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Recent developments in DMRG

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Outline

1. Introduction
2. Dynamical DMRG
3. DMRG and quantum information theory
4. Time-evolution
5. Finite-temperature dynamics
6. Conclusion

DMRG is a variational method

System energy $E(\psi) = \dfrac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}$

Minimization w.r.t. $|\psi\rangle \Rightarrow$ ground state $|\psi_0\rangle + O(\epsilon)$ and $E_0 + O(\epsilon^2)$

DMRG wave function: Matrix-Product State

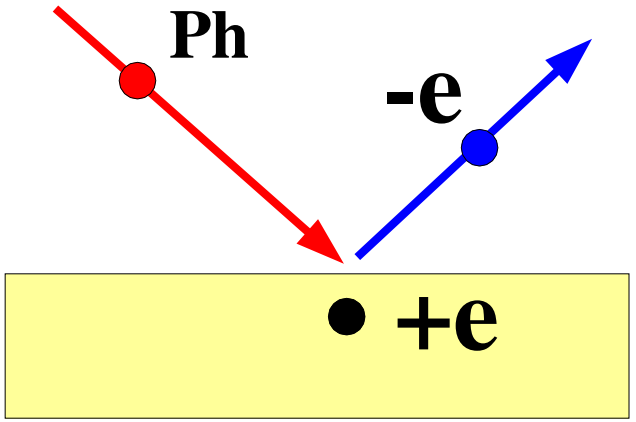
$$|\psi\rangle = \sum_{\{s_1,s_2,\ldots,s_N\}} (M_1[s_1] \cdot M_2[s_2] \cdot \ldots \cdot M_N[s_N])\ |s_1\rangle|s_2\rangle \ldots |s_N\rangle$$

with $M_i[s_i] = m \times m$ matrix and $|s_i\rangle, s_i = 1, \ldots, n_i =$ basis states of site i

Exact wave function for $m \to \sqrt{\mathcal{D}} = \sqrt{n_1 n_2 \ldots n_N}$

[S. Östlund and S. Rommer, Phys. Rev. Lett. **75**, 3537 (1995); PRB **55**, 2164 (1997)]

Photoemission



ARPES spectrum = spectral functions

$$A_\sigma(k,\omega\leq 0) = \lim_{\eta\to 0} Im\, G_\sigma(k,\hbar\omega - i\eta)$$

$$= \sum_n |\langle n|\hat{c}_{k,\sigma}|\psi_0\rangle|^2\, \delta(E_n - E_0 + \hbar\omega)$$

$$G_\sigma(k,\hbar\omega - i\eta) = \frac{1}{\pi}\,\langle\psi_0|\hat{c}^\dagger_{k,\sigma}\frac{1}{\hat{H} - E_0 + \hbar\omega - i\eta}\hat{c}_{k,\sigma}|\psi_0\rangle$$

Dynamical correlation functions with DMRG

$$\chi_{\hat{A}}(\omega + i\eta) = -\frac{1}{\pi}\langle\psi_0|\hat{A}^\dagger \frac{1}{E_0 + \omega + i\eta - \hat{H}}\hat{A}|\psi_0\rangle$$

Lanczos vector method

[K. Hallberg, PRB **52**, 9827 (1995)]

$$\begin{aligned} |\phi_0\rangle &= \hat{A}|\psi_0\rangle \\ |\phi_1\rangle &= \hat{H}|\phi_0\rangle - a_0|\phi_0\rangle \\ |\phi_{n+1}\rangle &= \hat{H}|\phi_n\rangle - a_n|\phi_n\rangle - b_n^2|\phi_{n-1}\rangle \end{aligned}$$

$\rho_{\mathrm{L}} = \psi_0\psi_0^*$+ Lanczos vectors

Correction vector method

[S. Ramasesha et *al.*, Synth. Met. **85**, 1019 (1997), T.D. Kühner and S.R. White, PRB **60**, 335 (1999)]

$$|CV\rangle = \frac{1}{E_0 + \omega + i\eta - \hat{H}}\hat{A}|\psi_0\rangle$$

$$\chi_{\hat{A}}(\omega + i\eta) = \frac{-1}{\pi}\langle\psi_0|\hat{A}^\dagger|CV\rangle$$

$\rho_{\mathrm{CV}} = \psi_0\psi_0^*$+ correction vectors

Variational principle for dynamical correlation functions

[E. Jeckelmann, PRB **66**, 045114 (2002)]

Functional

$$W_{\hat{A},\eta}(\omega,\psi) = \langle\psi| \left(\hat{H} - \omega - E_0\right)^2 + \eta^2 |\psi\rangle + \eta\langle\psi|\hat{A}|\psi_0\rangle + \eta\langle\psi_0|\hat{A}^\dagger|\psi\rangle$$

Minimization with respect to ψ

$$|\psi_{\min}\rangle = \frac{-\eta}{(E_0 + \omega - \hat{H})^2 + \eta^2}\, \hat{A}|\psi_0\rangle + \mathcal{O}(\epsilon)$$

$$W_{\hat{A},\eta}(\omega,\psi_{\min}) = -\pi\eta\ Im\ \chi_{\hat{A}}(\omega + i\eta) + \mathcal{O}(\epsilon^2)$$

$$Re\ \chi_{\hat{A}}(\omega + i\eta) = \frac{-1}{\pi\eta}\, \langle\psi_0|\hat{A}^\dagger(\hat{H} - E_0 - \omega)|\psi_{\min}\rangle$$

Note

$$|\psi_{\min}\rangle \quad \underset{(\eta \to 0)}{\longrightarrow} \quad -\pi \, \langle \psi_n | \hat{A} | \psi_0 \rangle \, \delta(\omega - E_n + E_0) \, |\psi_n\rangle$$

$$|CV\rangle \quad = \quad \frac{\hat{H} - E_0 - \omega + i\eta}{\eta} \, |\psi_{\min}\rangle$$

Dynamical DMRG (DDMRG)

[E. Jeckelmann, PRB 66, 045114 (2002)]

For the spectral function ($\hat{A} = \hat{c}_{k,\sigma}$)

$$W_{k,\sigma,\eta}(\omega,\psi) = \langle\psi| \left(\hat{H} + \omega - E_0\right)^2 + \eta^2 |\psi\rangle + \eta\langle\psi|\hat{c}_{k,\sigma}|\psi_0\rangle + \eta\langle\psi_0|\hat{c}^\dagger_{k,\sigma}|\psi\rangle$$

Minimization of $W_{k,\sigma,\eta}(\omega,\psi)$ **with a regular DMRG algorithm and** $\rho_{\rm CV} = (\psi_0\psi_0^* + \psi_{\rm min}\psi_{\rm min}^*$ **+ first Lanczos vector) yields**

$$\begin{aligned} A^\eta_\sigma(k,\omega) &= Im\, G_\sigma(\hbar\omega - i\eta) \\ &= \frac{-1}{\pi\eta} W_{k,\eta}(\omega,\psi_{\rm min}) \\ &= \frac{1}{\pi}\int_{-\infty}^{\infty} d\omega' A_\sigma(\omega') \frac{\eta}{(\omega-\omega')^2+\eta^2} \end{aligned}$$

Spectrum in the thermodynamic limit

[E. Jeckelmann, PRB 66, 045114 (2002)]

Lehmann spectral representation

$$I(\omega) = \mathrm{Im}\chi_{\hat{A}}(\omega) \quad = \quad \lim_{\eta\to 0} \lim_{N\to\infty} \sum_n \frac{\eta}{\pi} \frac{|\langle\psi_n|\hat{A}|\psi_0\rangle|^2}{(\omega - E_n + E_0)^2 + \eta^2}$$

Using $\eta(N) > \eta_0(N)$ **with** $\eta(N \to \infty) \to 0$

$$I(\omega) \quad = \quad \lim_{N\to\infty} \sum_n \frac{\eta(N)}{\pi} \frac{|\langle\psi_n|\hat{A}|\psi_0\rangle|^2}{(\omega - E_n + E_0)^2 + \eta(N)^2}$$

