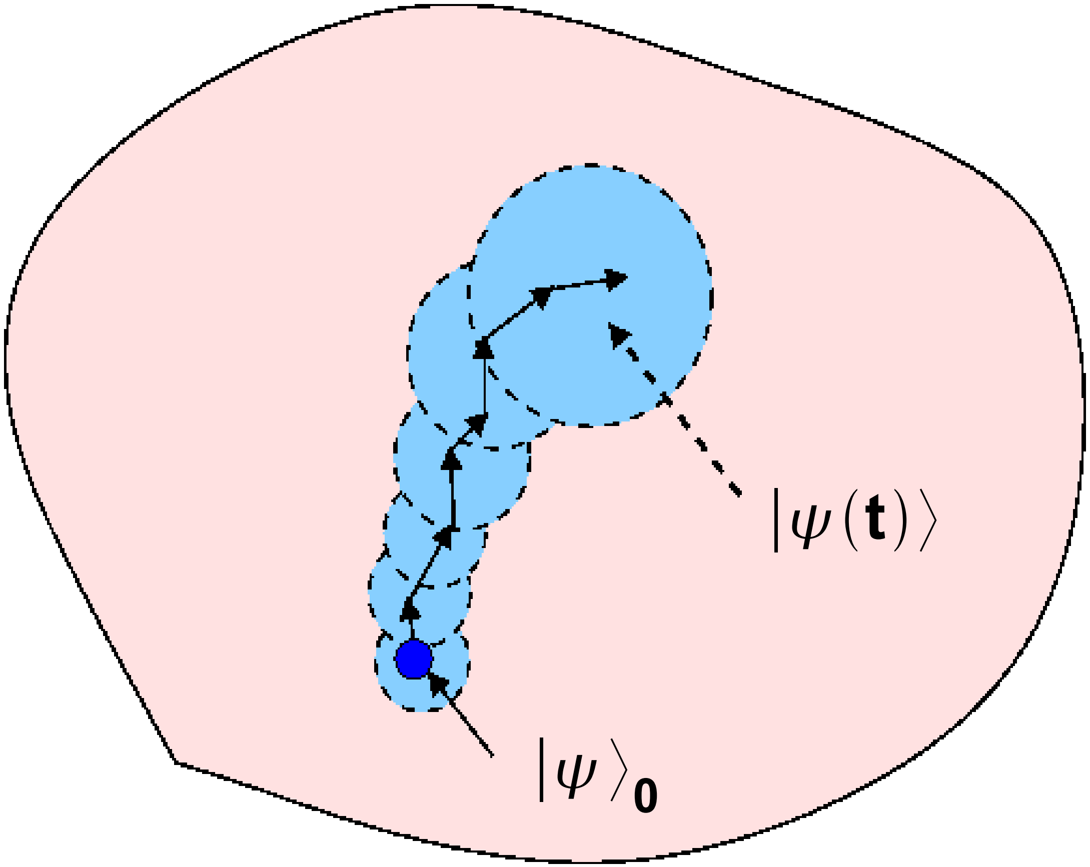
$$H_0|\psi\rangle_0 = E_0|\psi\rangle_0$$

Time $t=0^+$: $H_0 \to H$

$$|\psi(t)\rangle = \exp(-iHt/\hbar)|\psi\rangle_0$$

→ Explores Hilbert space

$$m \propto e^{S_{vN}}$$



Time evolution (worst case): $S_{vN,x}(t) \sim t$

Calabrese Cardy JstatM P04010 (2006)
Osborne PRL 97, 157202 (2006)

Stricter criteria using Renyi entropies:
Schuch, Wolf, Verstraete, Cirac, PRL 100, 030504 (2008)

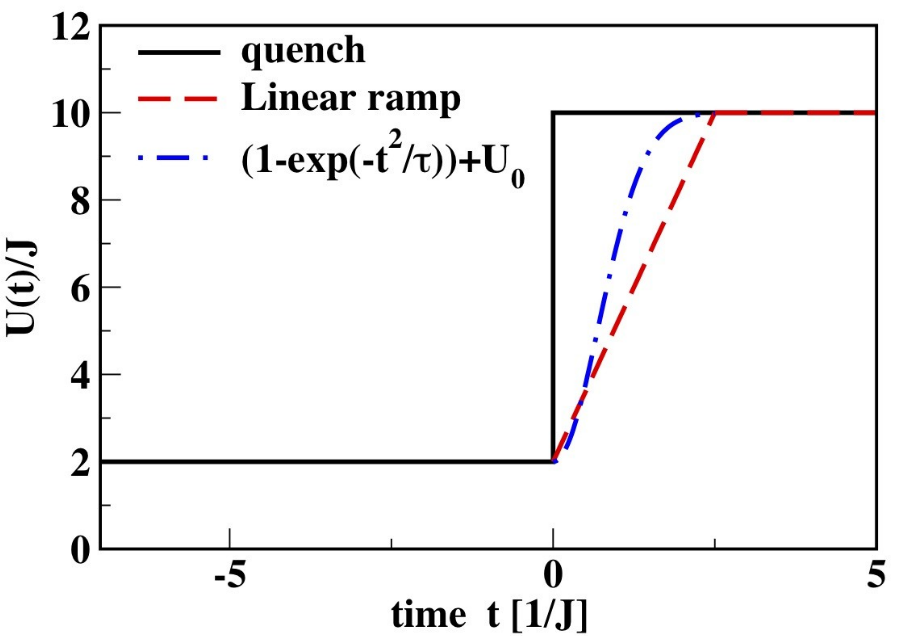
Example: Fermi-Hubbard model

$$H = -J\sum_{i=1}^{L-1}(c^\dagger_{i+1,\sigma}c_{i,\sigma} + h.c.) + \sum_i U_i(t)n_{i,\uparrow}n_{i,\downarrow}$$

