Density-Matrix Renormalisation Group/ Matrix Product States

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fundamental problem of solid state

- what do we need DMRG for? problem class:

  fundamental Hamiltonian (without lattice vibrations…!):

$$H = \sum_{j=1}^{e^-} \frac{\mathbf{p}_j^2}{2m_e} + \frac{1}{2}\frac{1}{4\pi\epsilon_0}\frac{q_e^2}{|\mathbf{r}_i - \mathbf{r}_j|} + \sum_{j}^{e^-} V_{\text{eff}}(\mathbf{r}_j)$$

kinetic energy | electron-electron interaction | lattice potential

- we don't know how to solve the Schrödinger equation!

  problem: electron-electron interactions

compression of information

- compression of information necessary and desirable
  - diverging number of degrees of freedom
  - emergent macroscopic quantities: temperature, pressure, ...

- classical spins
  - thermodynamic limit: $N \to \infty$ $2N$ degrees of freedom (linear)

- quantum spins
  - superposition of states
  - thermodynamic limit: $N \to \infty$ 2^N degrees of freedom (exponential)

classical simulation of quantum systems

- compression of exponentially diverging Hilbert spaces
- what can we do with classical computers?
  - exact diagonalizations
    - limited to small lattice sizes: 40 (spins), 20 (electrons)
  - stochastic sampling of state space
    - quantum Monte Carlo techniques
    - negative sign problem for fermionic systems
  - physically driven selection of subspace: decimation
    - variational methods
    - renormalization group methods
    - **how do we find the good selection? DMRG!**

DMRG: a young adult

09.11.1992 S.R.White: *Density Matrix Formulation for Quantum Renormalization Groups* (PRL 69, 2863 (1992))

„This new formulation appears extremely powerful and versatile, and we believe it will become the leading numerical method for 1D systems; and eventually will become useful for higher dimensions as well.“

~2004 old insight „DMRG is linked to MPS (Matrix Product States)“ goes viral

Östlund, Rommer, PRL 75, 3537 (1995), Dukelsky, Martin-Delgado, Nishino, Sierra, EPL43, 457 (1998)

Vidal, PRL 93, 040502 (2004), Daley, Kollath, Schollwöck, Vidal, J. Stat. Mech. P04005 (2004),
White, Feiguin, PRL 93, 076401 (2004), Verstraete, Porras, Cirac, PRL 93, 227205 (2004),
Verstraete, Garcia-Ripoll, Cirac, PRL 93, 207204 (2004), Verstraete, Cirac, cond-mat/0407066 (2004)

(some) reviews:

U. Schollwöck, Rev. Mod. Phys. 77, 259 (2005) - „old“ statistical physics perspective, applications
U. Schollwöck, Ann. Phys. 326, 96 (2011) - „new“ MPS perspective, technical
F. Verstraete, V. Murg, J. I. Cirac, Adv. Phys. 57, 143 (2008) - as seen from quantum information

matrix product states: definitions

quantum system living on *L* lattice sites

d local states per site $\{\sigma_i\}$ $\quad i \in \{1, 2, \ldots, L\}$

example: spin 1/2: $\quad d$=2 $\quad |\uparrow\rangle, |\downarrow\rangle$

Hilbert space:

$$\mathcal{H} = \otimes_{i=1}^{L} \mathcal{H}_i \qquad \mathcal{H}_i = \{|1_i\rangle, \ldots, |d_i\rangle\}$$

most general state (not necessarily 1D):

$$|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_L} c^{\sigma_1 \ldots \sigma_L} |\sigma_1 \ldots \sigma_L\rangle$$

abbreviations: $\quad \{\sigma\} = \sigma_1 \ldots \sigma_L \qquad c^{\{\sigma\}}$

(matrix) product states

exponentially many coefficients!
standard approximation: mean-field approximation

$$c^{\sigma_1 \cdots \sigma_L} = c^{\sigma_1} \cdot c^{\sigma_2} \cdot \ldots \cdot c^{\sigma_L} \qquad d^L \to dL \text{ coefficients}$$

often useful, but misses essential quantum feature: entanglement

consider 2 spin 1/2: $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \qquad \mathcal{H}_i = \{|\uparrow_i\rangle, |\downarrow_i\rangle\}$

$$|\psi\rangle = c^{\uparrow\uparrow}|\uparrow\uparrow\rangle + c^{\uparrow\downarrow}|\uparrow\downarrow\rangle + c^{\downarrow\uparrow}|\downarrow\uparrow\rangle + c^{\downarrow\downarrow}|\downarrow\downarrow\rangle$$

singlet state: $|\psi\rangle = \frac{1}{\sqrt{2}}|\uparrow\downarrow\rangle - \frac{1}{\sqrt{2}}|\downarrow\uparrow\rangle \qquad c^{\uparrow\downarrow} \neq c^{\uparrow} c^{\downarrow}$

generalize product state to matrix product state:

$$c^{\sigma_1} \cdot c^{\sigma_2} \cdot \ldots \cdot c^{\sigma_L} \to M^{\sigma_1} \cdot M^{\sigma_2} \cdot \ldots \cdot M^{\sigma_L}$$

matrix product states

useful generalization even for matrices of dimension 2:
AKLT (Affleck-Kennedy-Lieb-Tasaki) model

general matrix product state (MPS):

$$|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_L} M^{\sigma_1} M^{\sigma_2} \ldots M^{\sigma_L} |\sigma_1 \sigma_2 \ldots \sigma_L\rangle$$

matrix dimensions:

$$(1 \times D_1), (D_1 \times D_2), \ldots, (D_{L-2} \times D_{L-1}), (D_{L-1} \times 1)$$

non-unique: gauge degree of freedom

$$X X^{-1} = 1 \qquad M^{\sigma_i} \to M^{\sigma_i} X \qquad M^{\sigma_{i+1}} \to X^{-1} M^{\sigma_{i+1}}$$

matrix product states

Why are matrix product states interesting?

- any state can be represented as an MPS
  (even if numerically inefficiently)
- MPS are hierarchical: matrix size related to degree of entanglement
- MPS emerge naturally in renormalization groups
- MPS can be manipulated easily and efficiently
- MPS can be searched efficiently:
  which MPS has lowest energy for a given Hamiltonian?

singular value decomposition (SVD)

key workhorse of MPS manipulation and generally very useful!

general matrix *A* of dimension $(m \times n)$ $\quad k = \min(m, n)$

then $$A = USV^\dagger$$

with U dim.$(m \times k)$ $\quad U^\dagger U = I$ (ON col); if $m = k$: $\; UU^\dagger = I$

S dim.$(k \times k)$ diagonal: $s_1 \geq s_2 \geq s_3 \geq \ldots$ non-neg.: $s_i \geq 0$
singular values, non-vanishing = rank $r \leq k$

$V^\dagger$ dim.$(k \times n)$ $\quad V^\dagger V = I$ (ON row); if $k = n$: $\; VV^\dagger = I$

popular notation: (left) singular vectors $|u_i\rangle$

$$U = [|u_1\rangle|u_2\rangle \ldots]$$

SVD and EVD (eigenvalue decomp.)

singular value decomposition (always possible):

$$A = USV^\dagger \qquad s_1 \geq s_2 \geq s_3 \geq \dots \qquad s_i \geq 0$$

eigenvalue decomposition (for special square matrices):

$$AU = U\Lambda \qquad \lambda_i \qquad U = [|u_1\rangle|u_2\rangle \dots] \quad \text{eigenvectors}$$

connection by „squaring“ *A*: $A^\dagger A \qquad AA^\dagger$

$$AA^\dagger = USV^\dagger VSU^\dagger = US^2U^\dagger \Rightarrow (AA^\dagger)U = US^2$$
$$A^\dagger A = VSU^\dagger USV^\dagger = VS^2V^\dagger \Rightarrow (A^\dagger A)V = VS^2$$

eigenvalues = singular values squared
eigenvectors = left, right singular vectors

any state can be decomposed as MPS

reshape coefficient vector into matrix of dimension $(d \times d^{L-1})$ and SVD:

$$c^{\sigma_1\sigma_2\ldots\sigma_L} \rightarrow \Psi_{\sigma_1,\sigma_2\ldots\sigma_L} = \sum_{a_1} U_{\sigma_1,a_1} S_{a_1,a_1} V^{\dagger}_{a_1,\sigma_2\ldots\sigma_L}$$

slice *U* into *d* row vectors:

$$U_{\sigma_1,a_1} \rightarrow \{A^{\sigma_1}\} \quad \text{with} \quad A^{\sigma_1}_{1,a_1} = U_{\sigma_1,a_1}$$

rearrange SVD result:

$$c^{\sigma_1\sigma_2\ldots\sigma_L} = \sum_{a_1} A^{\sigma_1}_{1,a_1} c^{a_1\sigma_2\sigma_3\ldots\sigma_L} \qquad c^{a_1\sigma_2\sigma_3\ldots\sigma_L} = S_{a_1,a_1} V^{\dagger}_{a_1,\sigma_2\ldots\sigma_L}$$

reshape coefficient vector into matrix of dim. $(d^2 \times d^{L-2})$ and SVD:

$$c^{a_1\sigma_2\sigma_3\ldots\sigma_L} \rightarrow \Psi_{a_1\sigma_2,\sigma_3\ldots\sigma_L} = \sum_{a_2} U_{a_1\sigma_2,a_2} S_{a_2,a_2} V^{\dagger}_{a_2,\sigma_3\ldots\sigma_L}$$

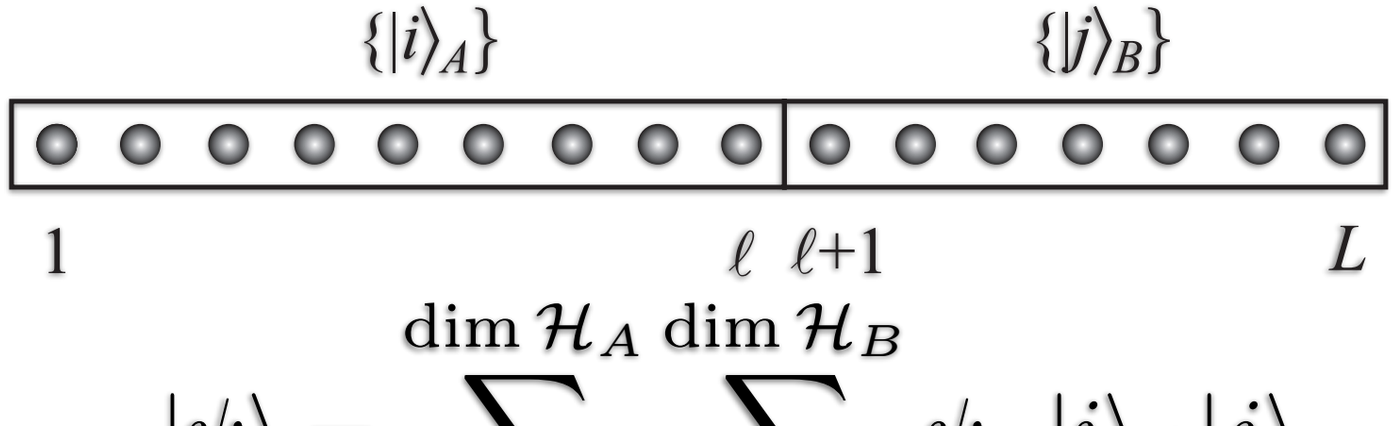
slice *U* into *d* matrices:

$$A^{\sigma_2}_{a_1,a_2} = U_{a_1\sigma_2,a_2}$$

rearrange SVD result: $c^{\sigma_1\sigma_2\ldots\sigma_L} = \sum_{a_1,a_2} A^{\sigma_1}_{1,a_1} A^{\sigma_2}_{a_1,a_2} c^{a_2\sigma_3\sigma_3\ldots\sigma_L}$ and so on!