Dense spectrum: $\eta_0(N) > E_{n+1}(N) - E_n(N)$
Discrete spectrum: $\eta_0(N) = 0$

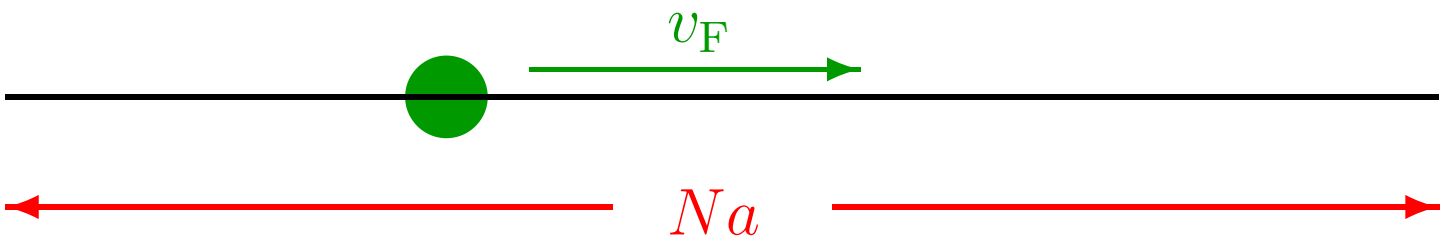
Methods

- convolution of an infinite-system spectrum for comparison
- extrapolation or scaling analysis for $N \to \infty, \eta(N) \to 0$
- deconvolution of finite-system spectrum
  (fit to a smooth infinite-system spectrum)

One-dimensional systems

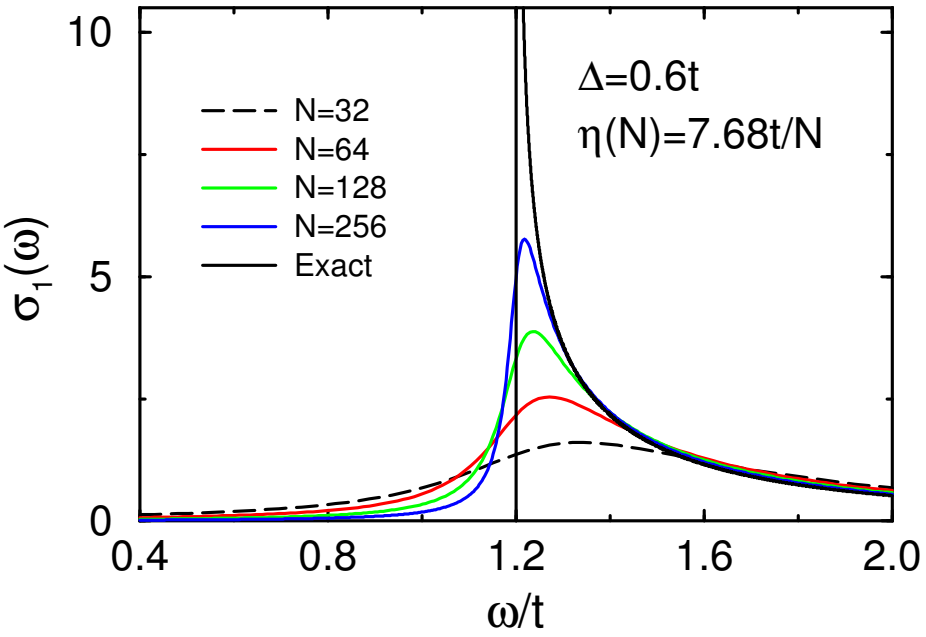
- $\eta(N) = cN^{-1}$ with $c >$ effective band width W
- $\eta^{-1} \sim$ measurement time Δt
- One-dimensional electron gas (Fermi velocity $v_{\mathrm{F}} \approx \frac{Wa}{2}$)