1) Global quench: $U_i \rightarrow U'_i$

2) Linear ramp U(t)=at+b

3) Local quench: $U_{i=i'} \rightarrow U'_{i=i'}$



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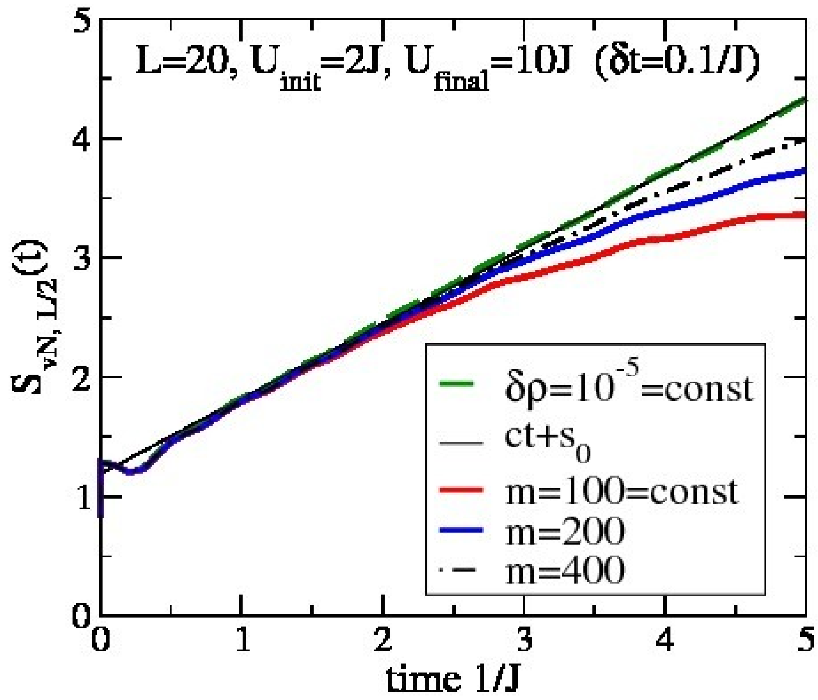
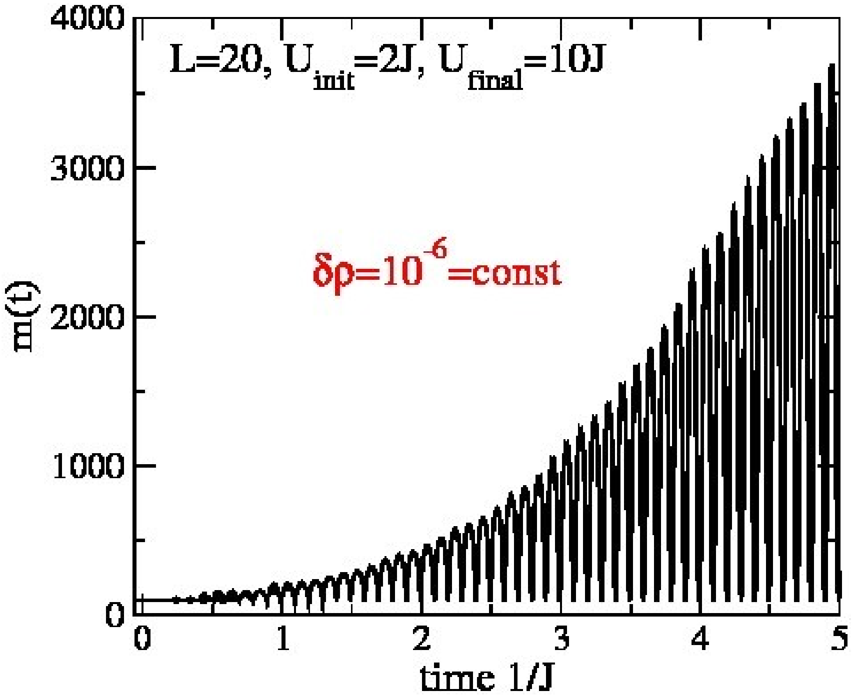
Constant m vs constant discarded weight

$$H = -J \sum_{i=1}^{L-1} (c^\dagger_{i+1,\sigma} c_{i,\sigma} + h.c.) + \sum_i U_i(t) n_{i,\uparrow} n_{i,\downarrow}$$

Global quench: U_{init}=2J, U_{final}=10J → $S_{vN} \sim t$





m=const: Run-away error

δρ=const: m grows

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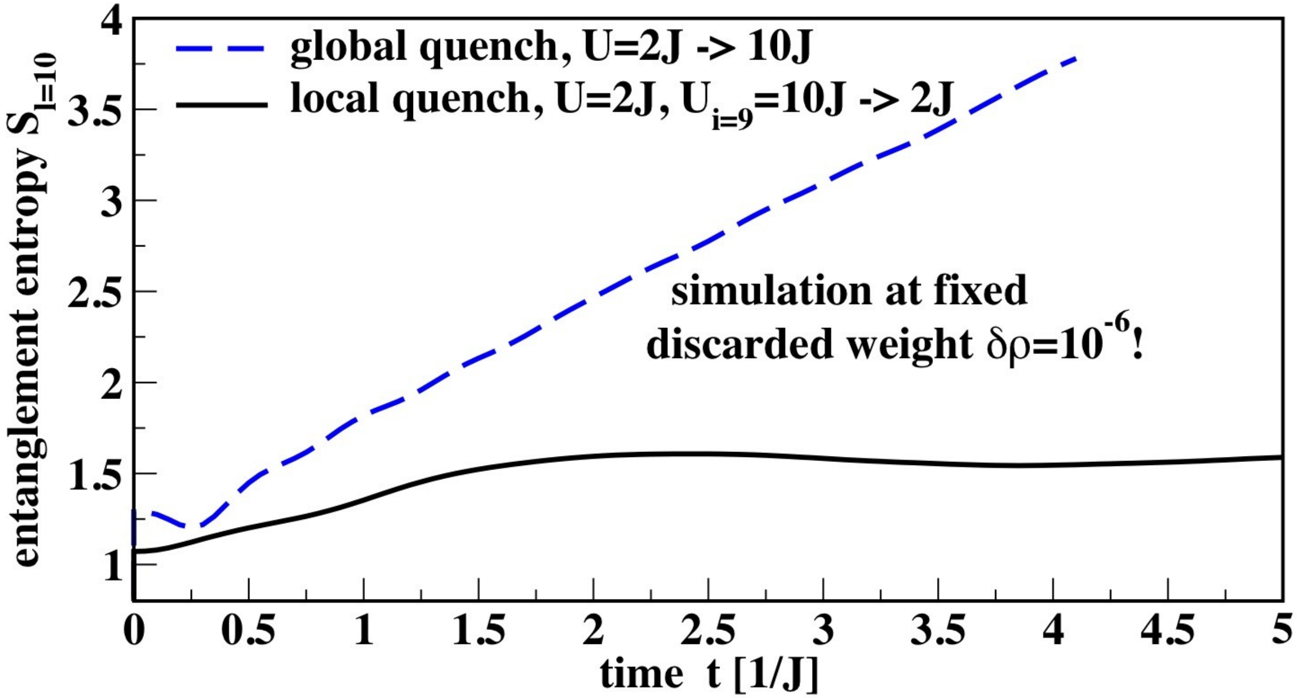
Entanglement growth: Global vs local quenches

$$H = -J \sum_{i=1}^{L-1} (c^\dagger_{i,\sigma} c_{i+1,\sigma} + h.c.) + \sum_i U_i(t) n_{i,\uparrow} n_{i,\downarrow}$$

Global quench: $U_i \rightarrow U'_i$ vs local quench: $U_{i=i'} \rightarrow U'_{i=i'}$

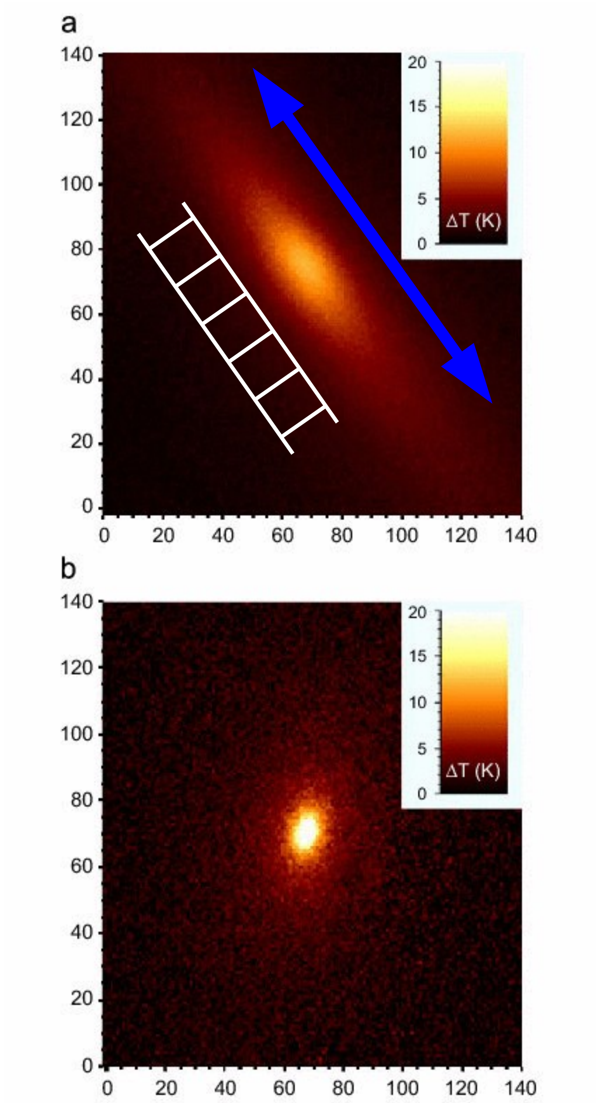


“hard” problem

“easy” problem

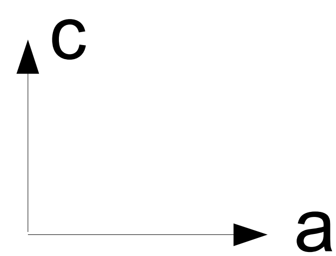
De Chiara et al. JstatM 2006, Calabrese, Cardy JStatM 2005, JStatM 2007, Cazalilla PRL 2006; Eisler, Peschel JStat M 2007; Gobert, Kollath, Schollwöck, Schütz PRE 2005 ...