Schmidt decomposition

bipartition of „universe“ AB into subsystems A and B:



$$\dim \mathcal{H}_A \quad \dim \mathcal{H}_B$$

$$|\psi\rangle = \sum_{i=1} \sum_{j=1} \psi_{ij} |i\rangle_A |j\rangle_B$$

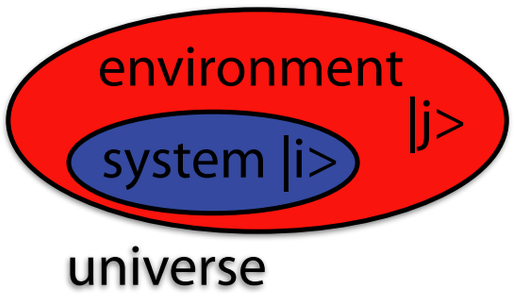
read coefficients as matrix entries, carry out SVD:

$$|\psi\rangle = \sum_{\alpha=1}^{r} s_\alpha |\alpha\rangle_A |\alpha\rangle_B$$ Schmidt decomposition

$$|\alpha\rangle_A = \sum_{i=1}^{\dim \mathcal{H}_A} U_{i\alpha} |i\rangle_A \qquad |\alpha\rangle_B = \sum_{j=1}^{\dim \mathcal{H}_B} V^*_{j\alpha} |j\rangle_B$$ orthonormal sets!

bipartite entanglement in MPS

- measuring bipartite entanglement *S*: reduced density matrix



$$|\psi\rangle = \sum \psi_{ij}|i\rangle|j\rangle \quad \hat{\rho} = |\psi\rangle\langle\psi| \rightarrow \hat{\rho}_S = \mathrm{Tr}_E \hat{\rho}$$

$$S = -\mathrm{Tr}[\hat{\rho_S} \log_2 \hat{\rho_S}] = -\sum w_\alpha \log_2 w_\alpha$$

- arbitrary bipartition

AAAAAAAA AAAAAAAAAAAAAAAA

$$|\psi\rangle = \sum_{\alpha}^{\mathbf{M}} \sqrt{w_\alpha} |\alpha_S\rangle |\alpha_E\rangle$$

use Schmidt decomposition

- reduced density matrix and bipartite entanglement

$$\hat{\rho_S} = \sum_\alpha w_\alpha |\alpha_S\rangle\langle\alpha_S|$$

$$S = -\sum_\alpha w_\alpha \log_2 w_\alpha \leq \log_2 M$$

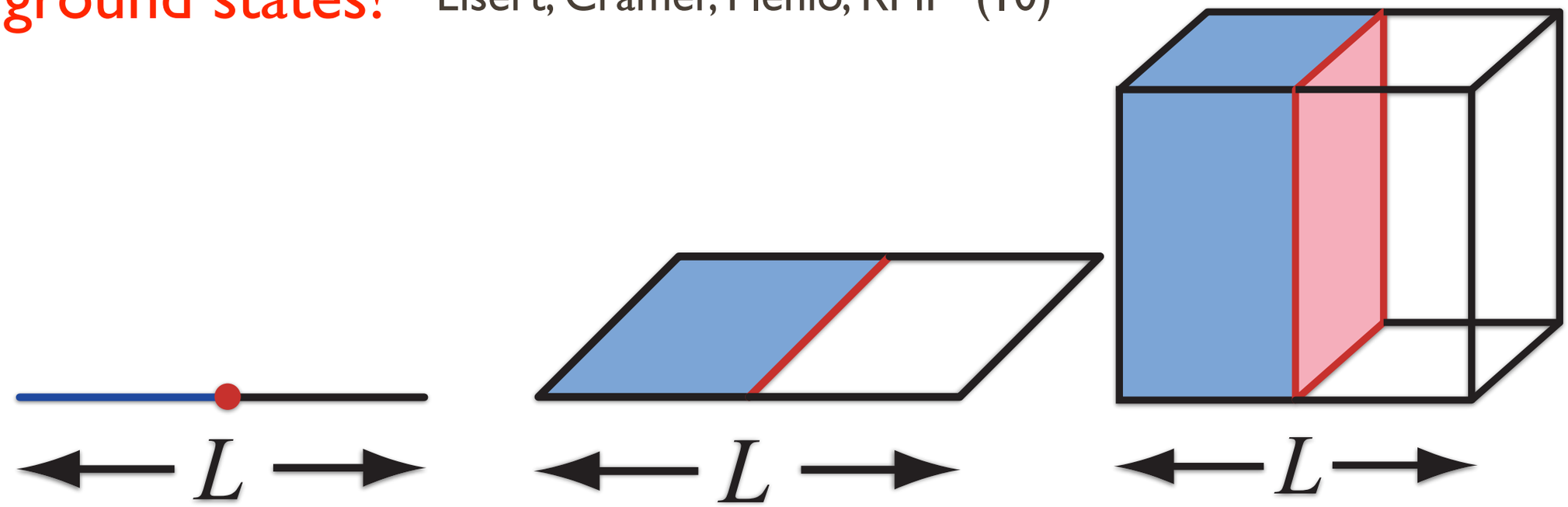
codable maximum

entanglement scaling: gapped systems

Latorre, Rico, Vidal, Kitaev (03)

- entanglement grows with system surface: area law
- for ground states! Eisert, Cramer, Plenio, RMP (10)

Bekenstein `73
Callan, Wilczek `94



gapped

$S(L) \sim \text{cst.}$ $S(L) \sim L$ $S(L) \sim L^2$

black hole

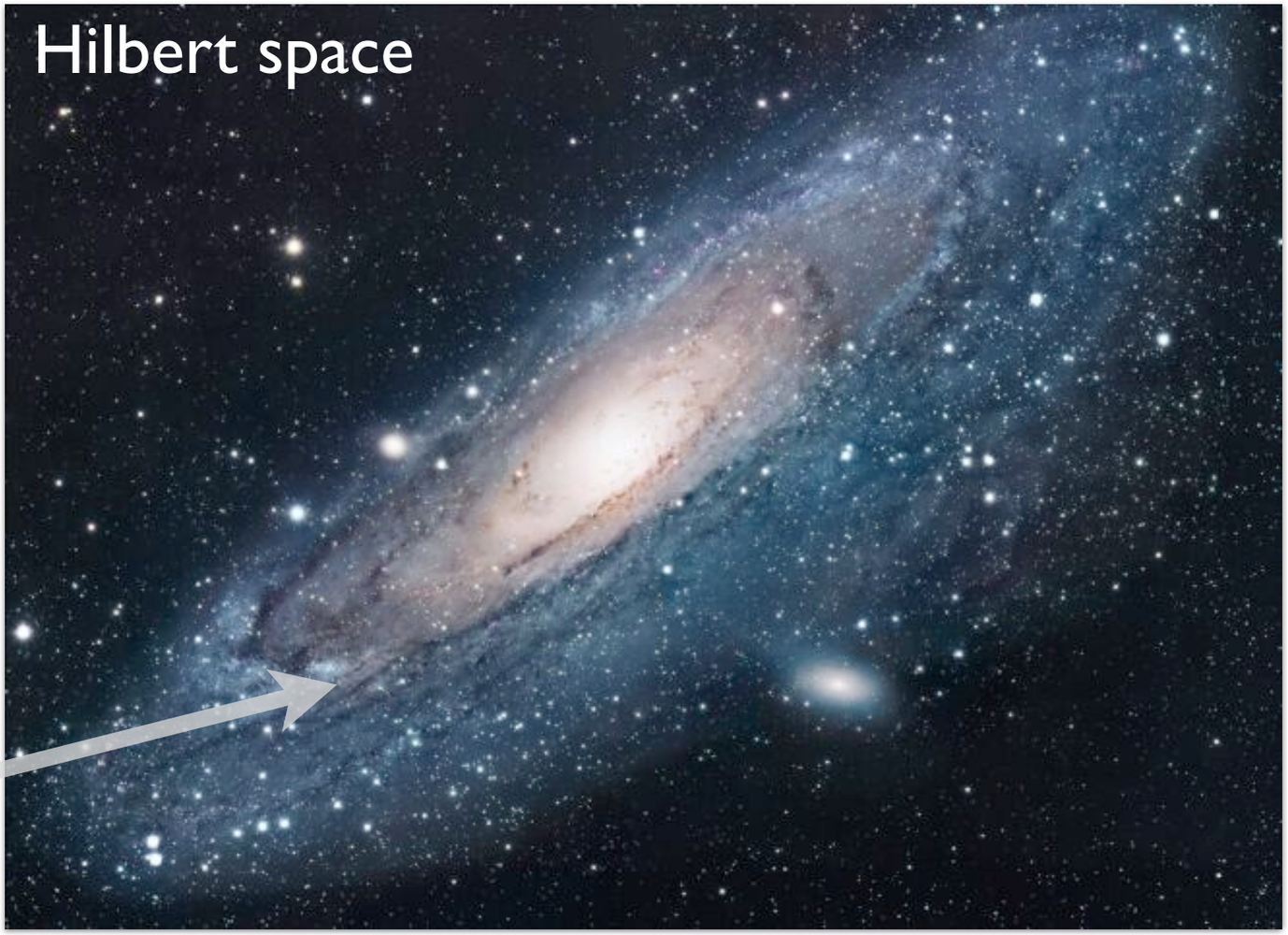
$$S \leq \log_2 M \Rightarrow M \geq 2^S$$

states

$M > 2^{cst.}$ $M > 2^L$ $M > 2^{L^2}$

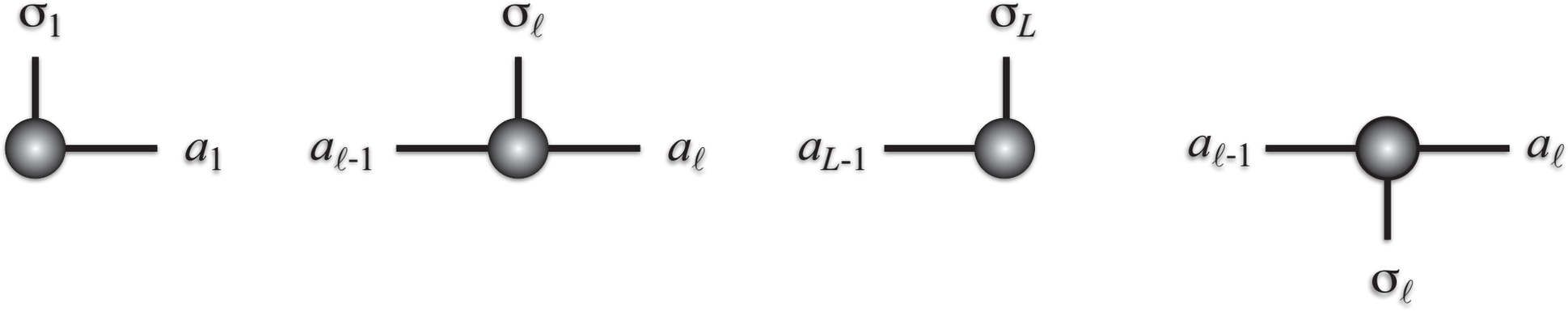
Hilbert space size: just an illusion?

- random state in Hilbert space: entanglement entropy extensive
- expectation value for entanglement entropy extensive and maximal
- states with non-extensive entanglement set of measure zero
- merit of MPS: parametrize this set efficiently!



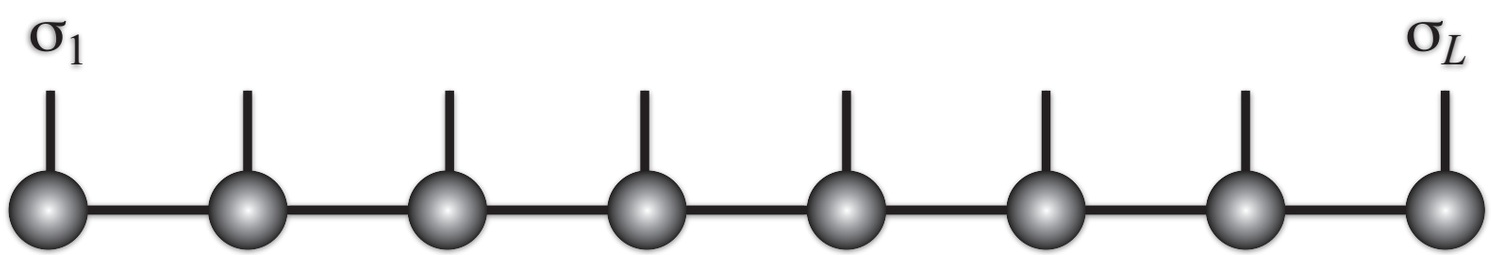
work with MPS: diagrammatics

matrix: vertical lines = physical states, horizontal lines = matrix indices



left edge | bulk | right edge | complex conjug.