$$v_{\mathrm{F}} \Delta t < \frac{Na}{2}$$

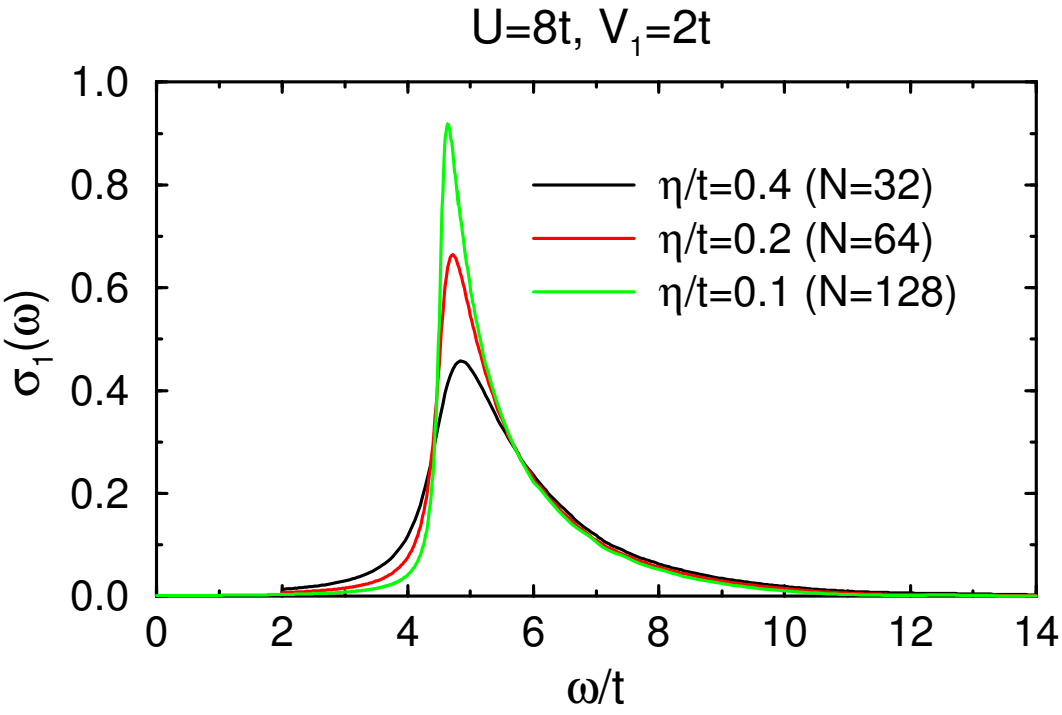


Examples: Optical conductivity of one-dimensional insulators

Peierls insulator



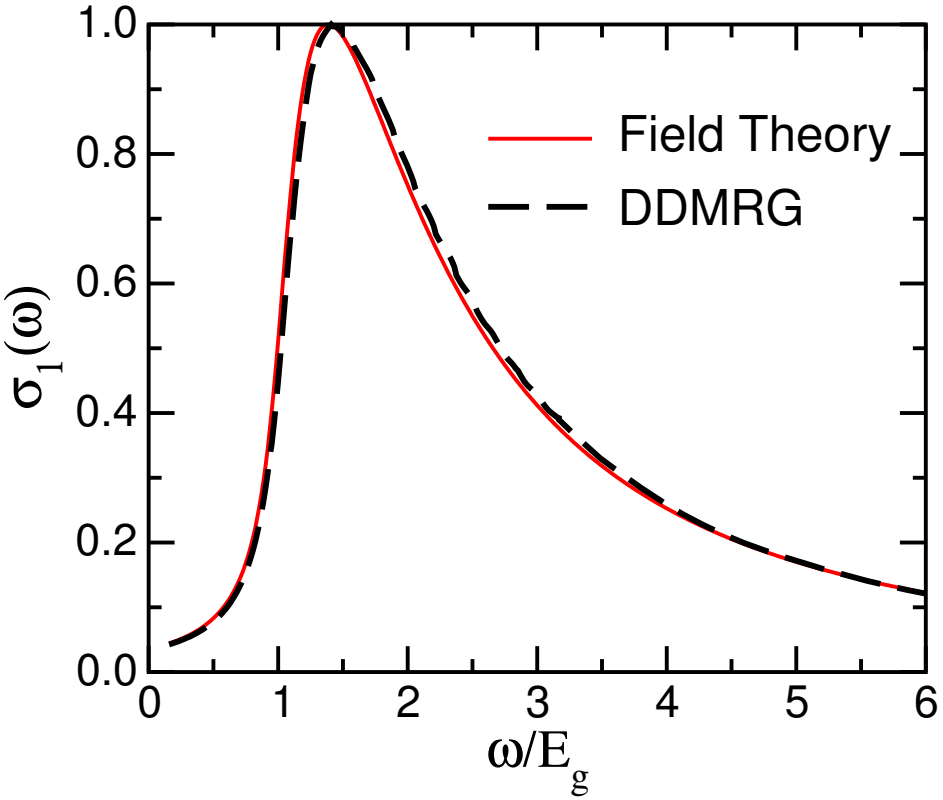
Half-filled 1D extended Hubbard model



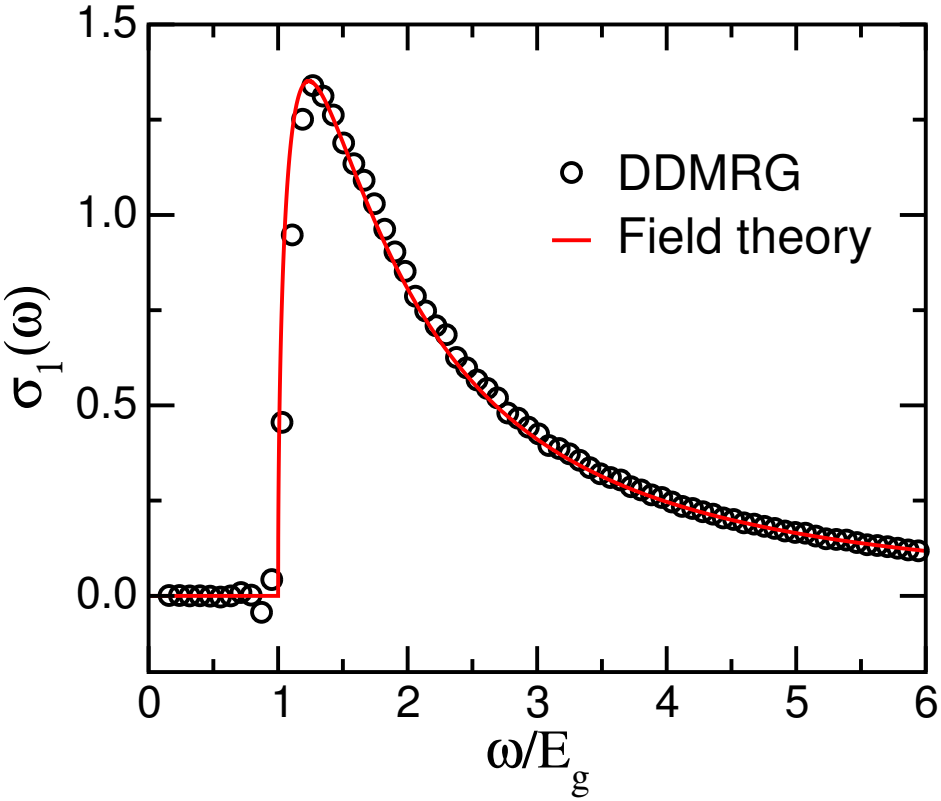
Optical conductivity of the 1D Hubbard model

(Half filling, $U = 3t$)

Broadening $\eta = 0.1t$



No broadening/deconvolved



Jeckelmann, Gebhard and Essler, PRL 85, 3910 (2000)
Jeckelmann and Fehske, cond-mat/0510637

Quasi-momentum for open boundary conditions

[H. Benthien, F. Gebhard, and E. Jeckelmann, Phys. Rev. Lett. **92**, 256401 (2004)]

Periodic boundary conditions

$\Rightarrow$ Bloch wavefunctions for momenta (wavevectors)

$$\hat{c}_{k\sigma} = \sqrt{\frac{1}{N}} \sum_n e^{ikn}\, \hat{c}_{n\sigma} \qquad k = \frac{2\pi}{N} z \quad \text{with} \quad z = 0, \pm 1, \pm 2, \ldots, \frac{N}{2}$$

Open boundary conditions

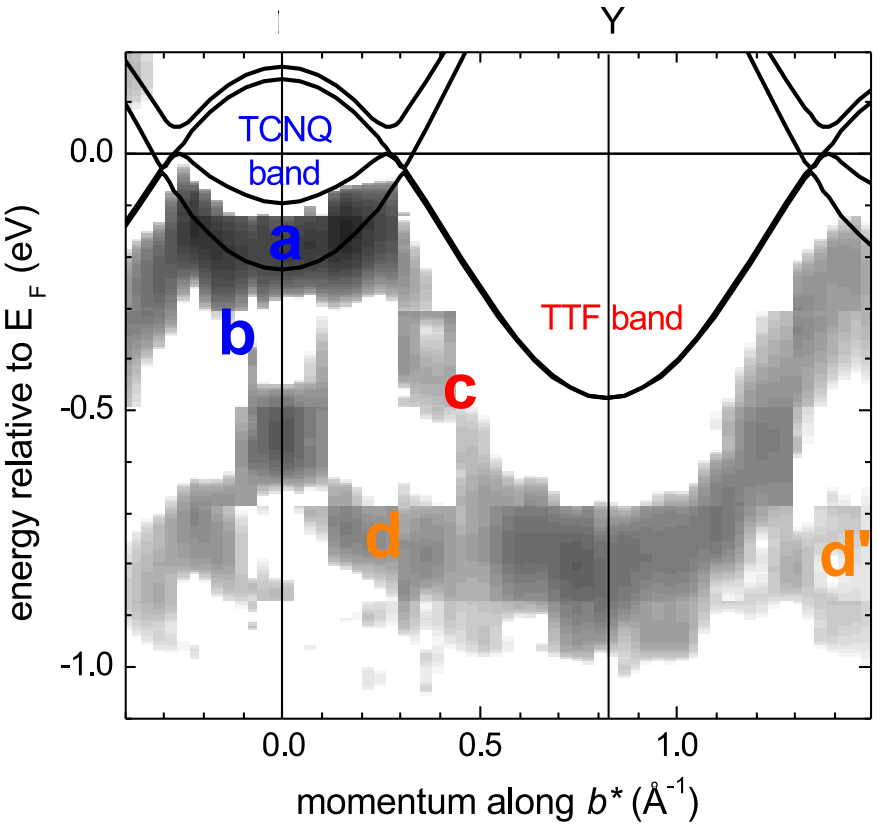
$\Rightarrow$ particle-in-the-box wavefunctions for quasi-momenta

$$\hat{c}_{k\sigma} = \sqrt{\frac{2}{N+1}} \sum_n \sin(kn)\, \hat{c}_{n\sigma}\ , \qquad k = \frac{\pi}{N+1}\, j \quad \text{with} \quad j = 1, 2, \ldots, N$$