Time-resolved experiments on heat transport

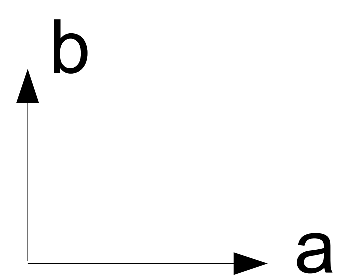


Otter et al. JMMM 2009

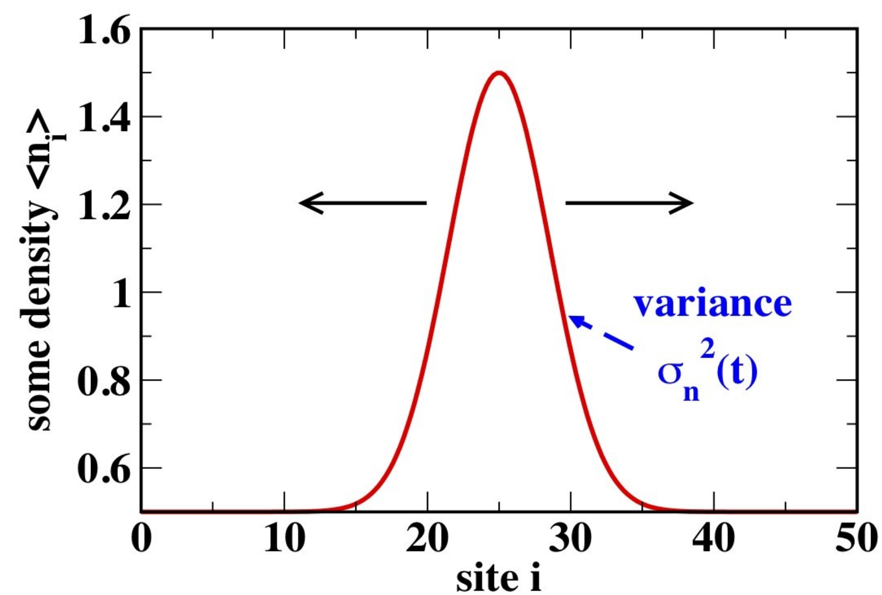
c-axis:
ladders!



top view:
ladder
plane



- **Real-time spin dynamics in pure spin systems: chains & ladders @ T=0**
  Langer, HM, Gemmer, McCulloch, Schollwöck PRB 2009
- **Real-time energy dynamics**
  Langer, Heyl, McCulloch, HM 2011



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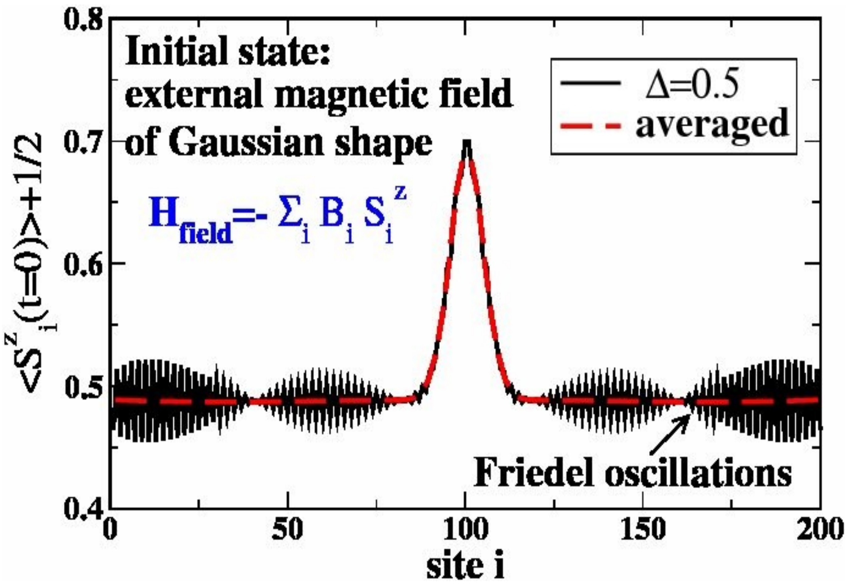
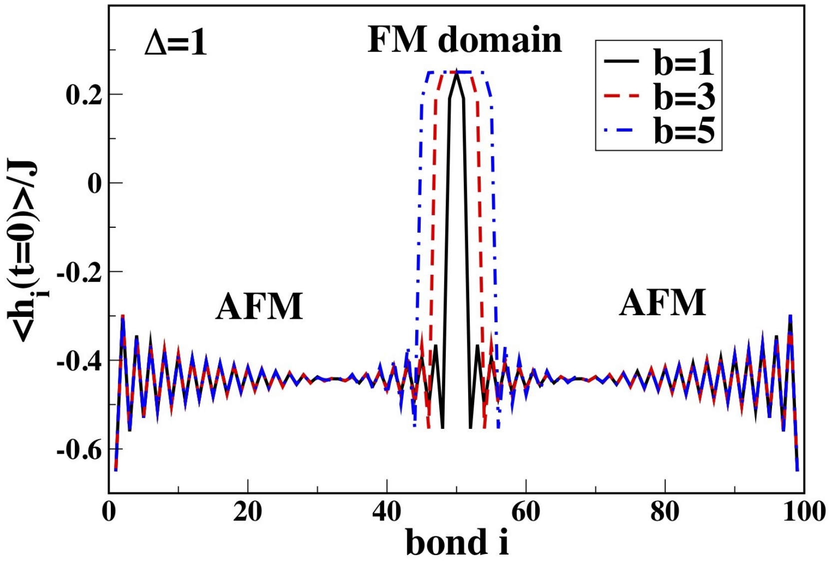
Example: Dynamics of density or spin density excitations