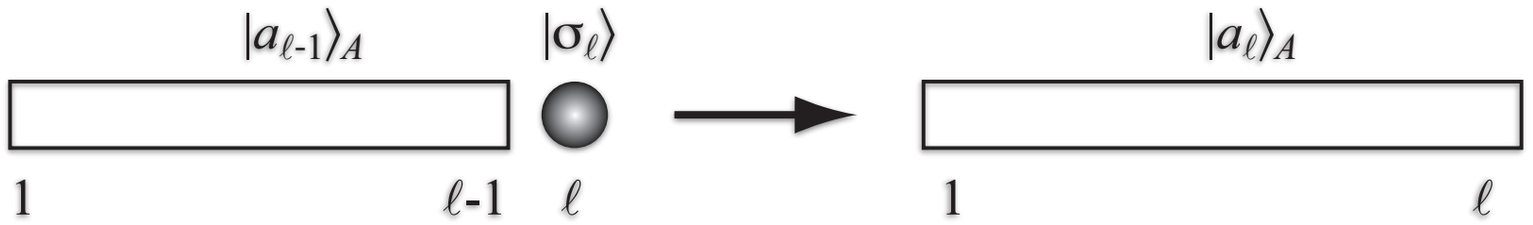
rule: connected lines are *contracted* (multiplied and summed)



matrix product state in graphical representation

block growth, decimation and MPS

RG schemes: grow blocks while decimating basis



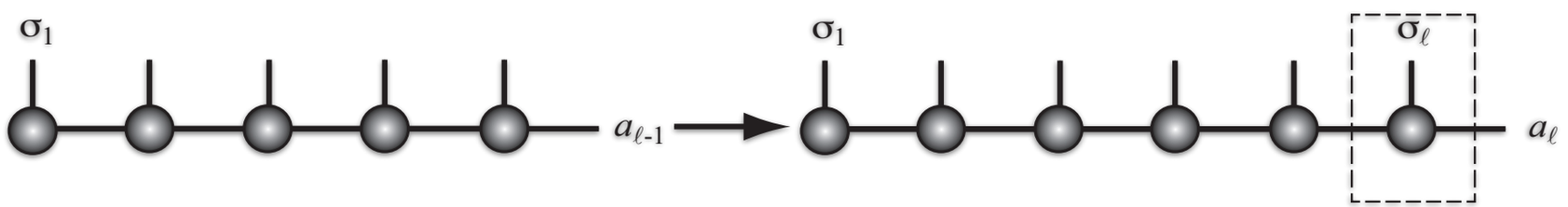
$$|a_\ell\rangle = \sum_{a_{\ell-1},\sigma_\ell} \langle a_{\ell-1},\sigma_\ell|a_\ell\rangle |a_{\ell-1}\rangle|\sigma_\ell\rangle \equiv \sum_{a_{\ell-1},\sigma_\ell} M^{\sigma_\ell}_{a_{\ell-1},a_\ell}|a_{\ell-1}\rangle|\sigma_\ell\rangle$$

simple rearrangement of expansion coefficients into matrices:

$$M^{\sigma_\ell}_{a_{\ell-1},a_\ell} = \langle a_{\ell-1},\sigma_\ell|a_\ell\rangle$$

recursion easily expressed as matrix multiplication:

$$|a_\ell\rangle = \sum_{\sigma_1,\ldots,\sigma_\ell} (M^{\sigma_1}M^{\sigma_2}\ldots M^{\sigma_\ell})_{1,a_\ell}|\sigma_1\sigma_2\ldots\sigma_\ell\rangle$$



(left and right) normalization

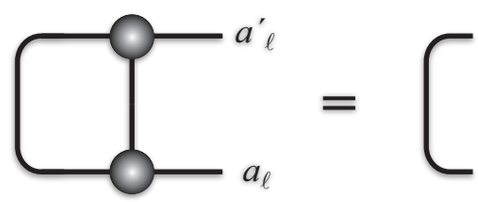
both state decomposition and block growth scheme give special gauge

$$\delta_{a'_\ell,a_\ell} = \langle a'_\ell|a_\ell\rangle = \sum_{a'_{\ell-1}\sigma'_\ell a_{\ell-1}\sigma_\ell} M^{\sigma'_\ell *}_{a'_{\ell-1},a'_\ell} M^{\sigma_\ell}_{a_{\ell-1},a'_\ell} \langle a'_{\ell-1}\sigma'_\ell|a_{\ell-1}\sigma_\ell\rangle$$

$$= \sum_{a_{\ell-1}\sigma_\ell} M^{\sigma_\ell *}_{a_{\ell-1},a'_\ell} M^{\sigma_\ell}_{a_{\ell-1},a'_\ell} = \sum_{\sigma_\ell} (M^{\sigma_\ell\dagger} M^{\sigma_\ell})_{a'_\ell,a_\ell}$$

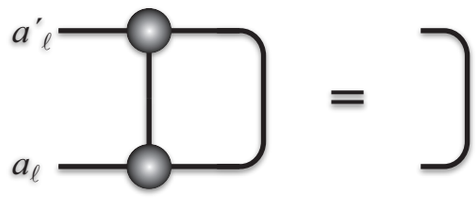
left normalization (called A); more compact representation:

$$I = \sum_{\sigma_\ell} M^{\sigma_\ell\dagger} M^{\sigma_\ell} \equiv \sum_{\sigma_\ell} A^{\sigma_\ell\dagger} A^{\sigma_\ell}$$



right normalization (called B):

$$I = \sum_{\sigma_\ell} B^{\sigma_\ell} B^{\sigma_\ell\dagger}$$



mixed normalization:

$$AAAAAMBBBBBBBBB$$

matrix product operators (MPO)

general operator:

$$\hat{O} = \sum_{\{\sigma\}} \sum_{\{\sigma'\}} c^{\sigma_1 \ldots \sigma_L, \sigma'_1 \ldots \sigma'_L} |\sigma_1 \ldots \sigma_L\rangle\langle\sigma'_1 \ldots \sigma'_L|$$

rearrange indices:

$$c^{\sigma_1 \ldots \sigma_L, \sigma_1 \ldots \sigma_L} \rightarrow c^{\sigma_1 \sigma_1 \sigma_2 \sigma_2 \ldots \sigma_L \sigma_L}$$

„mean-field“ very useful: $c^{\sigma_1 \sigma'_1 \sigma_2 \sigma'_2 \ldots \sigma_L \sigma'_L} \rightarrow c^{\sigma_1 \sigma'_1} \cdot c^{\sigma_2 \sigma'_2} \cdot \ldots \cdot c^{\sigma_L \sigma'_L}$

$$\hat{S}^z_i \rightarrow \hat{I}_1 \otimes \hat{I}_2 \otimes \ldots \otimes \hat{S}^z_i \otimes \ldots \otimes \hat{I}_L$$

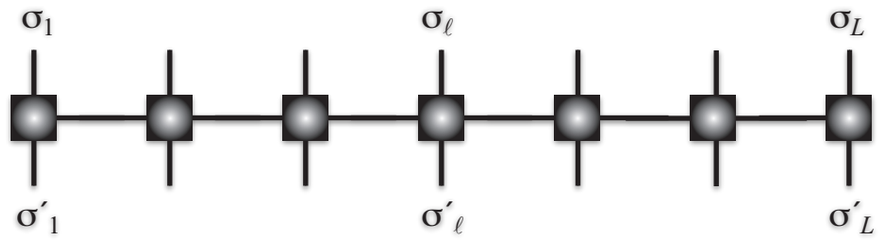
$$c^{\sigma_1 \sigma'_1 \sigma_2 \sigma'_2 \ldots \sigma_L \sigma'_L} = \delta_{\sigma_1, \sigma'_1} \cdot \delta_{\sigma_2, \sigma'_2} \cdot \ldots \cdot (\hat{S}^z)_{\sigma_i, \sigma'_i} \cdot \ldots \cdot \delta_{\sigma_L, \sigma'_L}$$

matrix product operator:

$$\hat{O} = \sum_{\{\sigma\}} \sum_{\{\sigma'\}} M^{\sigma_1 \sigma'_1} M^{\sigma_2 \sigma'_2} \ldots M^{\sigma_L \sigma'_L} |\sigma_1 \ldots \sigma_L\rangle\langle\sigma'_1 \ldots \sigma'_L|$$

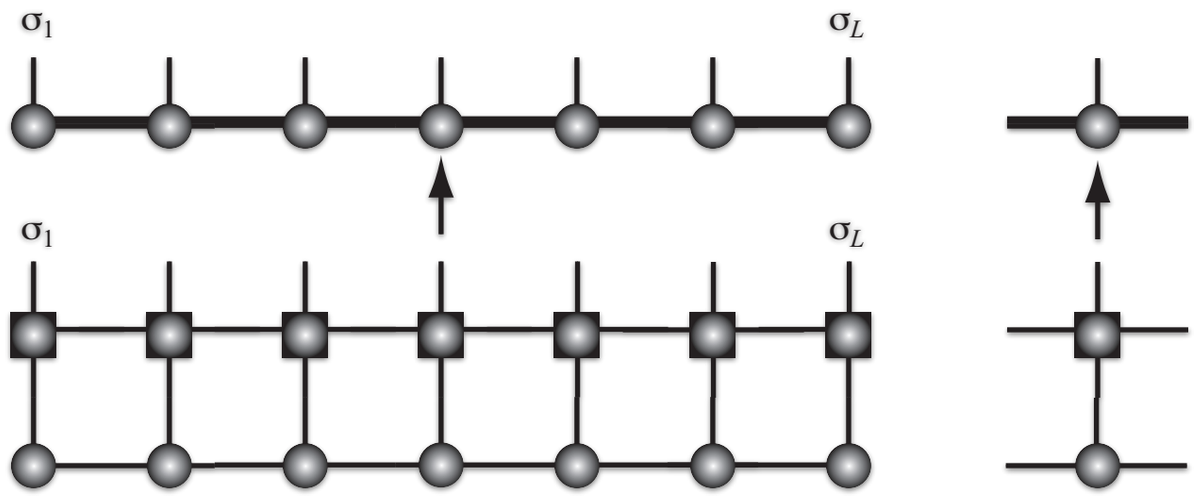
applying an MPO to an MPS

graphical representation with ingoing and outgoing physical states:



applying an MPO to an MPS: new MPS with matrix dims multiplied

$$\tilde{M}^{\sigma_i}_{(ab),(a'b')} = \sum_{\sigma'_i} N^{\sigma_i \sigma'_i}_{aa'} M^{\sigma'_i}_{bb'}$$



normalization and compression I

problem: matrix dimensions of MPS grow under MPO application

solution: compression of matrices with minimal state distance

assume state is given in mixed normalized form:

$$|\psi\rangle = \sum_{\{\sigma\}} A^{\sigma_1} A^{\sigma_2} \dots A^{\sigma_\ell} M^{\sigma_{\ell+1}} B^{\sigma_{\ell+2}} \dots B^{\sigma_L} |\sigma_1 \dots \sigma_L\rangle$$

stack *M* matrices into one:

$$M_{a_\ell, \sigma_{\ell+1} a_{\ell+1}} = M^{\sigma_{\ell+1}}_{a_\ell, a_{\ell+1}}$$

carry out SVD, and use results: $M = USV^\dagger$

$$A^{\sigma_\ell} \leftarrow A^{\sigma_\ell} U$$ orthonormality of *U* !

$$B^{\sigma_{\ell+1}}_{a_\ell, a_{\ell+1}} = V^\dagger_{a_\ell, \sigma_{\ell+1} a_{\ell+1}}$$

normalization and compression II

now introduce orthonormal states:

$$|a_\ell\rangle_A := \sum_{\sigma_1,\ldots,\sigma_\ell} (A^{\sigma_1}\ldots A^{\sigma_\ell})_{1,a_\ell}|\sigma_1\ldots\sigma_\ell\rangle$$

$$|a_\ell\rangle_B := \sum_{\sigma_{\ell+1},\ldots,\sigma_L} (B^{\sigma_{\ell+1}}\ldots B^{\sigma_L})_{a_\ell,1}|\sigma_{\ell+1}\ldots\sigma_L\rangle$$

read off Schmidt decomposition: $|\psi\rangle = \sum_{a_\ell} s_{a_\ell}|a_\ell\rangle_A|a_\ell\rangle_B$

compress matrices $A^{\sigma_\ell}, B^{\sigma_{\ell+1}}$ by keeping *D* largest singular values

$$A^{\sigma_\ell}S \to M^{\sigma_\ell}$$

$$|\psi\rangle = \sum_{\{\sigma\}} A^{\sigma_1}A^{\sigma_2}\ldots A^{\sigma_{\ell-1}}M^{\sigma_\ell}B^{\sigma_{\ell+1}}\ldots B^{\sigma_L}|\sigma_1\ldots\sigma_L\rangle$$

mixed rep shifted by 1 site: sweep through chain; also normalization

time-evolution

assume initial state in MPS representation; time evolution:

$$|\psi(t)\rangle = \mathrm{e}^{-\mathrm{i}\hat{H}t}|\psi(0)\rangle$$

how to express the evolution operator as an MPO?