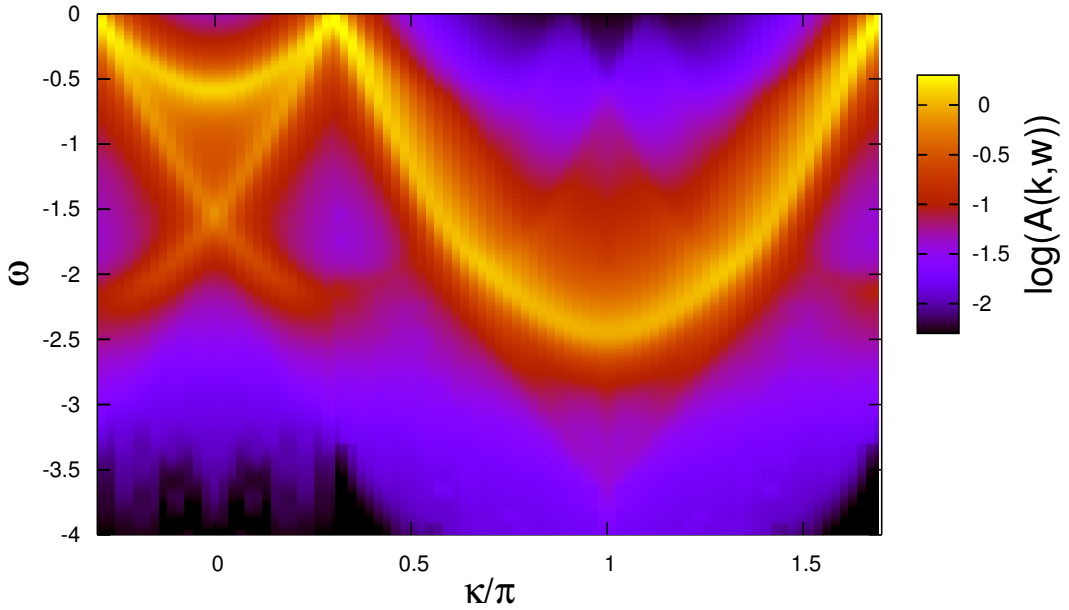
ARPES spectrum of TTF-TCNQ

[R. Claessen *et al.*, PRL 88, 096402 (2002); M. Sing *et al.*, PRB 68, 125111 (2003)]
[Benthien, Gebhard, and Jeckelmann, PRL 92, 256401 (2004)]

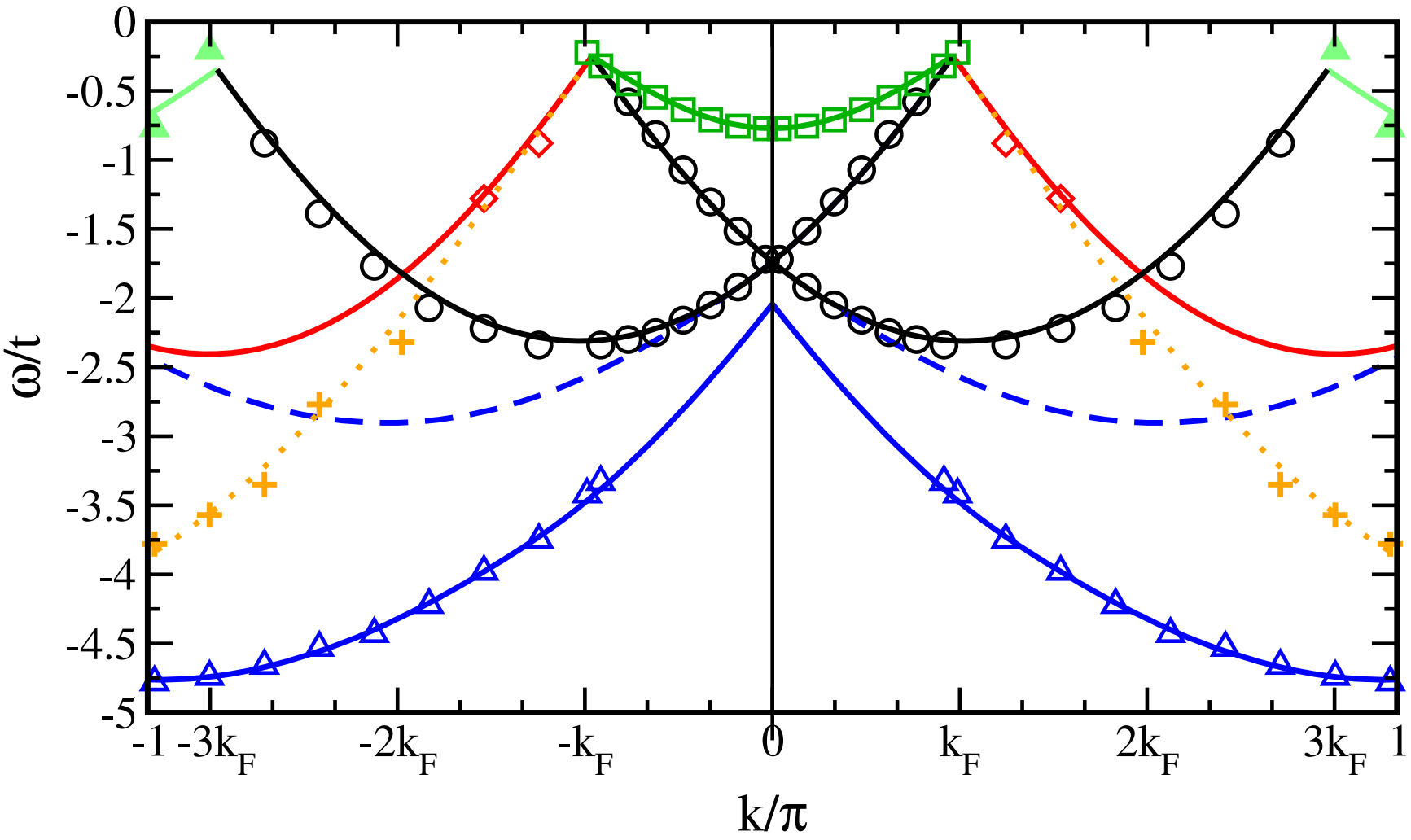
Experiment



Hubbard model



DDMRG vs Bethe Ansatz ($\rho = 0.6$, $U = 4.9t$)



Spectral properties of $SrCuO_2$

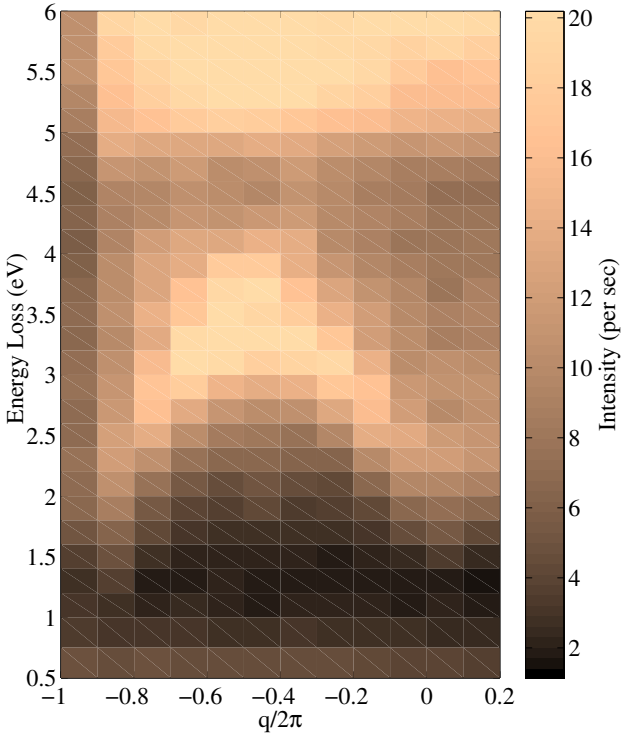
[H. Benthien and E. Jeckelmann, e-print cond-mat/0606748]

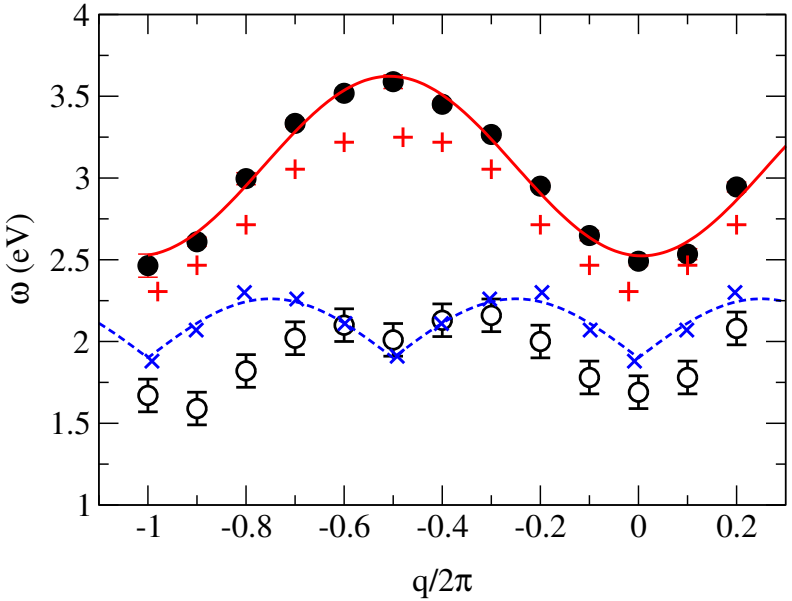
Quantitative description of
- **optical absorption,**
- **angle-resolved photoemission spectrum,**
- **resonant inelastic X-ray scattering (RIXS),**
- **and neutron scattering**

with the one-dimensional half-filled extended Hubbard model

RIXS spectrum

[Y.-J. Kim *et al.*, Phys. Rev. Lett. 92, 137402 (2004)]