Spin and energy dynamics:

$$H=\sum_i h_i=\sum_i J[(S_i^+ S_{i+1}^- + h.c.)/2+\Delta S_i^z S_{i+1}^z]$$



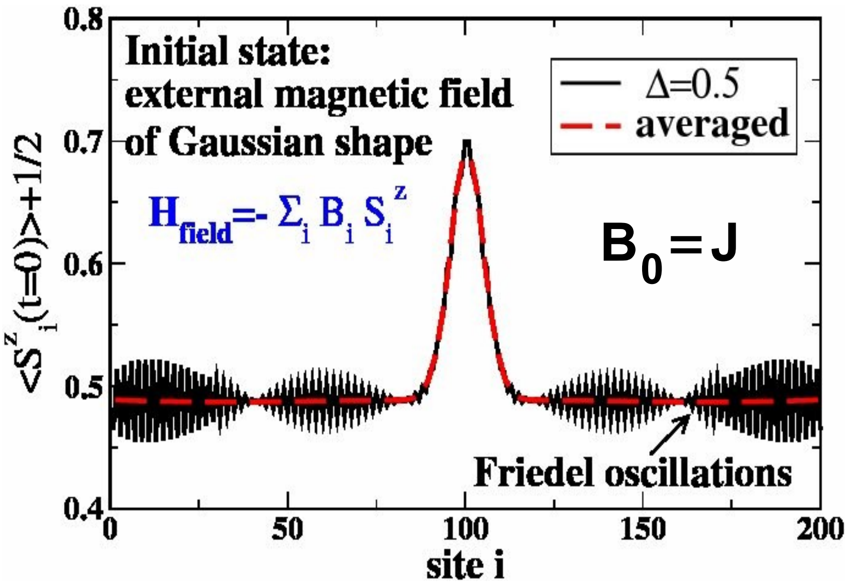


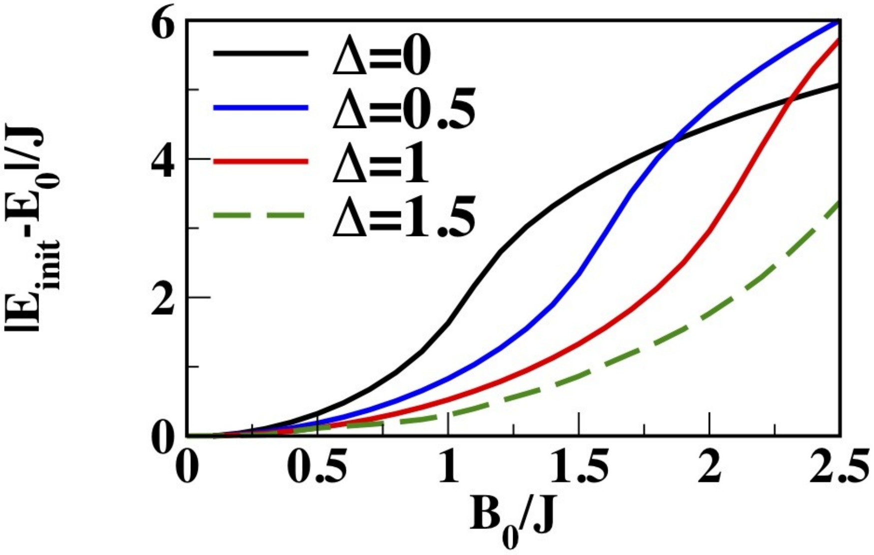
Langer, HM, Gemmer, McCulloch, Schollwöck, PRB 2009; Langer, Heyl, McCulloch, HM PRB 2012

Example: Dynamics of density or spin density excitations

Spin and energy dynamics:

$$B_i = B_0 \exp(-(i-i_0)^2/\sigma_B^2)$$



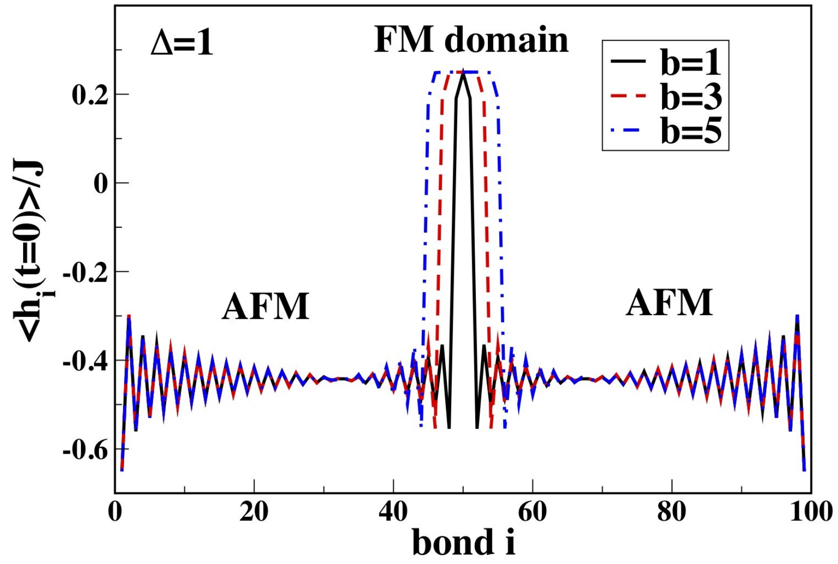


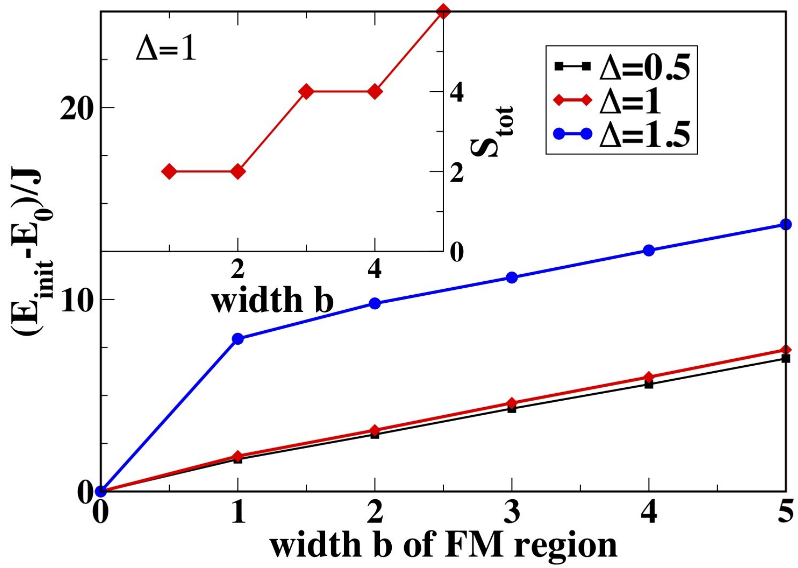
Langer, HM, Gemmer, McCulloch, Schollwöck, PRB 2009; Langer, Heyl, McCulloch, HM PRB 2012

Example: Dynamics of density or spin density excitations

Only energy dynamics:

$$\langle S_i^z(t) \rangle = \text{const}$$

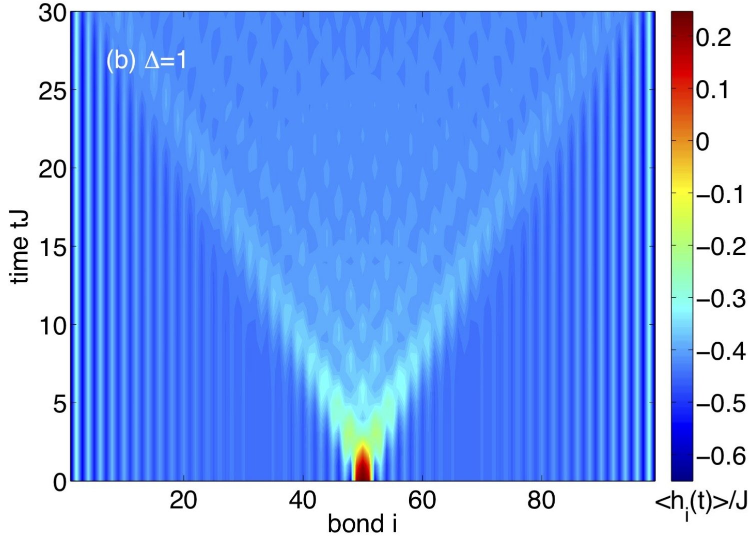


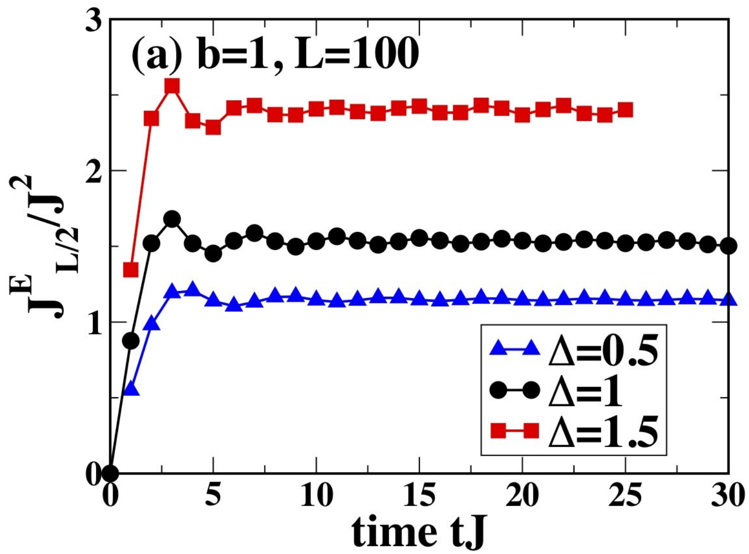


Langer, HM, Gemmer, McCulloch, Schollwöck, PRB 2009; Langer, Heyl, McCulloch, HM PRB 2012

Example: Dynamics of density or spin density excitations

Real-time dynamics of bond-energies and energy current:



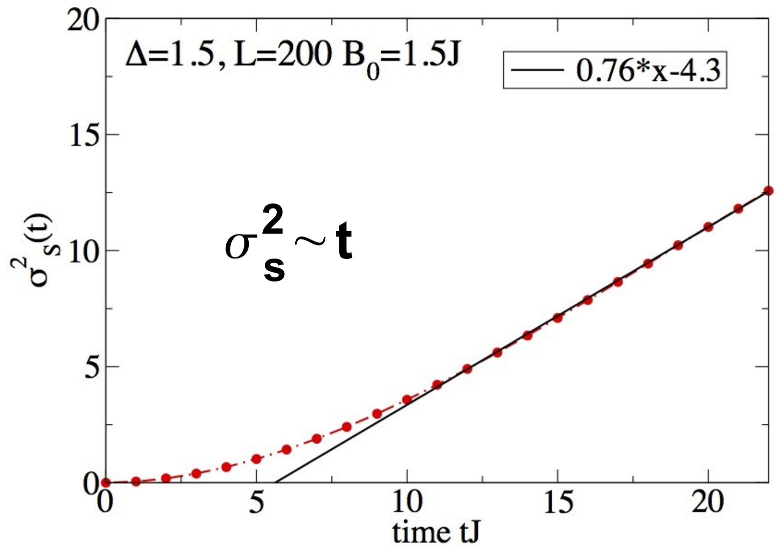


Langer, Heyl, McCulloch, HM PRB 2012

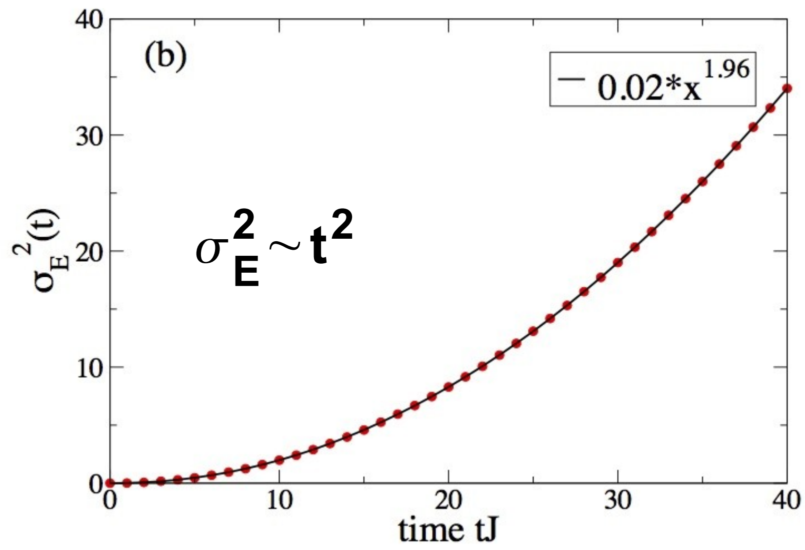
Example: Dynamics of density or spin density excitations

Spin and energy dynamics in the massive phase Δ>1:

$$\sigma_s^2(t) \sim \sum_i \langle S_i^z(t) \rangle (i - i_0)^2 \qquad \sigma_E^2(t) \sim \sum_i \langle h_i(t) \rangle (i - i_0)^2$$



$\sigma_s^2 \sim t$



$\sigma_E^2 \sim t^2$

Spin: not ballistic – diffusive!?

Energy: ballistic

Langer, HM, Gemmer, McCulloch, Schollwöck, PRB 2009; Langer, Heyl, McCulloch, HM PRB 2012
Jesenko, Znidaric PRB 2012

Example: Dynamics of density or spin density excitations

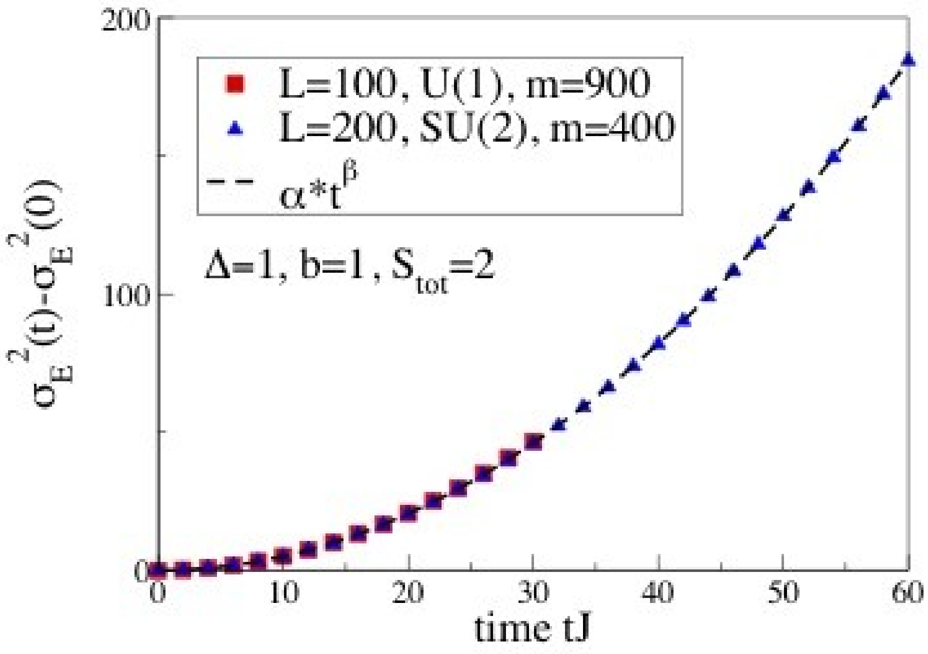
Spin and energy dynamics:

$$H = \sum_i h_i = J \sum_i \vec{S}_i \cdot \vec{S}_{i+1}$$

If possible: Exploiting SU(2) symmetry allows one to go to at least twice as long time-scales!