one solution: Trotterization of evolution operator into small time steps

$$N \to \infty \qquad \tau \to 0 \qquad N\tau = T \qquad \tau \sim 0.01$$

Heisenberg model: $\hat{H} = \sum_{i=1}^{L-1} \hat{h}_i \qquad \hat{h}_i = \mathbf{S}_i \cdot \mathbf{S}_{i+1}$

$$\mathrm{e}^{-\mathrm{i}\hat{H}T} = \prod_{i=1}^{N} \mathrm{e}^{-\mathrm{i}\hat{H}\tau} = \prod_{k=1}^{N} \mathrm{e}^{-\mathrm{i}\sum_{i=1}^{L-1}\hat{h}_i\tau} \overset{!}{=} \prod_{k=1}^{N}\prod_{i=1}^{L-1} \mathrm{e}^{-\mathrm{i}\hat{h}_i\tau}$$

first-order Trotter decomposition

Trotter decomposition

calculation of $\mathrm{e}^{-\mathrm{i}\hat{h}_i\tau}$ as $(d^2 \times d^2)$ matrix:

$$H_i U = U\Lambda \quad H_i = U\Lambda U^\dagger \quad \Rightarrow \quad \mathrm{e}^{-\mathrm{i}H_i\tau} = U\mathrm{e}^{-\mathrm{i}\Lambda\tau}U^\dagger = U \cdot \mathrm{diag}(\mathrm{e}^{-\mathrm{i}\lambda_1\tau}, \mathrm{e}^{-\mathrm{i}\lambda_2\tau}, \ldots) \cdot U^\dagger$$

problem: exponential does not factorize if operators do not commute

$$\mathrm{e}^{\hat{A}+\hat{B}} = \mathrm{e}^{\hat{A}}\mathrm{e}^{\hat{B}}\mathrm{e}^{\frac{1}{2}[\hat{A},\hat{B}]}$$

but error is negligible as $\tau \to 0$

$$[\hat{h}_i\tau, \hat{h}_{i+1}\tau] \propto \tau^2$$

convenient rearrangement:

$$\hat{H} = \hat{H}_{\mathrm{odd}} + \hat{H}_{\mathrm{even}}; \qquad \hat{H}_{\mathrm{odd}} = \sum_i \hat{h}_{2i-1}, \quad \hat{H}_{\mathrm{even}} = \sum_i \hat{h}_{2i}$$

$$\mathrm{e}^{-\mathrm{i}\hat{H}T} = \mathrm{e}^{-\mathrm{i}\hat{H}_{\mathrm{even}}\tau}\mathrm{e}^{-\mathrm{i}\hat{H}_{\mathrm{odd}}\tau}; \qquad \mathrm{e}^{-\mathrm{i}\hat{H}_{\mathrm{even}}\tau} = \prod_i \mathrm{e}^{-\mathrm{i}\hat{h}_{2i}\tau}, \quad \mathrm{e}^{-\mathrm{i}\hat{H}_{\mathrm{odd}}\tau} = \prod_i \mathrm{e}^{-\mathrm{i}\hat{h}_{2i-1}\tau}$$

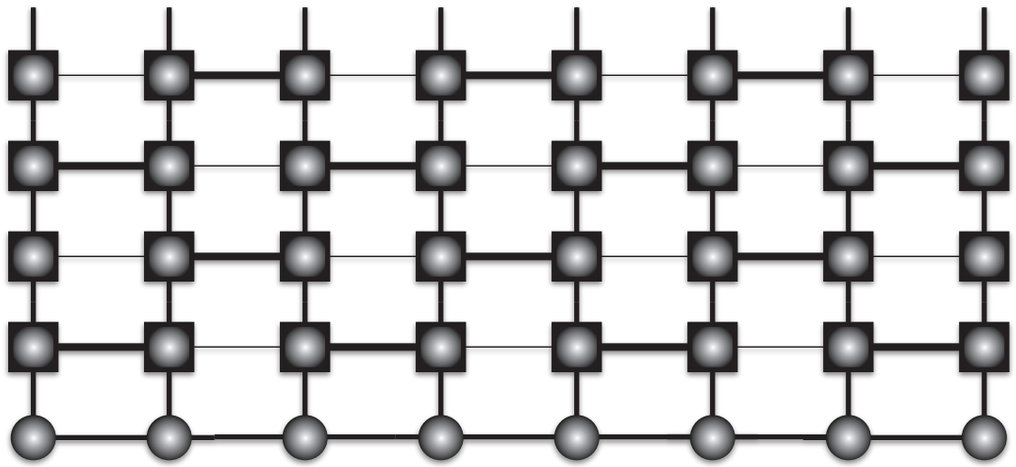
tDMRG, tMPS, TEBD

bring local evolution operator into MPO form:

$$U^{\sigma_1\sigma_2,\sigma_1'\sigma_2'} = \langle\sigma_1\sigma_2|\mathrm{e}^{-\mathrm{i}\hat{h}_1\tau}|\sigma_1'\sigma_2'\rangle$$

$$U^{\sigma_1\sigma_2,\sigma_1'\sigma_2'} = \overline{U}_{\sigma_1\sigma_1',\sigma_2\sigma_2'} \overset{SVD}{=} \sum_b W_{\sigma_1\sigma_1',b} S_{b,b} W_{b,\sigma_2\sigma_2'}$$

$$= \sum_b M^{\sigma_1\sigma_1'}_{1,b} M^{\sigma_2\sigma_2'}_{b,1}$$



even bonds

odd bonds

initial state

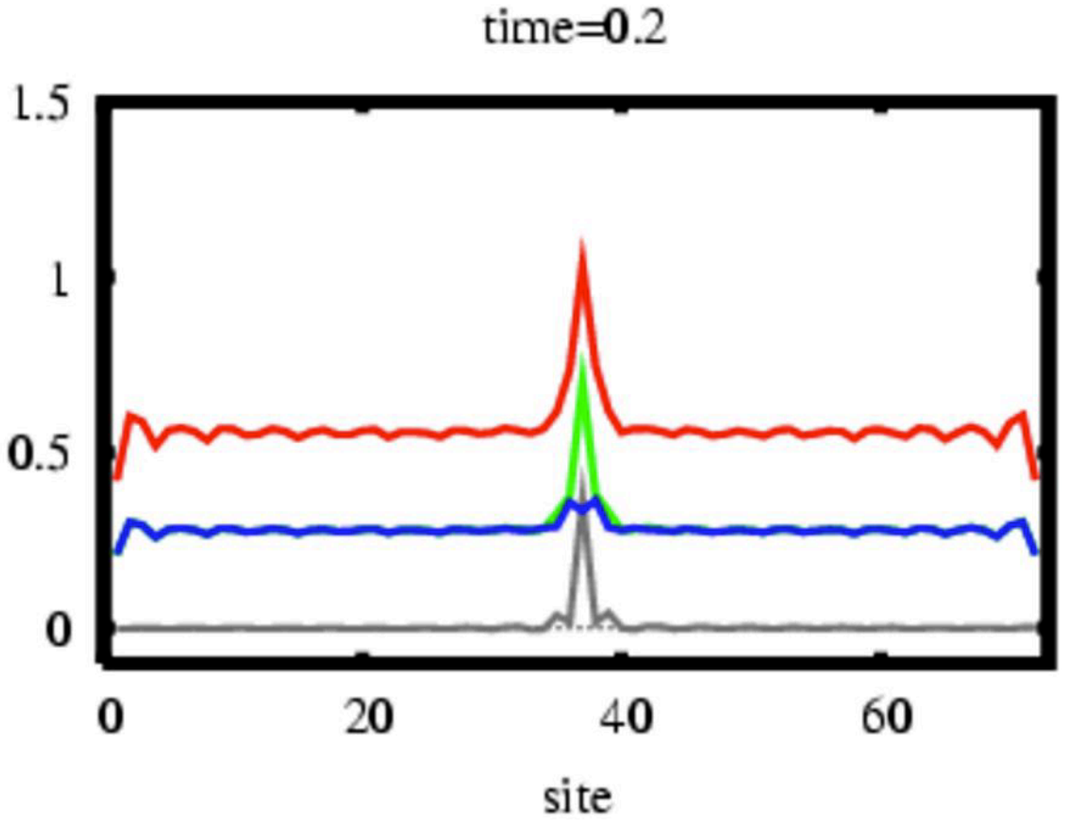
one time step: dimension grows as d^2

- apply one infinitesimal time step in MPO form
- compress resulting MPS

single-particle excitation

- quarter-filled Hubbard chain: $U/t=4$
- add spin-up electron at chain center at time=0
- measure charge and spin density

time-dependent DMRG



charge

spin

- separation of charge and spin

Kollath, US, Zwerger, PRL 95, 176401 ('05)

some comments ...

real time evolution limited by entanglement growth:

$$S(t) \leq S(0) + \nu t \qquad S \sim \ln D$$

in the worst case, matrix dimensions grow exponentially!

ground states can be obtained by imaginary time evolution (SLOW!):

$$|\psi\rangle = \sum_n c_n |n\rangle \qquad \hat{H}|n\rangle = E_n|n\rangle \qquad E_0 \leq E_1 \leq E_2 \leq \dots$$

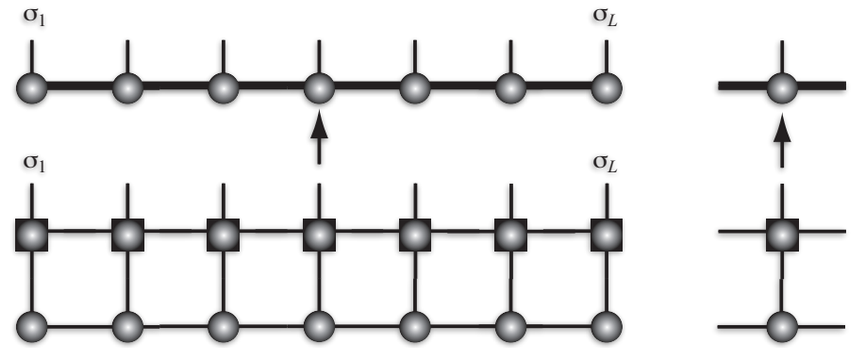
$$\lim_{\beta\to\infty} \mathrm{e}^{-\beta\hat{H}}|\psi\rangle = \lim_{\beta\to\infty} \sum_n \mathrm{e}^{-\beta E_n} c_n|n\rangle = \lim_{\beta\to\infty} \mathrm{e}^{-\beta E_0}(c_0|0\rangle + \sum_{n>0} \mathrm{e}^{-\beta(E_n-E_0)} c_n|n\rangle$$

$$= \lim_{\beta\to\infty} \mathrm{e}^{-\beta E_0} c_0|0\rangle$$

long-ranged interaction: Krylov

what can we do if interactions are long-ranged and Trotter fails?
Krylov time evolution

- bring Hamiltonian into MPO form: exact, small dimension
- calculate successive powers $|\psi\rangle, H|\psi\rangle, H^2|\psi\rangle, \ldots$ Krylov vectors
  - apply Hamiltonian MPO
  - compress resulting MPS



- orthonormalize powers
- tridiagonalize Hamiltonian in new basis, calculate $e^{iH\Delta t}|\psi\rangle$
- for small time steps, 4 to 5 Krylov vectors sufficient; quasi-exact

limitations …

- do correlations in non-relativistic systems spread at finite velocity?

$$\|[A_0(0), B_d(t)]\| \leq cst. \|A\| \|B\| \exp[-(d - vt)]$$

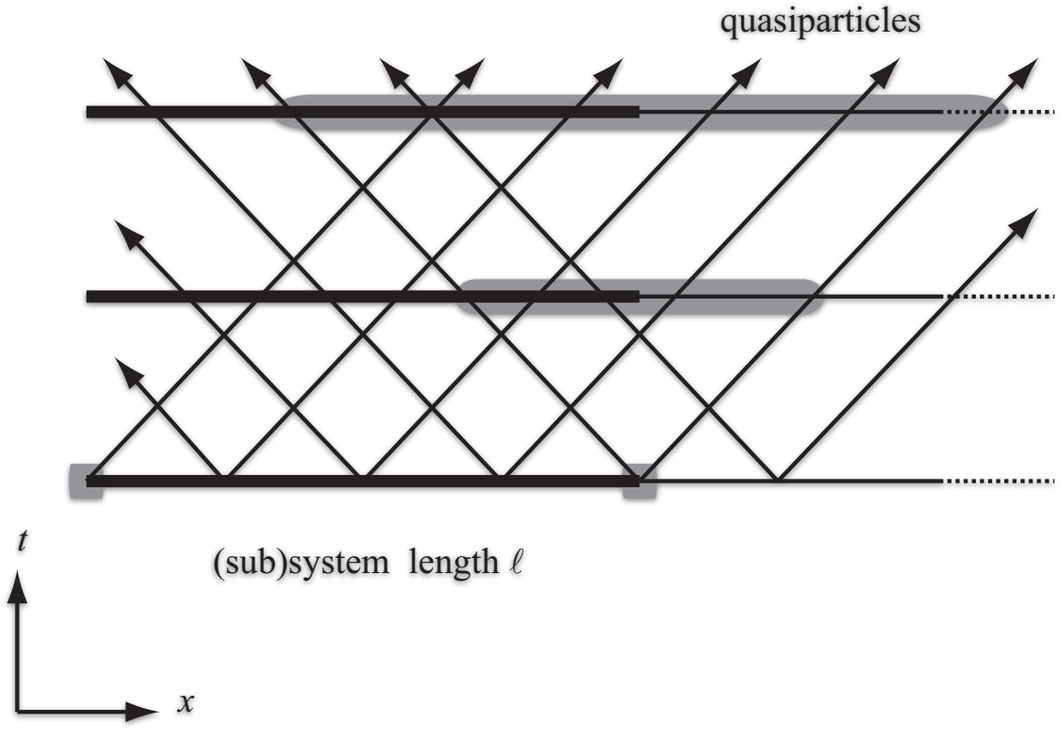
- correlations

Lieb-Robinson theorem (CMP, 1972)