$\epsilon_c(k) \sim 2t\cos(q)$ $\epsilon_s(k) \sim \frac{\pi J}{2}|\sin(q)|$

DMRG and quantum information theory: A new perspective

The Hilbert space truncation in DMRG is optimal because

- $||\psi_{\rm exact} - \psi_{\rm DMRG}||$ **is maximal**
  [Noack and White in I. Peschel *et al.*, Density Matrix Renormalization, Springer, 1999]
- **the maximal entanglement between system and environment is preserved**
  [G. Vidal *et al.*, PRL **90**, 227902 (2003)]

Measure of entanglement: Von Neumann entropy

$$S = -Tr\rho \ln_2(\rho) = -\sum_\mu \lambda_\mu \ln_2(\lambda_\mu)$$

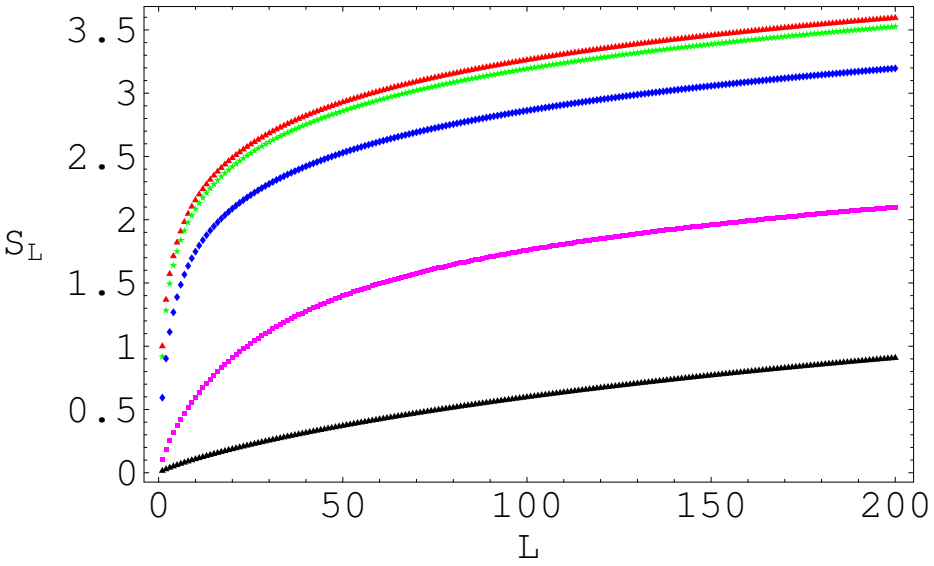
Examples

- $\lambda_1 = 1, \lambda_{\mu>1} = 0 \Rightarrow S = 0$**, i.e. no entanglement**
- $\lambda_\mu = 1/m \Rightarrow S = \ln_2(m)$**, i.e. maximal entanglement**

Entanglement entropy S_L of a L-site cluster in an infinite chain

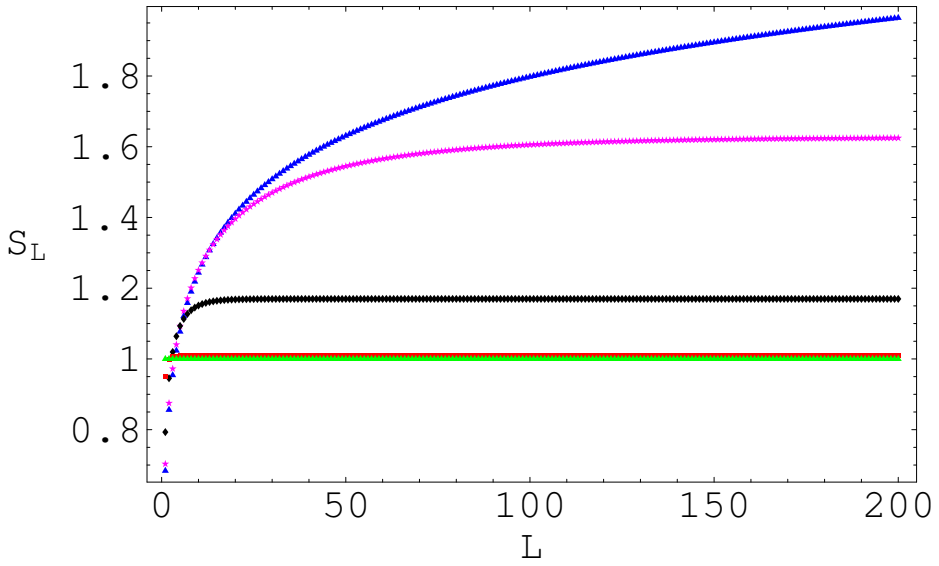
- S_L **diverges for** $L \to \infty$ **at criticality**
- S_L **saturates for** $L \to \infty$ **in the non-critical regime**

Isotropic XX chain in a magnetic field



S_L vanishes for $H = H_c$

Ising chain in a transverse field



$S_L = 0$ for $H = 0$

S_L diverges at criticality $H = H_c$

[Latorre, Rico, and Vidal, arXiv:quant-ph/0304098]

Geometric arguments $\Rightarrow S_L \sim L^{d-1}$ **for a hypercubic cluster in dimension** $d > 1$

Number of density matrix eigenstates $m(L)$ for a fixed accuracy in the thermodynamic limit $L \to \infty$

- **In $d = 1$ away from criticality, $m(L) \to$ finite value**
- **In $d = 1$ at criticality, $\lim_{L\to\infty} m(L) = \infty$**
- **For $d > 1$, $m(L) \sim n^{L^{d-1}}$**

Optimization using entanglement entropy
(for non-local systems)

DMRG procedure = successive density-matrix truncations

- **Fixed number m of density-matrix eigenstates is not optimal**
- **Dynamical block state selection is better: $P_m \leq const.$**
  [Legeza *et al.*, PRB 67, 125114 (2003)]
- **Even better: quantum information loss $\chi(S) \leq const.$**
  [Legeza and Sólyom, PRB 70, 205118 (2004)]

Site ordering in non-local systems

- **Optimal ordering using quantum information entropy**
  [Legeza and Sólyom, PRB 68, 195116 (2003)]