tJ~60

McCulloch, Gulasci EPL 2002



Langer, Heyl, McCulloch, HM PRB 2012

Fabian Heidrich-Meisner
LMU München

Example: Dynamics of density or spin density excitations

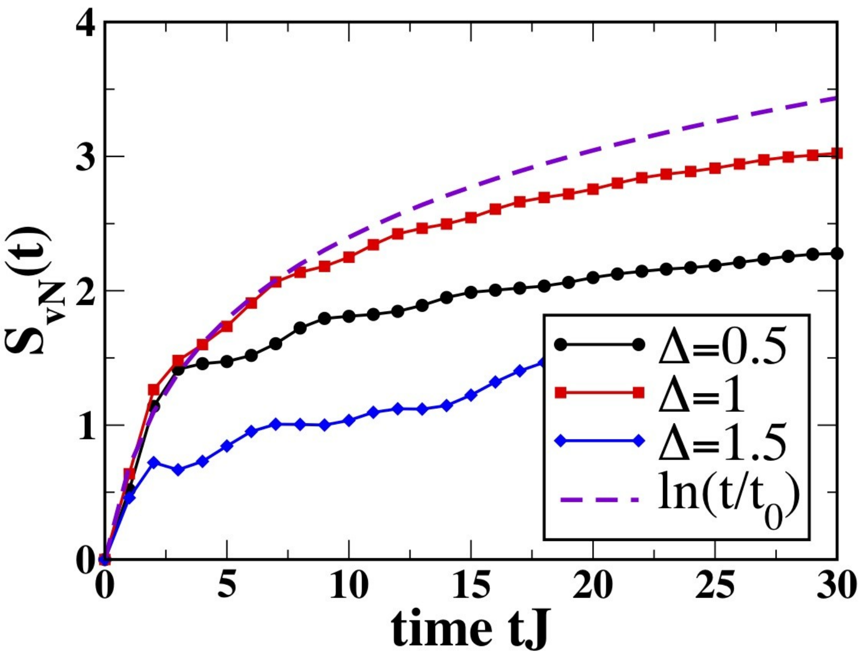
Spin and energy dynamics:

$$H = \sum_i h_i = J \sum_i \vec{S}_i \cdot \vec{S}_{i+1}$$

If possible: Exploiting SU(2) symmetry allows one to go to at least twice as long time-scales!

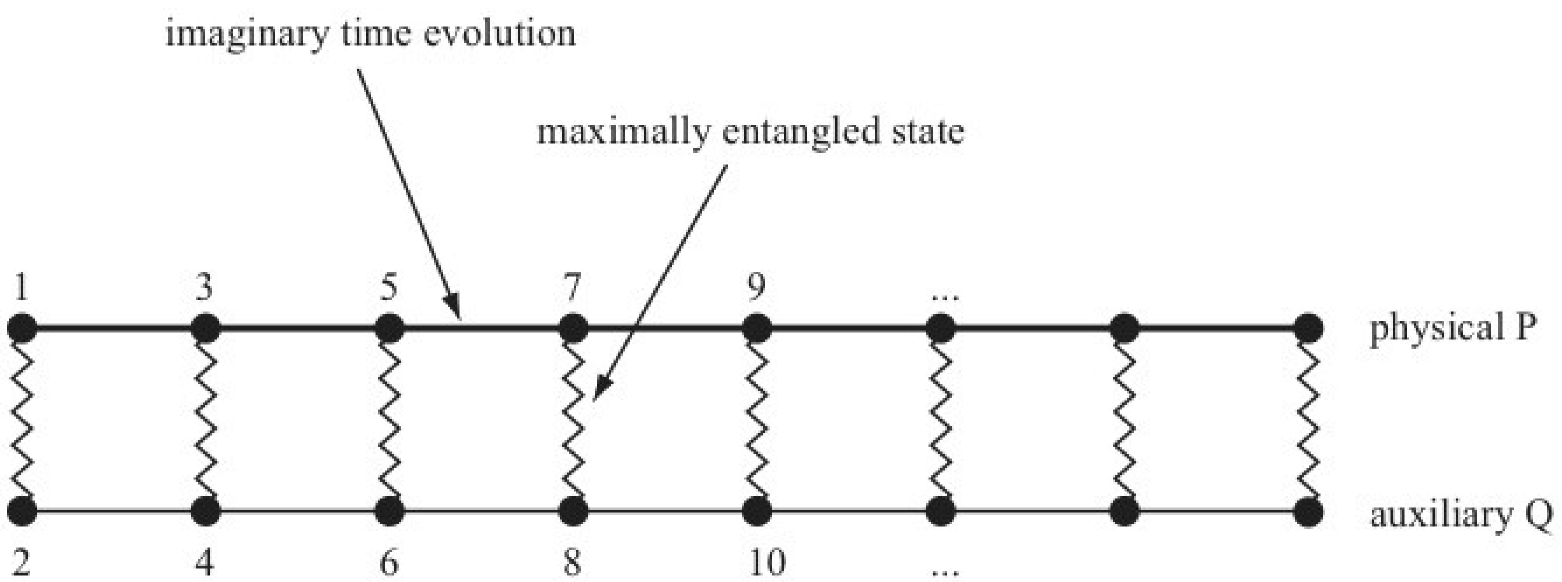
tJ~60

McCulloch, Gulasci EPL 2002



Langer, Heyl, McCulloch, HM PRB 2012

Finite-temperature methods: Purification



Schollwöck Ann. Phys. 2011

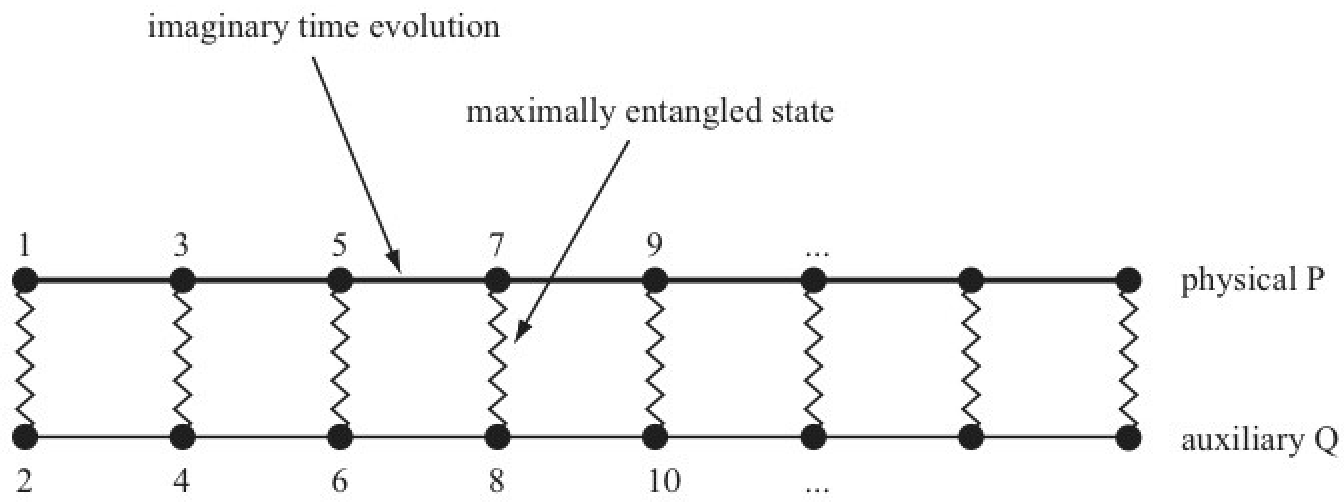
$$\hat{\rho}_P = \sum_\alpha s_\alpha^2 |\alpha_P\rangle\langle\alpha_P| \rightarrow |\psi\rangle = \sum_\alpha s_\alpha |\alpha_P\rangle|\alpha_Q\rangle \rightarrow \hat{\rho}_P = \mathrm{tr}_Q |\psi\rangle\langle\psi|$$

$$\hat{\rho}_\beta = Z(\beta)^{-1} e^{-\beta H} = Z(\beta)^{-1} e^{-\beta H/2}\,\hat{1}\,e^{-\beta H/2}$$