- entanglement bound:

$$S(t) \leq S(0) + cst. \times 2vt$$

linear in time
exponential resources



out-of-equilibrium cartoon:

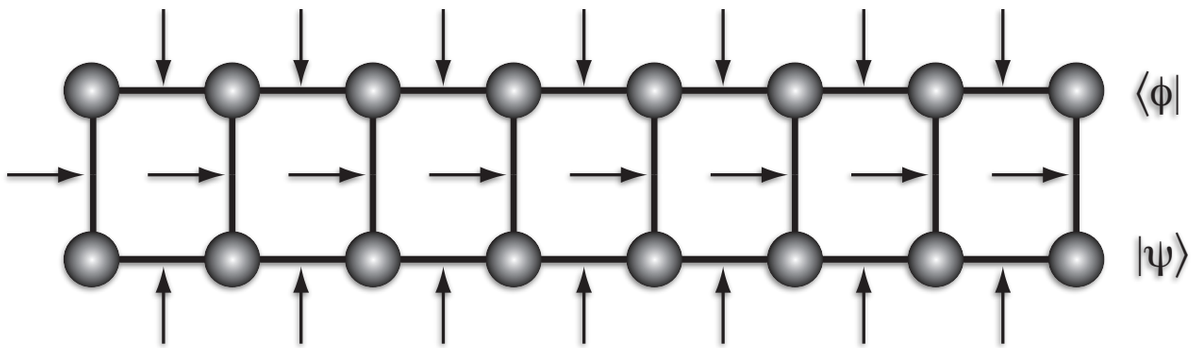
quasiparticles entangle in „light“ cone

Calabrese, Cardy (since 2004) and others

overlaps

$$\langle \psi(t)|\psi(0)\rangle \qquad \langle S_i^z(t)\rangle = \langle \psi(t)|\hat{S}_i^z|\psi(t)\rangle$$

overlap contractions:

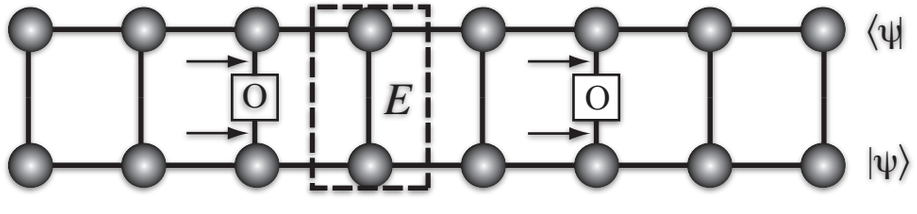


$$\langle \phi|\psi\rangle = \sum_{\{\sigma\}}\sum_{\{\sigma'\}}\langle\{\sigma'\}|\tilde{M}^{\sigma_1'*}\dots\tilde{M}^{\sigma_L'*}M^{\sigma_1}\dots M^{\sigma_L}|\{\sigma\}\rangle = \sum_{\{\sigma\}}\tilde{M}^{\sigma_1*}\dots\tilde{M}^{\sigma_L*}M^{\sigma_1}\dots M^{\sigma_L}$$

$$\begin{aligned}\langle \phi|\psi\rangle &= \sum_{\{\sigma\}}\tilde{M}^{\sigma_1*}\dots\tilde{M}^{\sigma_L*}M^{\sigma_1}\dots M^{\sigma_L}\\ &= \sum_{\{\sigma\}}\tilde{M}^{\sigma_L\dagger}\dots\tilde{M}^{\sigma_1\dagger}M^{\sigma_1}\dots M^{\sigma_L}\\ &= \sum_{\sigma_L}\tilde{M}^{\sigma_L\dagger}\left(\dots\left(\sum_{\sigma_2}\tilde{M}^{\sigma_2\dagger}\left(\sum_{\sigma_1}\tilde{M}^{\sigma_1\dagger}M^{\sigma_1}\right)M^{\sigma_2}\right)\dots\right)M^{\sigma_L}\end{aligned}$$

order of contractions:
zip through the ladder;
cost $O(dLD^3)$

two-point correlators: long-range or superposition of exponentials



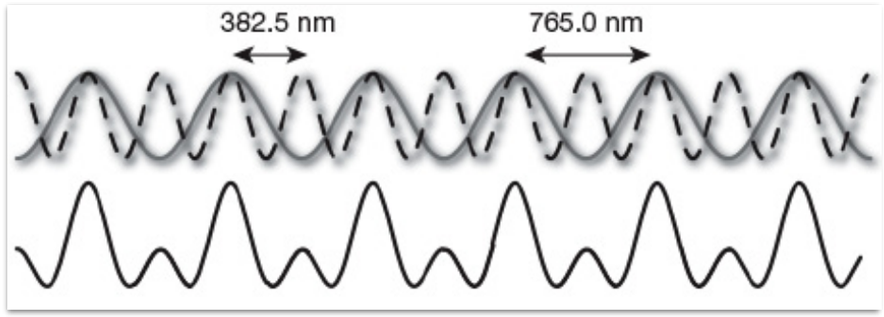
$$E^{(a_{\ell-1}a'_{\ell-1}),(a_\ell,a'_\ell)} := \sum_{\sigma_\ell} A^{\sigma_\ell *}_{a_{\ell-1},a_\ell} A^{\sigma_\ell}_{a'_{\ell-1},a'_\ell}$$

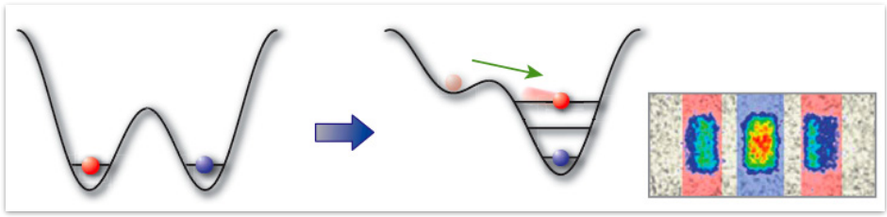
hence: power laws only „by approximation“

dynamical quantum simulator

coherent dynamics! controlled preparation? local measurements?

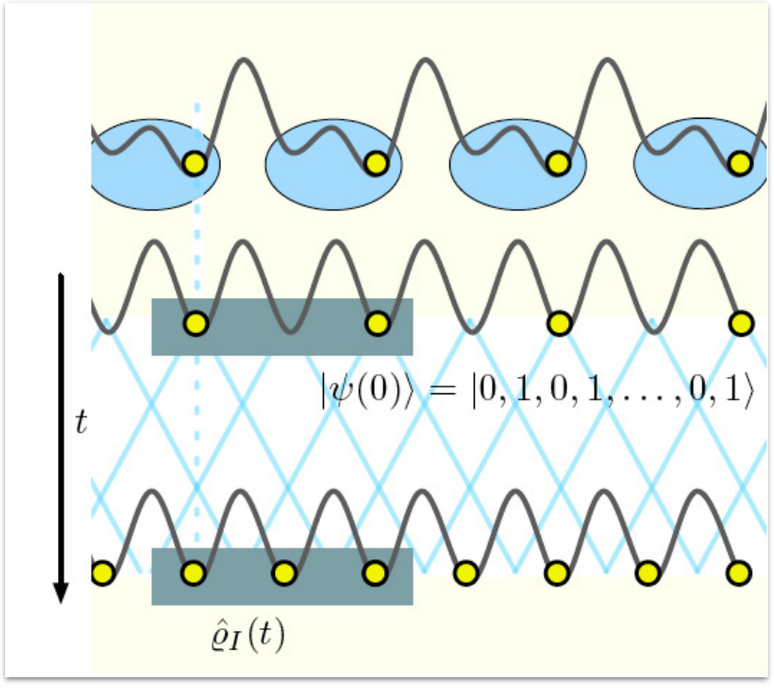
first experiments:
period-2 superlattice
- double-well formation
- staggered potential bias





- pattern loading
- odd/even resolved measurement

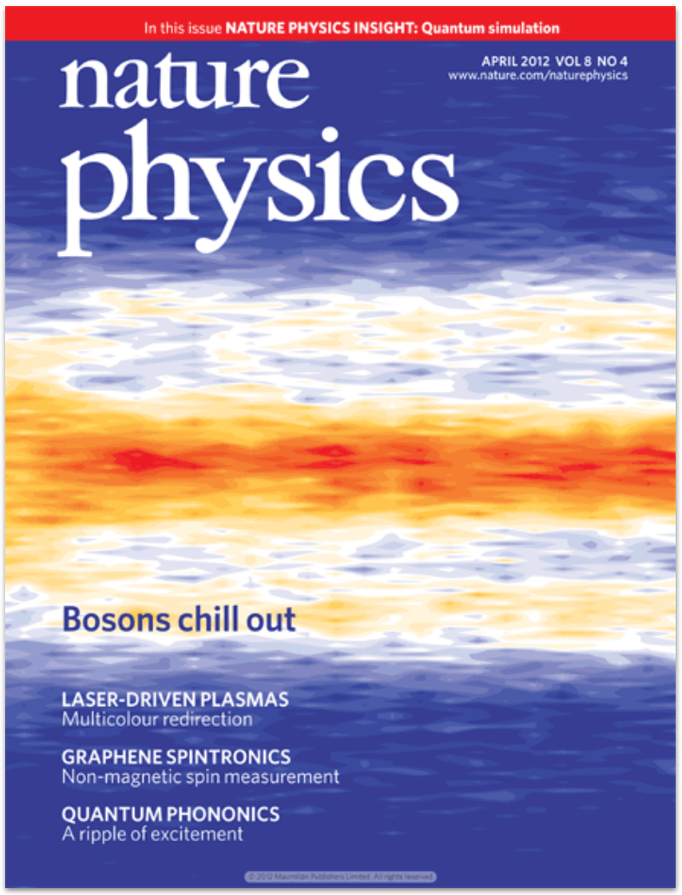
(Fölling *et al.* (2007))



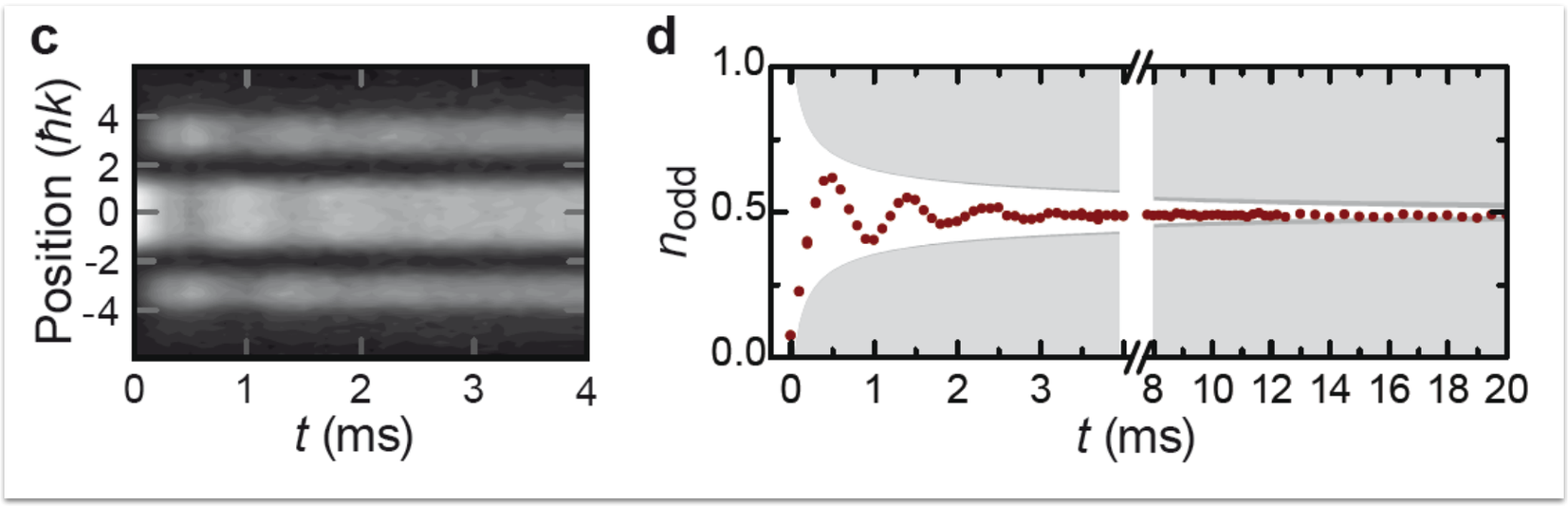
first theory proposals:
- prepare $|\psi\rangle = |1,0,1,0,1,0,\ldots\rangle$
- switch off superlattice
- observe Bose-Hubbard dynamics