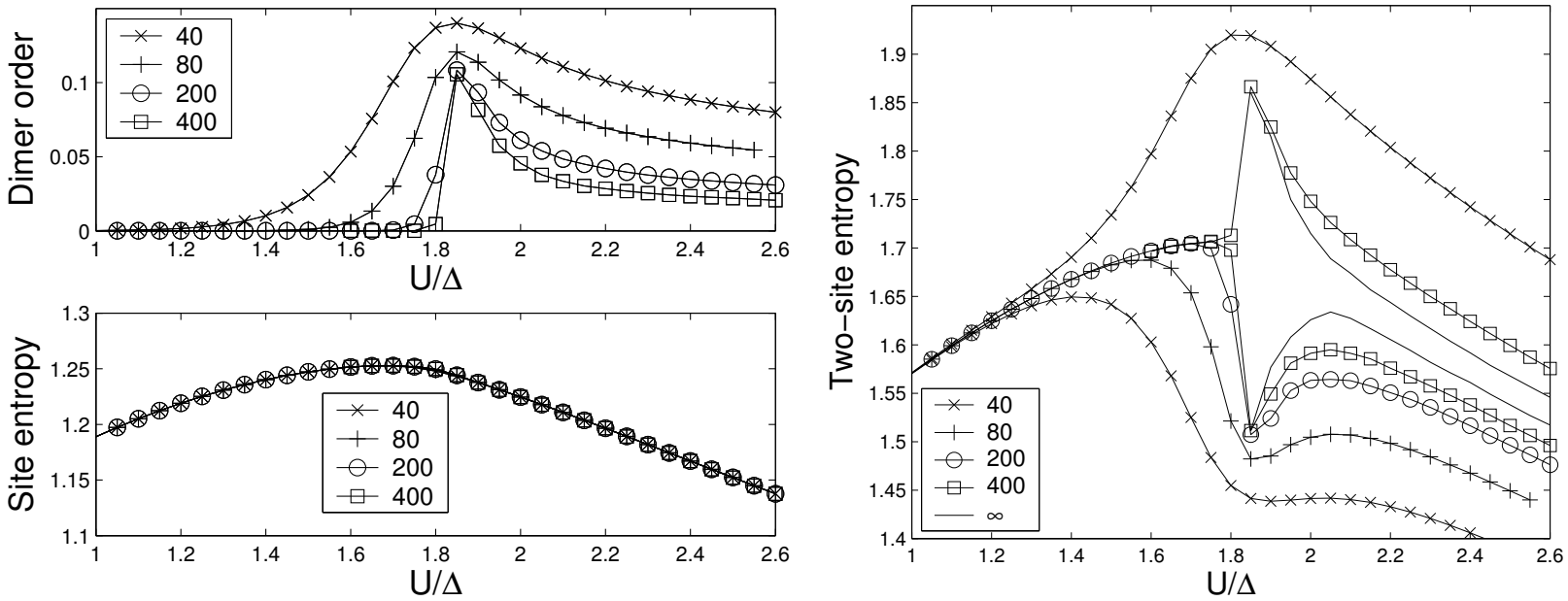
Entropy and quantum phase transitions

Quantum phase transition ≡ singularity in the ground state entanglement
[Wu, Sarandy, and Lidar, PRL 93, 250404 (2004)]

Problem: measure of entanglement ?

- **Cluster entropy S_L for $L \to \infty$ [G. Vidal *et al.*, PRL 90, 227902 (2003)]**
- **Concurrence (only for spin systems) [A. Osterloh, Nature 416, 608 (2005)]**
- **One-site entropy (often insensitive) [Gu *et al.*, PRL 93, 086402 (2004)]**
- **Two-site entropy [Legeza and Sólyom, PRL 96, 116401 (2006)]**

Ionic Hubbard model ($\Delta = t$)



Variational matrix-product states

Reformulation of DMRG as a variational optimization of matrix-product states

[F. Verstraete, D. Porras, and J.I. Cirac, PRL **93**, 227205 (2004)]

- **As good as DMRG for open chains**
- **In theory, improvement for periodic systems**
- **In theory, extension to higher dimensions with projected entangled pair states (PEPS)**
  [F. Verstraete and J. I. Cirac, cond-mat/0407066]

Time-dependent DMRG

$$i\hbar\frac{\partial\psi(t)}{\partial t} = H(t)\psi(t)$$

First approach: integration in a static superblock (Runge-Kutta)

- $\rho = \psi_0\psi_0^*$ **(incorrect)**

  [Cazalilla and Marston, PRL 88, 256403 (2002)]

- $\rho = \sum_i \psi_(t_i)\psi^*(t_i)$ **(not practical)**

  [Luo, Xiang, and Wang, PRL 91, 049701 (2003)]

Second approach: Taylor-expansion of $\exp(-iHt)$

- $\rho = \sum_n \psi_n\psi_n^*$ **with** $\psi_n = H^n\psi(t=0)$ **(not practical)**

  [Schmitteckert, PRB 70, 121302 (2004)]

Vidal's algorithm [G. Vidal, PRL **93**, 040502 (2004)]

Only one-dimensional nearest-neighbor Hamiltonians

$$H = \sum_{k=1}^{N-1} H_{k,k+1}$$

Trotter-Suzuki decomposition

$$\exp(-iH\tau) = \prod_{k=1}^{N/2} \exp(-i\tau H_{2k-1,2k}) \prod_{k=1}^{N/2-1} \exp(-i\tau H_{2k,2k+1}) + \mathcal{O}(\tau^2)$$

(More accurate for higher order decomposition)

Matrix-product representation

$$\exp(-i\tau H_{k,k+1})\psi(t) \Rightarrow M_k[s_k], M_{k+1}[s_{k+1}] \rightarrow M'_k[s_k], M'_{k+1}[s_{k+1}]$$

Time step = sweep through the lattice $k = 1, \ldots, N-1$

$$\psi(t+\tau) = \exp(-i\tau H)\psi(t)$$

(Adaptive) time-dependent DMRG (t-DMRG)

[A.J. Daley, C. Kollath, U. Schollwöck, and G. Vidal, JSTAT (2004);
S.R. White and A.E. Feiguin, PRL **93**, 076401 (2004)]

Efficient implementation of Vidal's algorithm within DMRG

The DMRG superblock basis is adapted at every step

$$\rho(t,k) = \psi(t,k)\psi^*(t,k)$$

DMRG step: Adding one site to the left block or to the right block

$$\psi(t,k{+}1) = \exp(-i\tau H_{k,k+1})\psi(t,k) \quad \textbf{or} \quad \psi(t,k) = \exp(-i\tau H_{k,k+1})\psi(t,k{+}1)$$

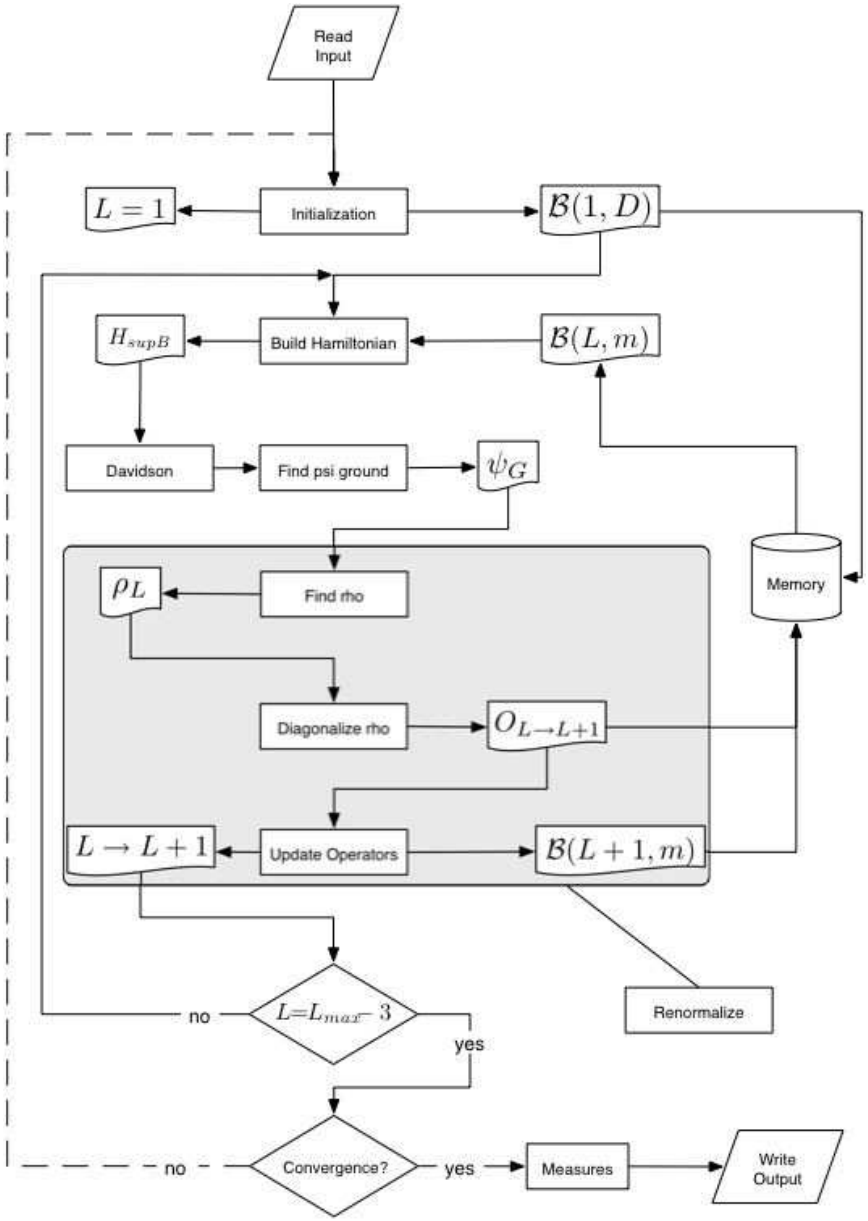
Time step = one sweep from (L) left to right or (R) right to left