→ **We only need purification of infinite-T DM:** $\hat{1} = Z(0)\hat{\rho}_0$

Verstraete, Garcia-Ripoll, Cirac PRL 2005, Feiguin, White PRB 2005

Finite-temperature methods: Purification



Choose an initial state at β=0: Maximally entangled

$$|\psi(\beta=\mathbf{0})\rangle = \prod_i \sum_{s_i} |s_i \tilde{s}_i\rangle$$

Evolve in imaginary time:

$$|\psi(\beta)\rangle = e^{-\beta H/2} |\psi(\beta=\mathbf{0})\rangle$$

Verstraete, Garcia-Ripoll, Cirac PRL 2005,
Feiguin, White PRB 2005

At desired β, evolve in real time:

$$|\psi(t)\rangle_\beta = e^{-iHt} |\psi(\beta)\rangle$$

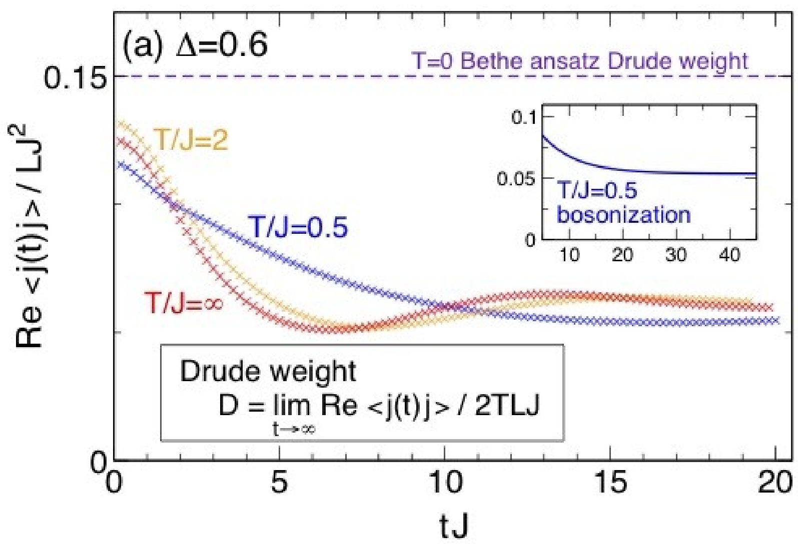
Unitary trafo on *ancillas:* disentangler!

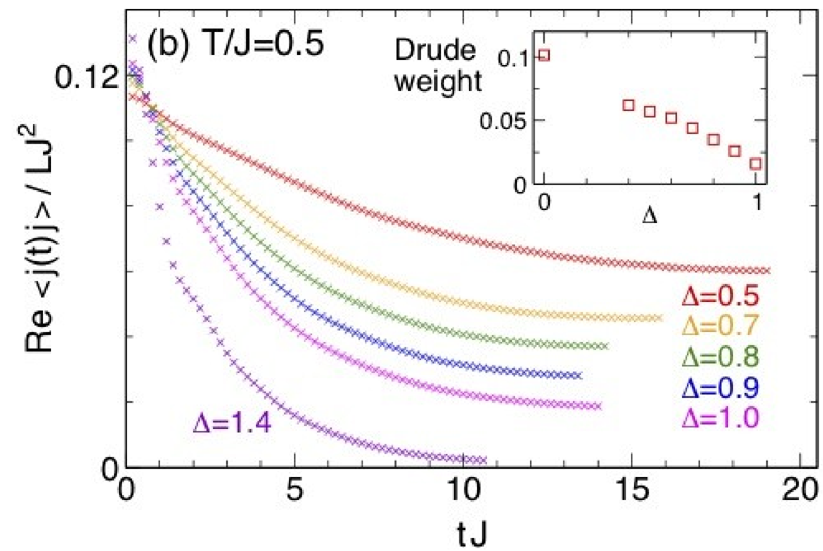
$$U_{aux} = e^{+iHt}$$

Karrasch, Bardarson, Moore PRL 2012
Barthel, Schollwöck, White PRB 2009

Current-current correlation functions

$$H = J \sum_{i=1}^{L} \left[\frac{1}{2} (S_i^+ S_{i+1}^- + h.c.) + \Delta S_i^z S_{i+1}^z \right]$$





If Drude D_s weight finite, then:

$$C(t) = \langle j(t) j \rangle \rightarrow D_s$$

Finite-T tDMRG:

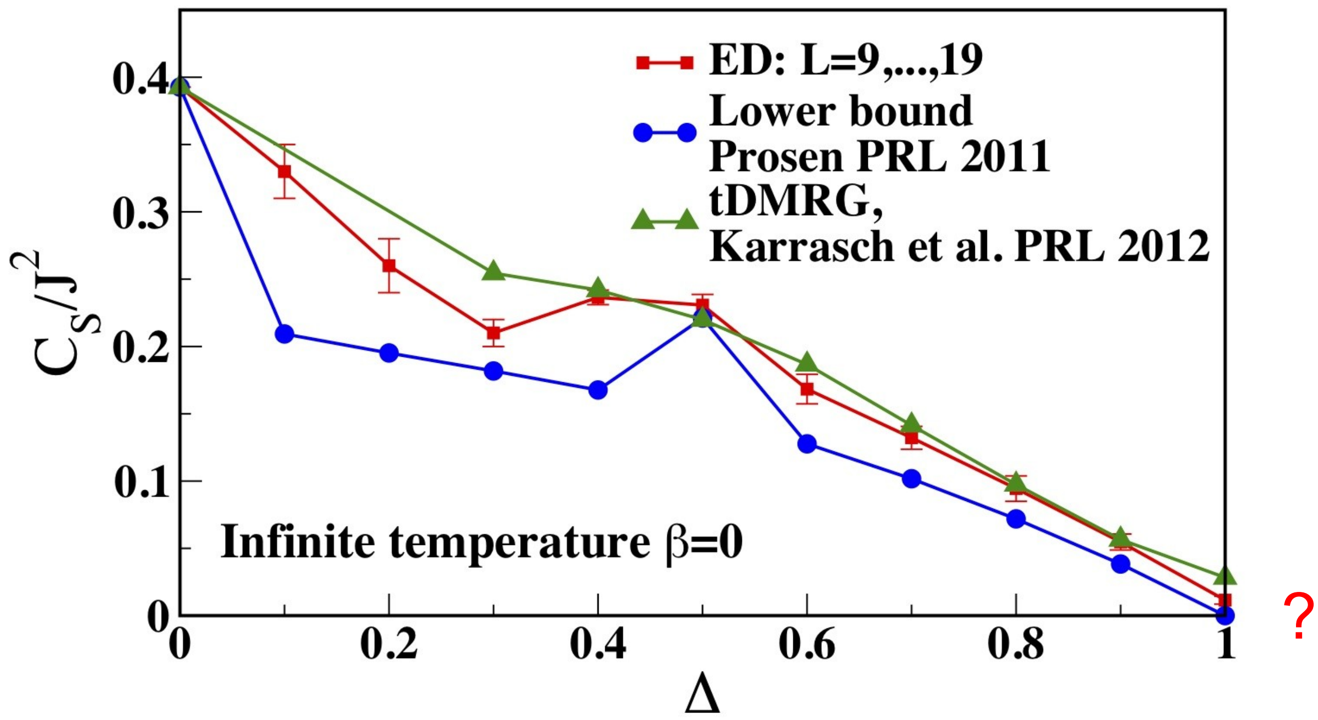
$$D_s(T>0) > 0 \text{ for } |\Delta| \leq 1$$