Cramer *et al.*, PRL 101, 063001 (2008)
Flesch *et al.*, PRA 78, 033608 (2008)

dynamical quantum simulator

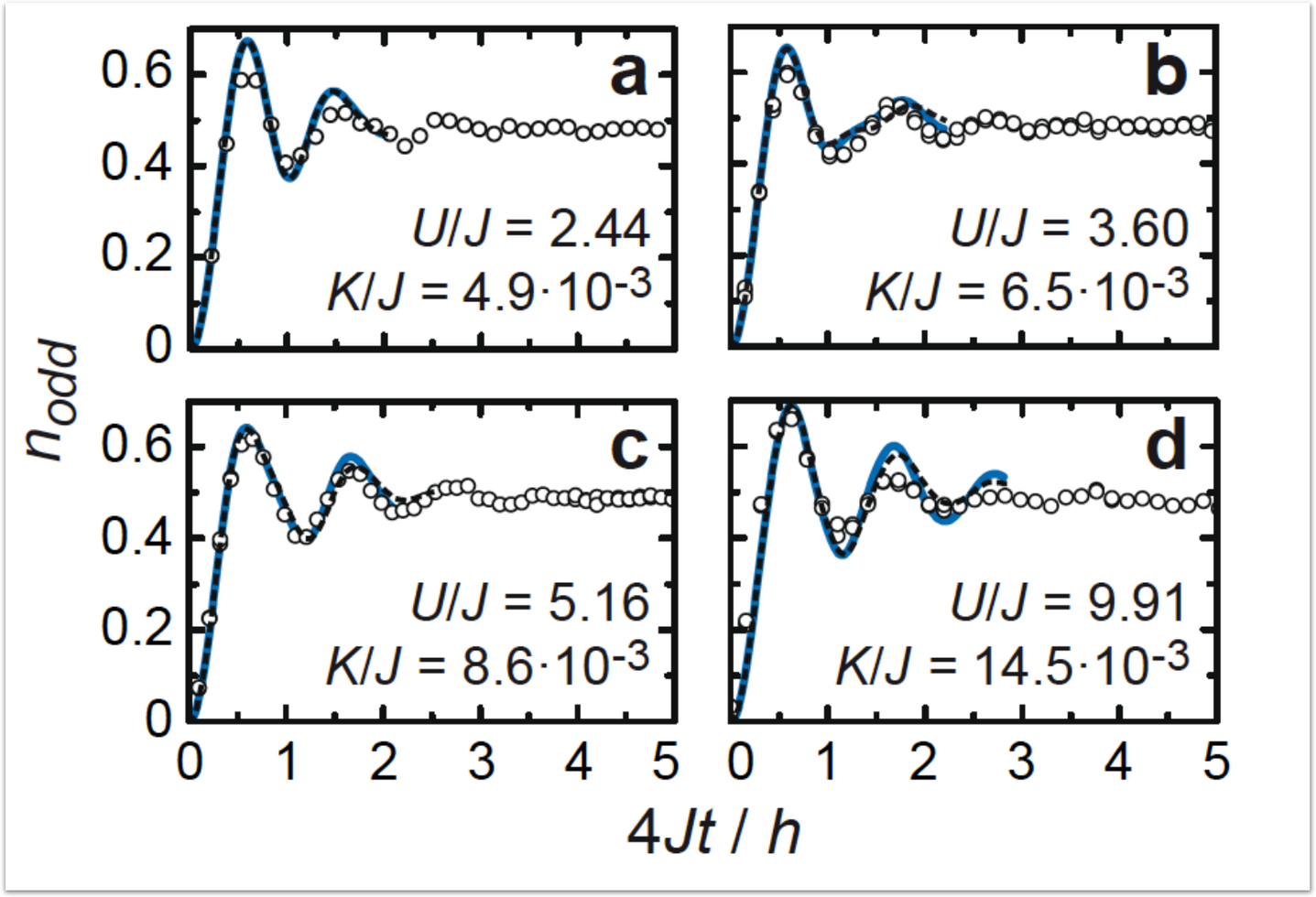


Trotzky *et al.*, Nat. Phys. 8, 325(2012)



45,000 atoms,
U=5.2
momentum
distribution

densities II



no free fit parameters!

fully controlled relaxation in closed quantum system!

*validation of **dynamical** quantum simulator*

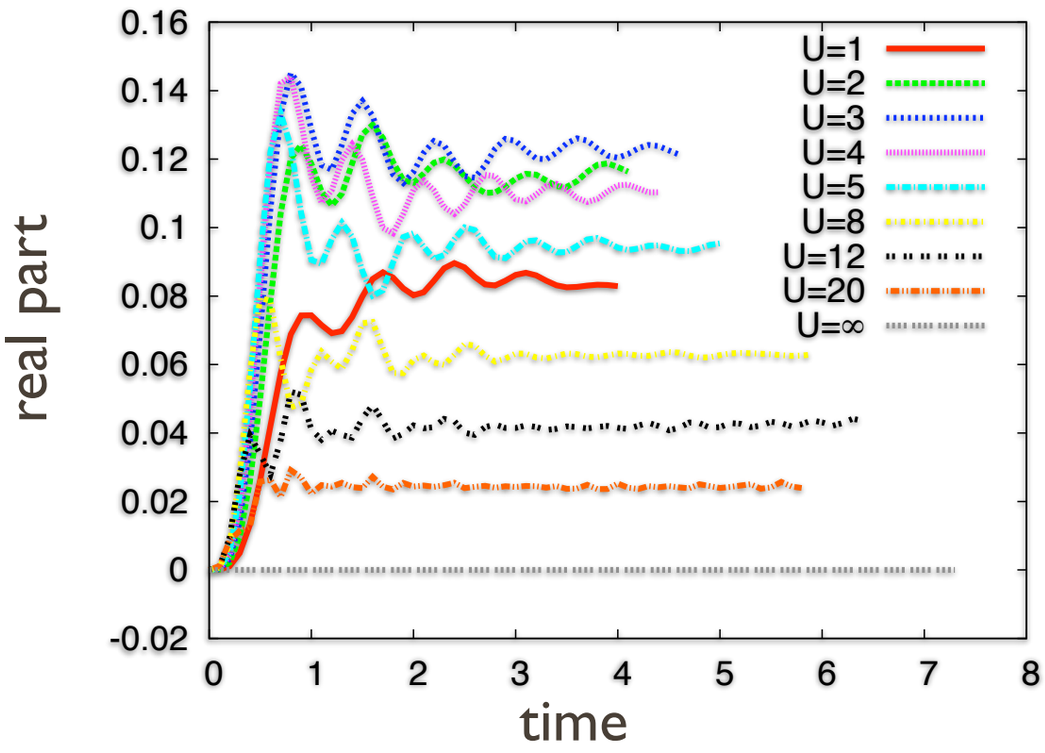
time range of experiment > 10 x time range of theory

real „analog computer“ that goes beyond theory

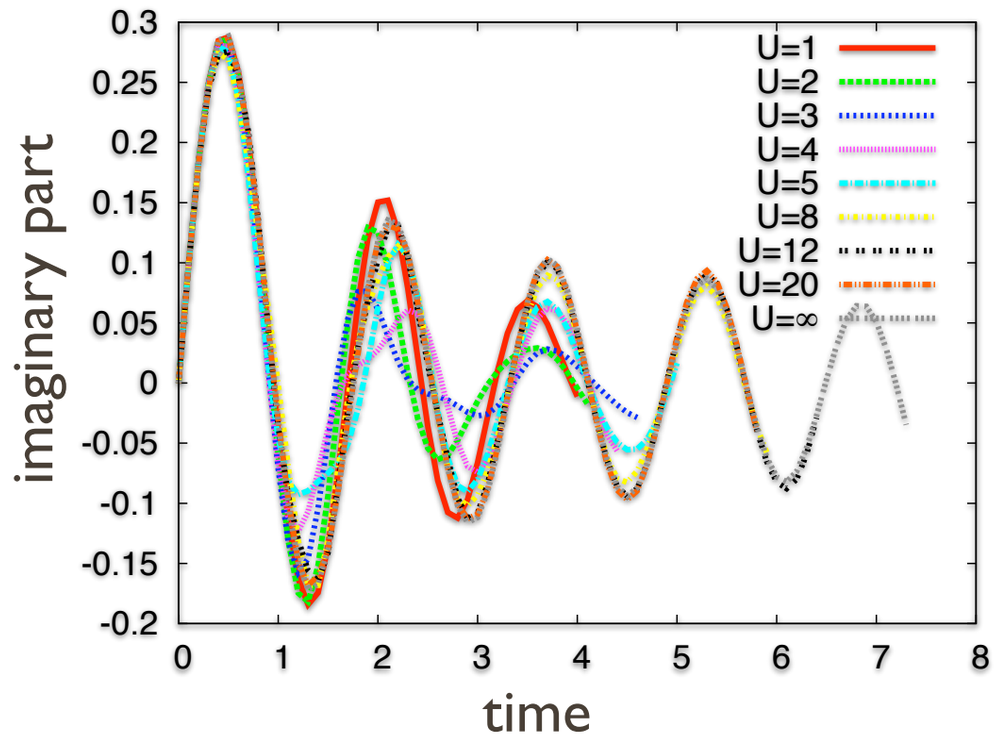
nearest-neighbour correlators

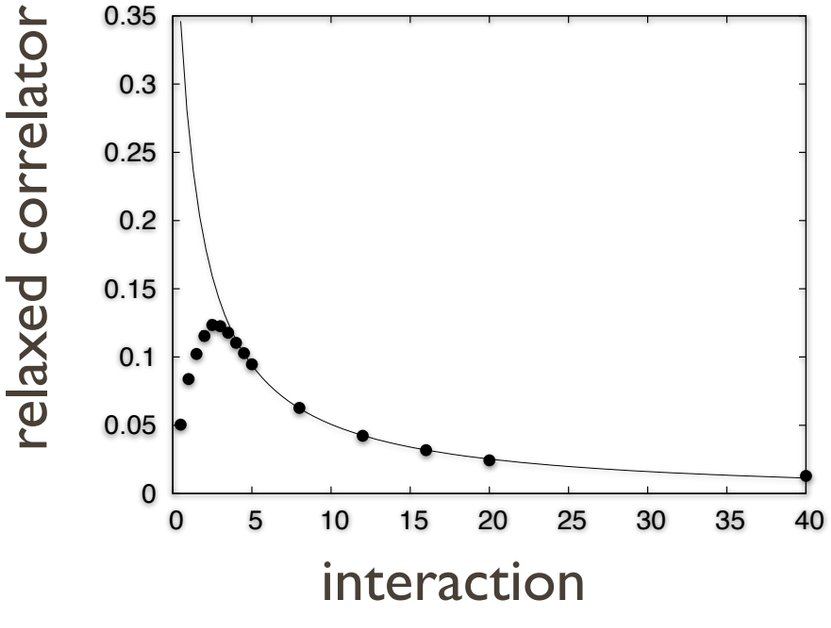
$$\langle \hat{b}_n^\dagger(t)\hat{b}_{n+1}(t)\rangle$$

correlator



current



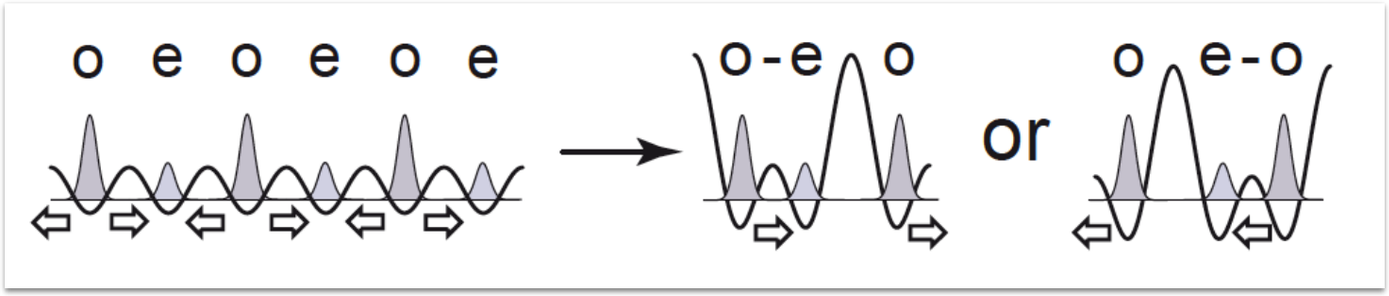


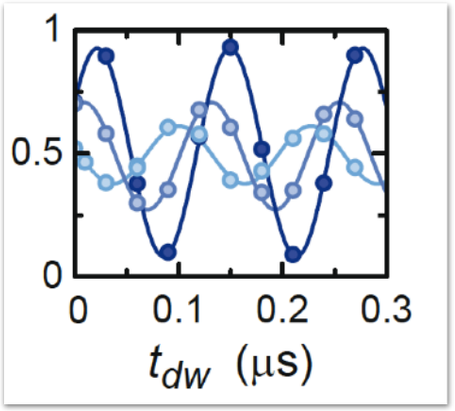
- again three regimes
- $U \approx 3$: crossover regime