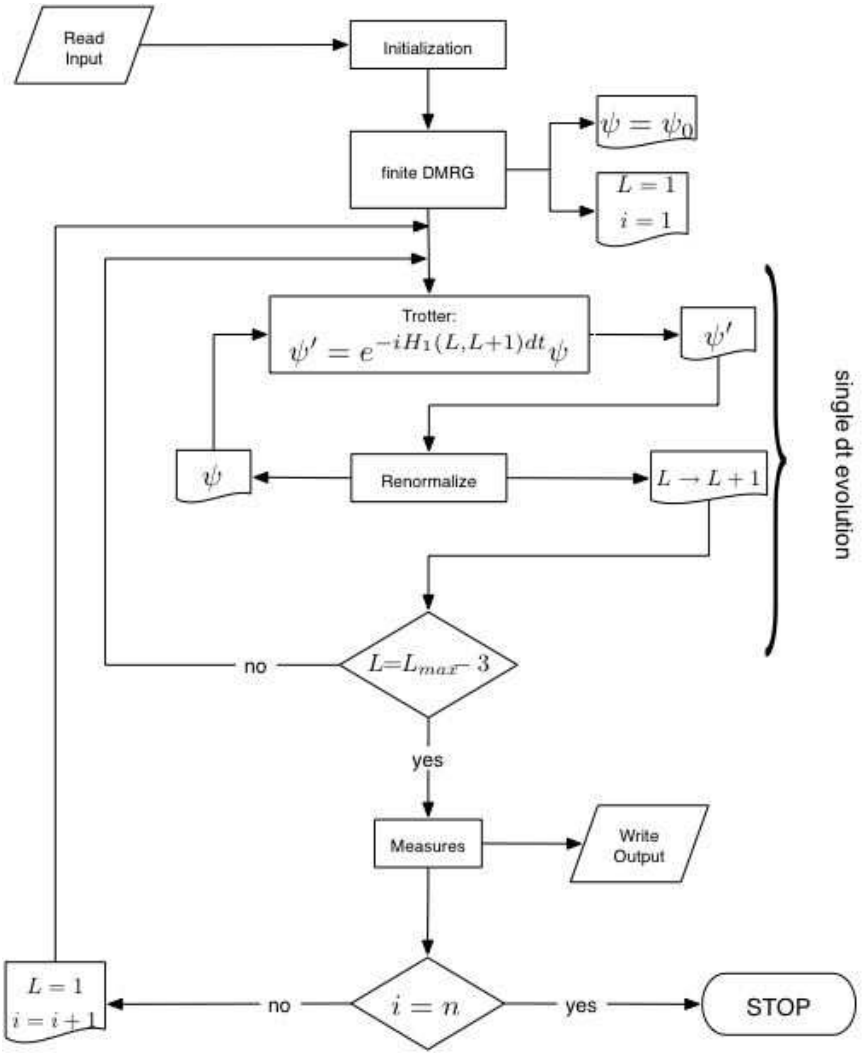
$$\text{(L)} \quad \psi(t+\tau) = \psi(t,k=N) = \exp(-i\tau H)\psi(t,k=1) = \exp(-i\tau H)\psi(t)$$

$$\text{(R)} \quad \psi(t+\tau) = \psi(t,k=1) = \exp(-i\tau H)\psi(t,k=N) = \exp(-i\tau H)\psi(t)$$

For longer-range interactions or higher dimensions: Adaptive Runge-Kutta approach
[Feiguin and White, PRB **72**, 020404 (2005)]