Karrasch, Bardarson, Moore PRL 2012

(exceeds Sirker, Pereira, Affleck PRL 2009 by a factor of 2)

Spin Drude weight: Comparison with ED

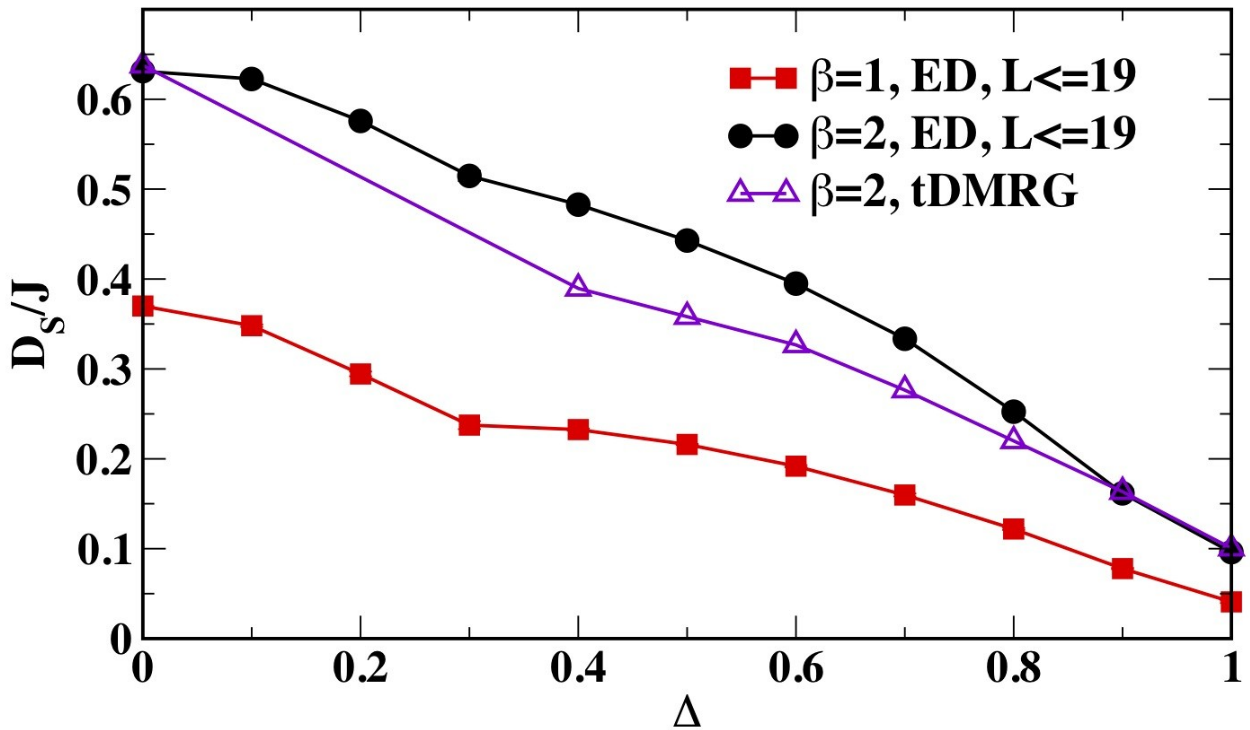
$$H = J \sum_{i=1}^{L} \left[\frac{1}{2} (S_i^+ S_{i+1}^- + h.c.) + \Delta S_i^z S_{i+1}^z \right]$$



ED: extrapolated in 1/L, L odd only, "grand-canonical"
→ Fairly good agreement at commensurate Δ

Spin Drude weight: Comparison with ED

$$H = J \sum_{i=1}^{L} \left[\frac{1}{2} \left(S_i^+ S_{i+1}^- + h.c. \right) + \Delta S_i^z S_{i+1}^z \right]$$



$D_s(\Delta=1)>1$

→ **Yet the extrapolation function needs justification**

→ **Discrepancy with extrapolation of canonical data remains**
Herbrych et al. PRB 2011

→ **Error bars for the tDMRG?**

Outlook: Beating the entanglement growth & Finite temperature

1) **Transverse-folding method**
Banuls, Hastings, Verstraete, Cirac Phys. Rev. Lett. 2009

2) **TD-DMRG in the Heisenberg picture**
Hartmann, Prior, Clark, Plenio Phys. Rev. Lett. 2009
Znidaric, Prosen J. Stat, Mech 2009

3) **Finite-temperatures: need mixed states instead of pure states !**

Using **purification** Feiguin, White Phys. Rev. B 2005
Zwolak, Vidal Phys. Rev. Lett. 2004
Verstraete, Garcia-Ripoll, Cirac Phys. Rev. Lett. 2004
Karrasch, Bardarson, Moore PRL 2012

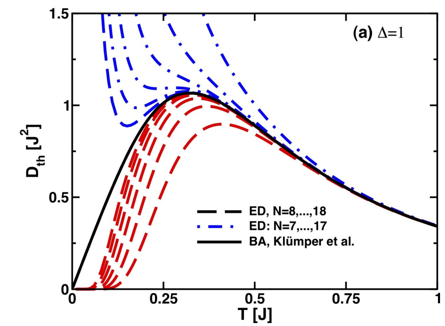
Using **transfer-matrix RG**: Sirker, Klümper Phys. Rev. B 2005

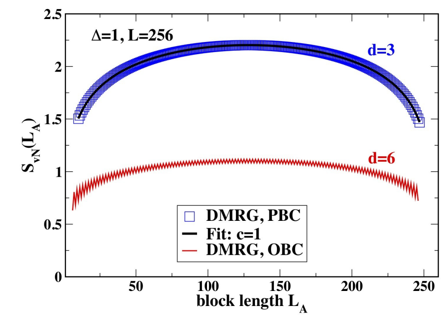
Minimally entangled states – **Metts**: White Phys. Rev. Lett. 2009
Stoudemire, White New. J. Phys. 2010

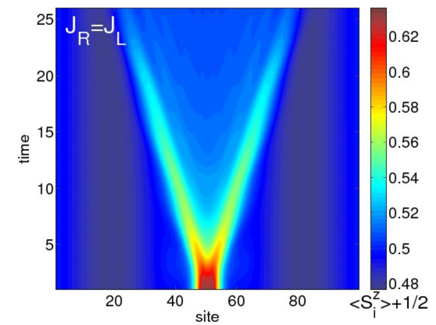
Simulating **master equations**:
Kantian, Dalmonte, Diehl. Hofstetter, Zoller, Daley Phys. Rev. Lett. 2009
Znidaric, Prosen J. Stat, Mech 2009; Hartmann, Prior, Clark, Plenio Phys. Rev. Lett. 2009

Summary

- **Exact diagonalization**
- **DMRG**
- **Time-dependent DMRG**
- **Selected applications:**
  - current-current correlations
  - Drude weight
  - thermodynamics
  - real-time dynamics







Reviews: Sandvik AIP Conf. Proc 2011,
Schollwöck Rev. Mod. Phys. 2005 & Ann. Phys. 2011

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University of Ljubljana

Thank you for your attention!

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