- at large U, $1/U$ fit of relaxed correlator can be understood as perturbation to locally relaxed subsystems

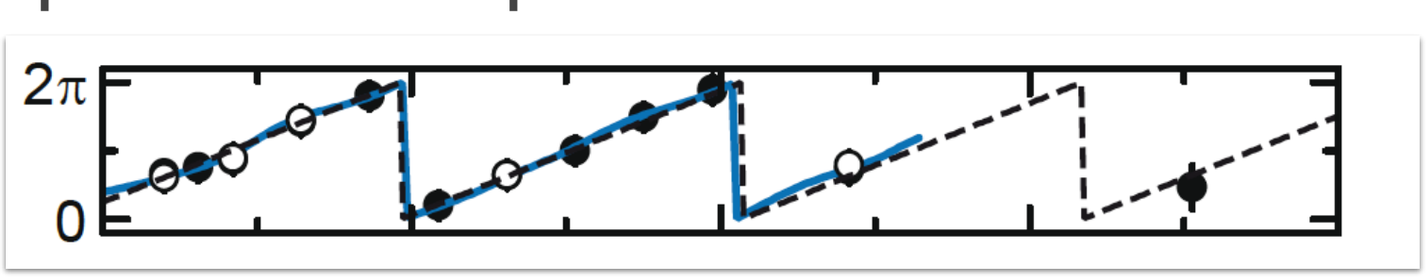
currents

measurement: split in double wells, measure well oscillations

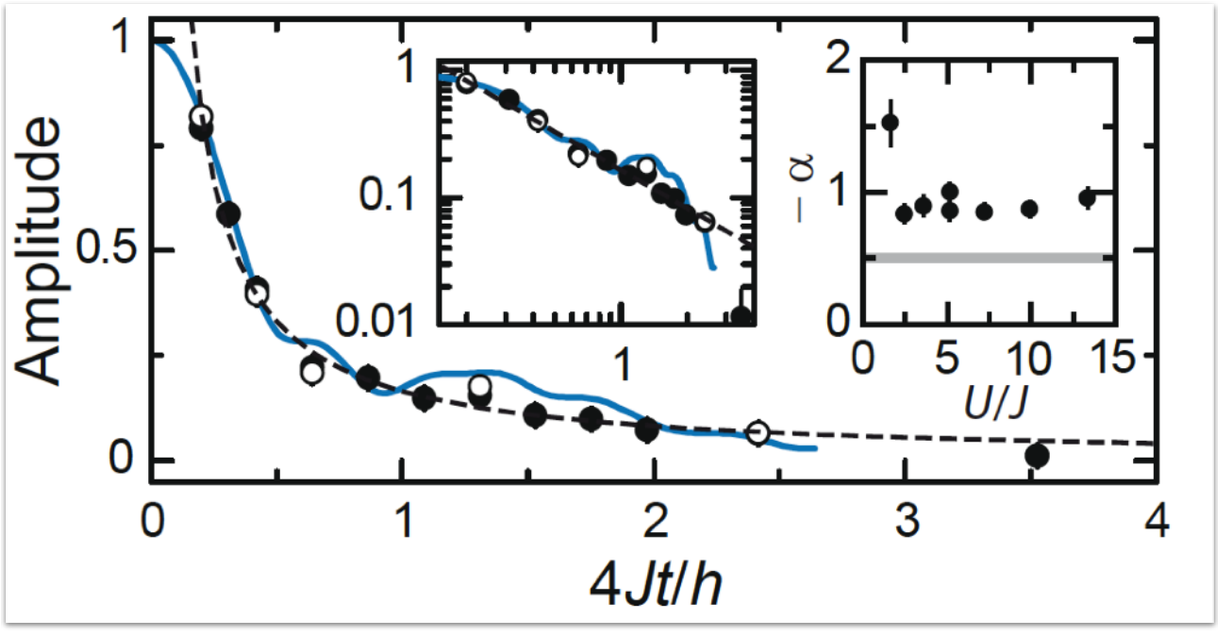




phase and amplitude

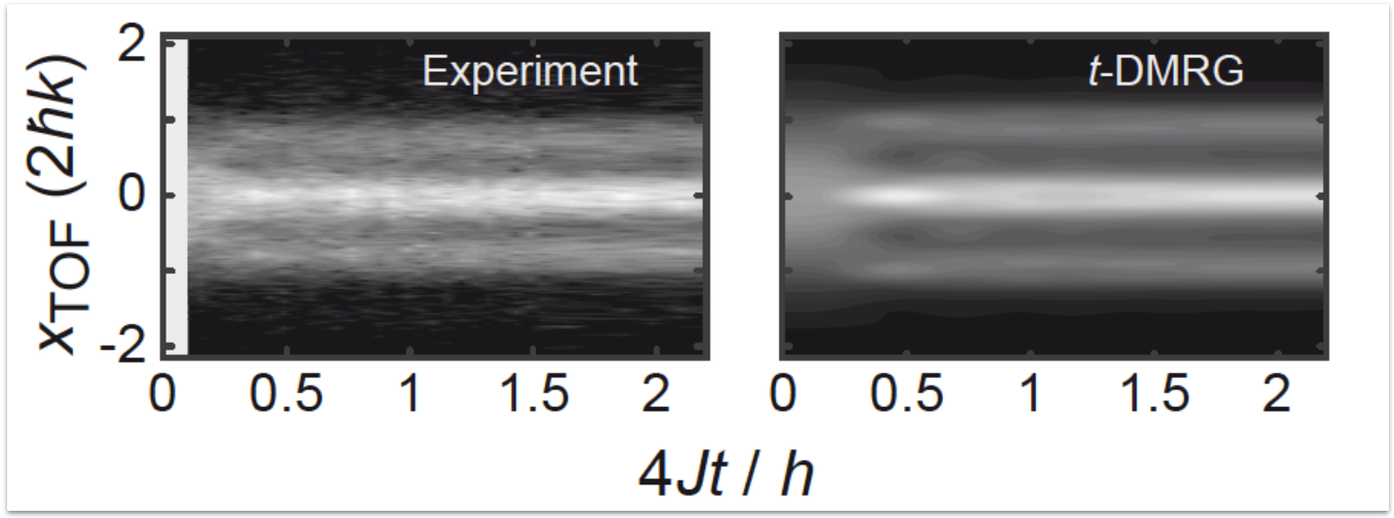


sloshing;
no c.m. motion



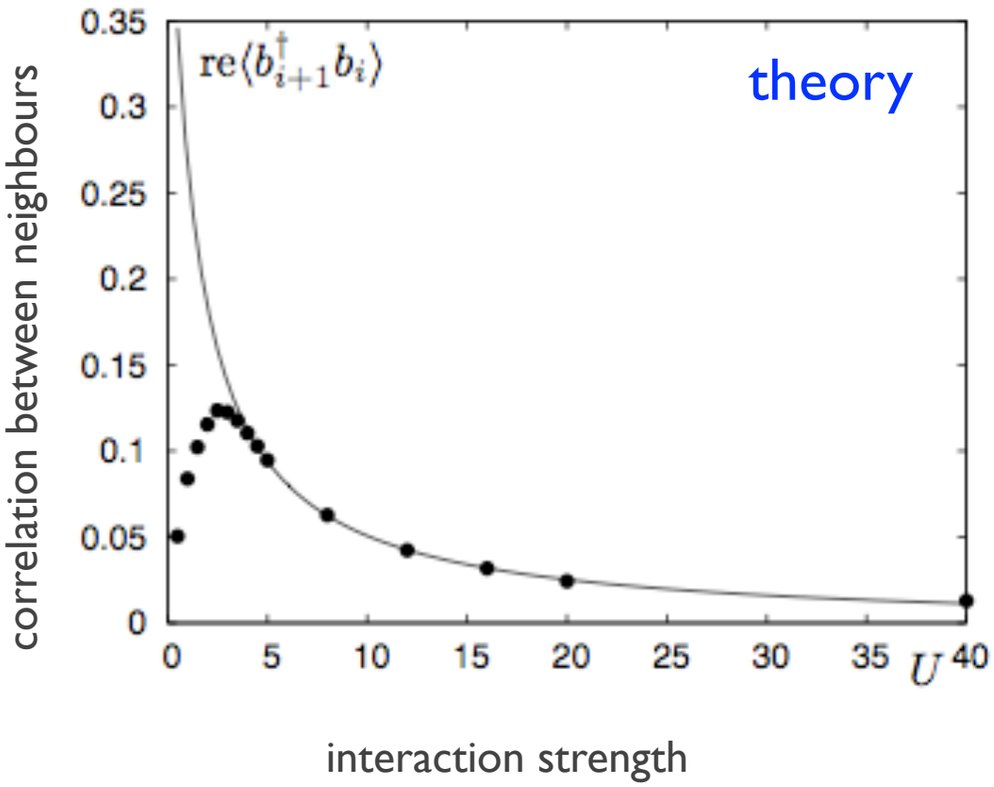
current decay as power law?