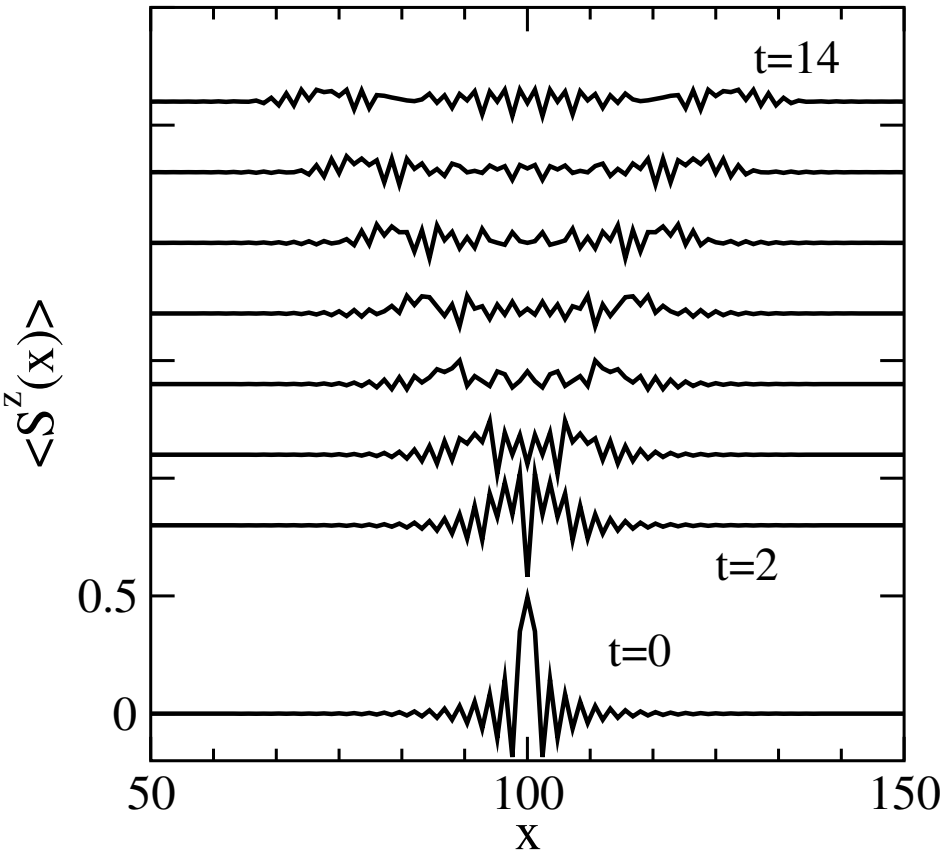
t-DMRG code





From De Chiara *et al.*, e-print arXiv:cond-mat/0603842

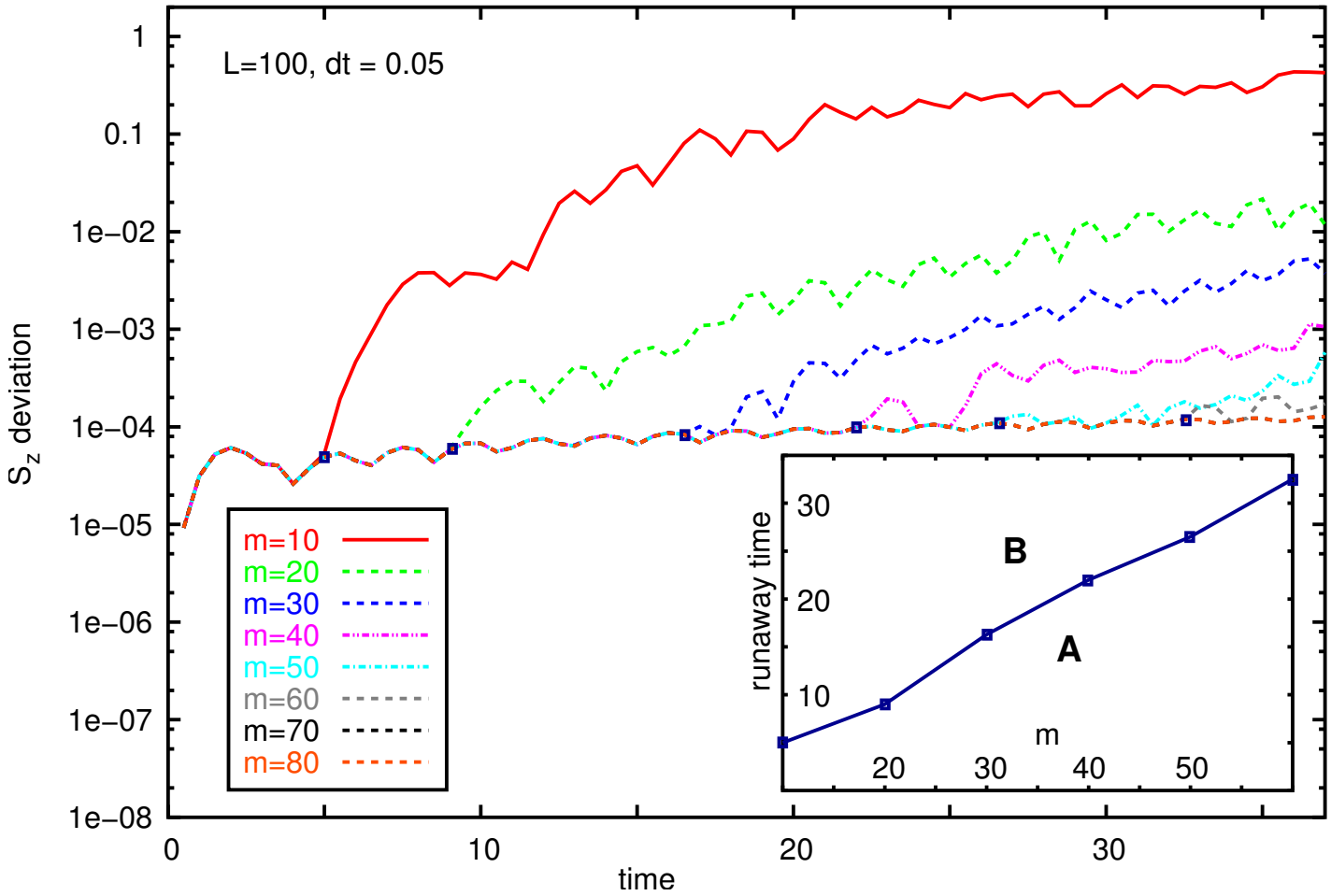
Spin chain dynamics



Time evolution of the local magnetization $\langle S^z(x)\rangle$ of a 200 site spin-1 Heisenberg chain after $S^+(100)$ is applied ($\tau = 0.1$).

From S.R. White and A.E. Feiguin, PRL **93**, 076401 (2004)

Problem: runaway time

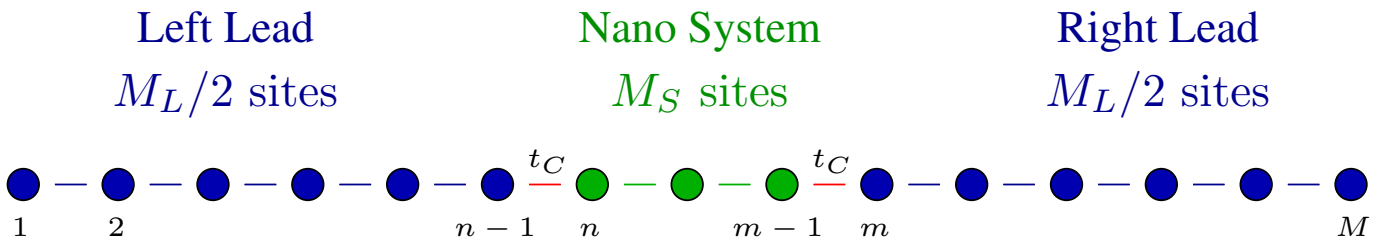


Error in the local magnetization as a function of time in the XX model ($\tau = 0.05$).

From Gobert, Kollath, Schollwöck, Schütz, PRE **71**, 036102 (2005)

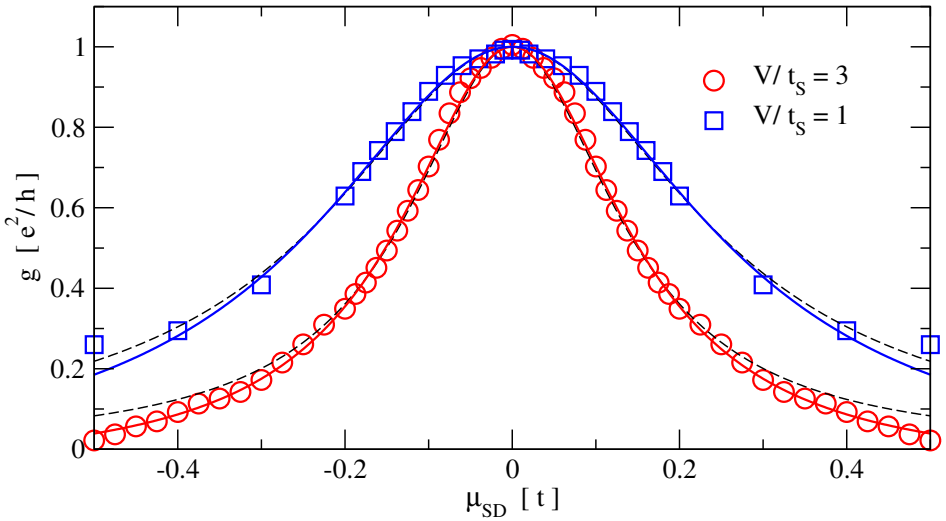
Transport through nanostructures

Interacting spinless fermion system coupled to non-interacting leads



Finite-size effects are important $\Rightarrow$ no steady state

Differential conductance vs bias voltage ($M_S = 7$)
($M = 144, m = 600$ for weak coupling, $M = 192, m = 800$ for strong coupling)



From Schneider and Schmitteckert, arXiv:cond-mat/0601389

Finite-temperature dynamics

Density operator ρ in Hilbert space of dimension D
$\equiv$ wavefunction in space of dimension D^2

$\Rightarrow$ matrix-product representation of ρ

$$\rho = \sum_{\{s_1,\ldots,s_N\}} \sum_{\{t_1,\ldots,t_N\}} (M_1[s_1,t_1] \cdot \ldots \cdot M_N[s_N,t_N])\ |s_1\rangle \ldots |s_N\rangle\langle t_1| \ldots \langle t_N|$$

with $M_i[s_i,t_i] = m \times m$ matrix and $|s_i\rangle, s_i = 1,\ldots,n_i$ = basis states of site i

Imaginary and real time evolution

$$\frac{d\rho}{d\beta} = -H\rho \text{ and } \rho(\beta = 0) = Id \Leftrightarrow \rho = \exp(-\beta H)$$

$$\frac{d\rho}{dt} = -i[H,\rho] \Leftrightarrow \rho(t+\tau) = \exp(-iH\tau)\rho(t)\exp(iH\tau)$$

[Verstraete *et al.*, PRL **93**, 207204 (2004); Zwolak and Vidal, PRL **93**, 207205 (2004); Feiguin and White, PRB **72**, 220401 (2005)]

Summary

- DMRG is a variational method
- Connection to matrix-product states
- Relation to quantum information theory (entanglement)
- Optimization using entanglement entropy
- Criticality and entanglement
- Time-dependent DMRG
- Finite-temperature dynamics
- Bright prospects for the future

Thanks

Holger Benthien (Marburg)

Florian Gebhard (Marburg)

Satoshi Nishimoto (Dresden)

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