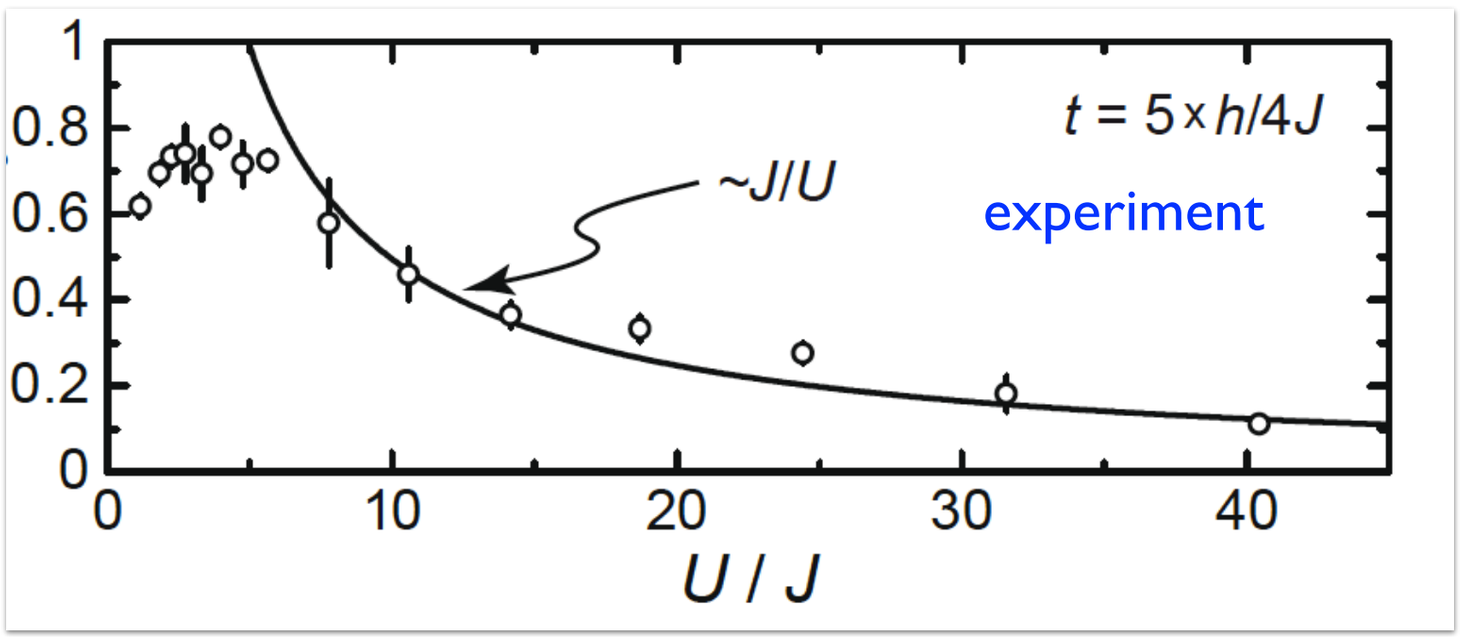
nearest neighbour correlations



momentum distribution

visibility proportional to nearest neighbour correlations

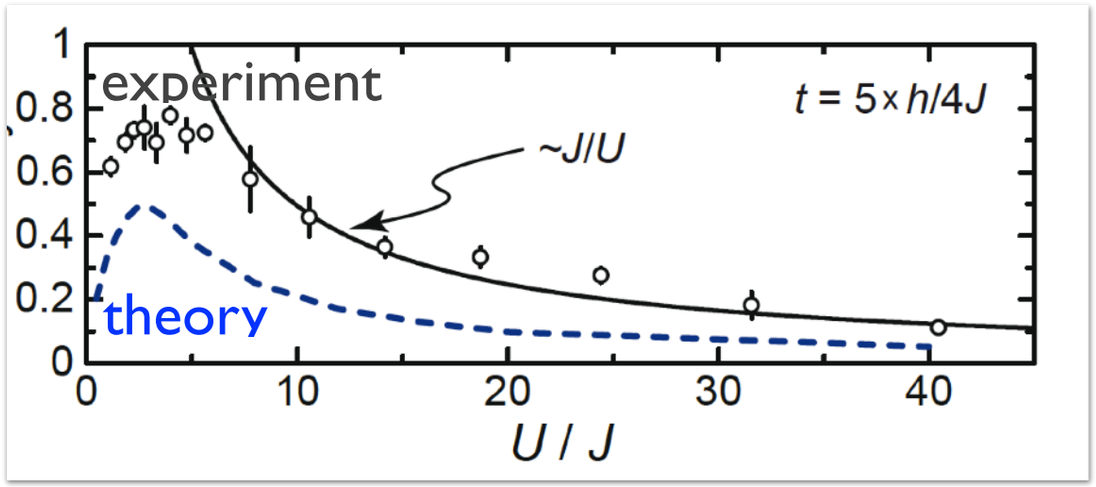




build-up of quantum coherence

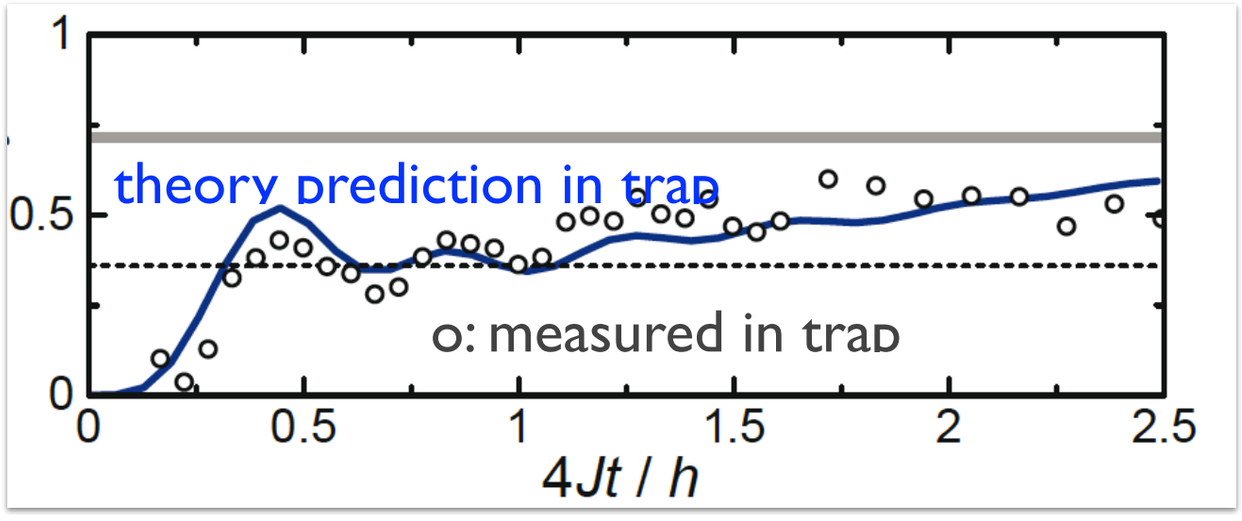
general trend, 1/U correct!

build-up of quantum coherence



long-time limit of nearest-neighbor correlations (here: visibility of momentum distribution)

discrepancy because original theory ignored trap:

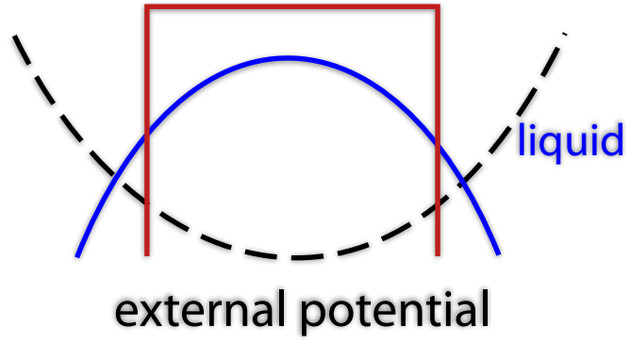


measurement at „long time“

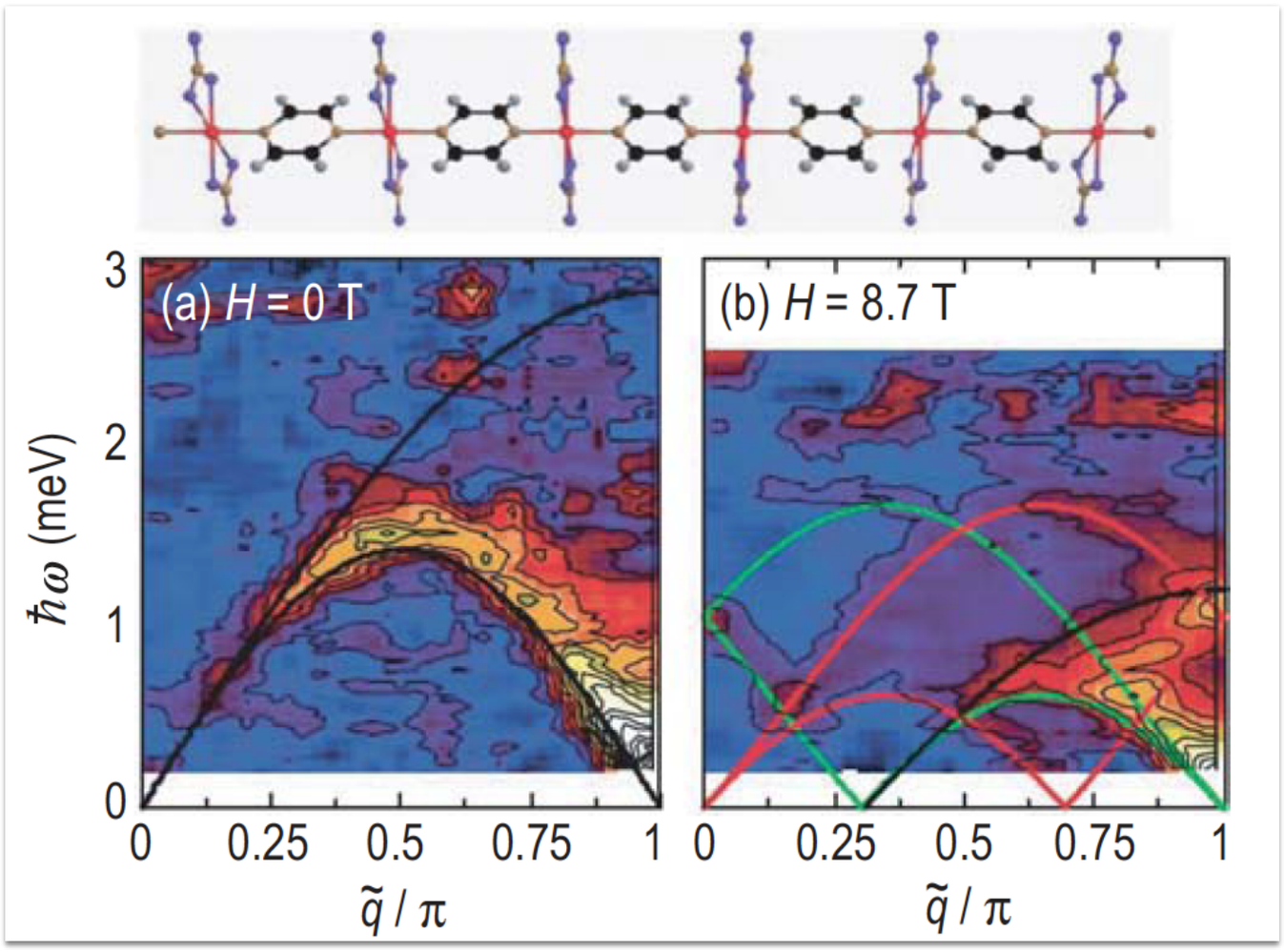
old theory prediction for long times without trap

trap allows particle migration to the „edges“
energy gained in kinetic energy:

$$E_{kin} = -J\langle b_i^\dagger b_{i+1} + b_{i+1}^\dagger b_i \rangle$$



neutron scattering at $T>0$



structure function
by neutron scattering
(Broholm group)

high flux

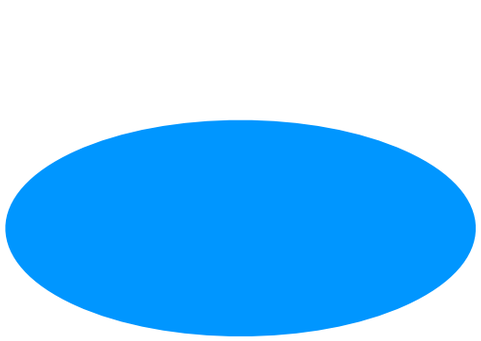
precise lineshapes

- problem: experiment usually T=4.2K, energy scales at J=O(10K)
  definitely not at T=0!
- desired feature because of achievable field strengths:
  H should be of order J --- rule of thumb 1K=1T

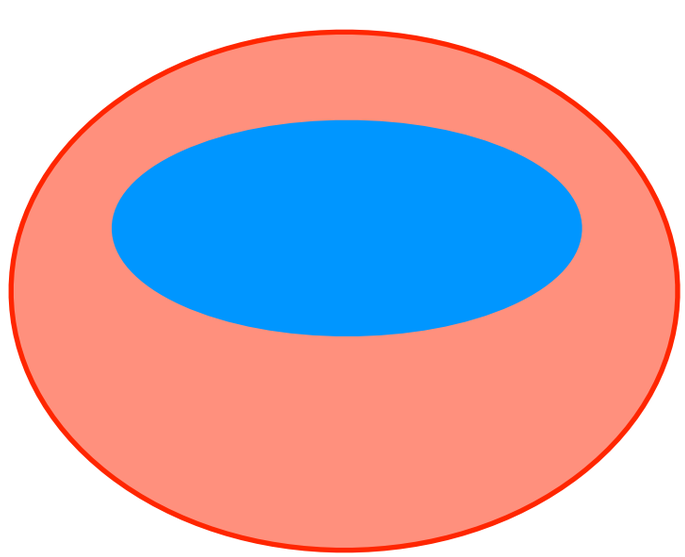
finite-temperature dynamics

- purification

  density matrix of physical system:
  pure state of physical system plus auxiliary system



$$\hat{\rho}_{phys} = \mathrm{Tr}_{aux} |\psi\rangle\langle\psi|$$



- finite-temperature dynamics

  evolution of pure state in enlarged state space

Verstraete, Garcia-Ripoll, Cirac, PRL '04

purification and finite-T evolution

purification: any mixed state can be expressed by a pure state on a larger system (P: physical, Q: auxiliary state space)

$$\hat{\rho}_P = \sum_n \rho_n |n\rangle_P \ {}_P\langle n| \qquad |\psi\rangle_{PQ} = \sum_n \sqrt{\rho_n}|n\rangle_P |n\rangle_Q$$

$$\hat{\rho}_P = \mathrm{tr}_Q |\psi\rangle_{PQ} \ {}_{PQ}\langle\psi|$$

simplest way: Q copy of P

expectation values as before:

$$\langle \hat{O}_P \rangle_{\hat{\rho}_P} = \mathrm{tr}_P \hat{O}_P \hat{\rho}_P = \mathrm{tr}_P \hat{O}_P \mathrm{tr}_Q |\psi\rangle_{PQ} \ {}_{PQ}\langle\psi| = \mathrm{tr}_{PQ} \hat{O}_P |\psi\rangle_{PQ} \ {}_{PQ}\langle\psi| = \ {}_{PQ}\langle\psi|\hat{O}_P|\psi\rangle_{PQ}$$

time evolution as before:

$$\hat{\rho}_P(t) = \mathrm{e}^{-\mathrm{i}\hat{H}t} \hat{\rho}_P \mathrm{e}^{+\mathrm{i}\hat{H}t} = \mathrm{e}^{-\mathrm{i}\hat{H}t} \mathrm{tr}_Q |\psi\rangle_{PQ} \ {}_{PQ}\langle\psi| \mathrm{e}^{+\mathrm{i}\hat{H}t} = \mathrm{tr}_Q |\psi(t)\rangle_{PQ} \ {}_{PQ}\langle\psi(t)|$$

$$|\psi(t)\rangle_{PQ} = \mathrm{e}^{-\mathrm{i}\hat{H}t} |\psi\rangle_{PQ}$$

time-evolution of thermal states

problem: usually we do not have mixed state in eigenrepresentation

thermal states: easy way out by imaginary *t*-evolution

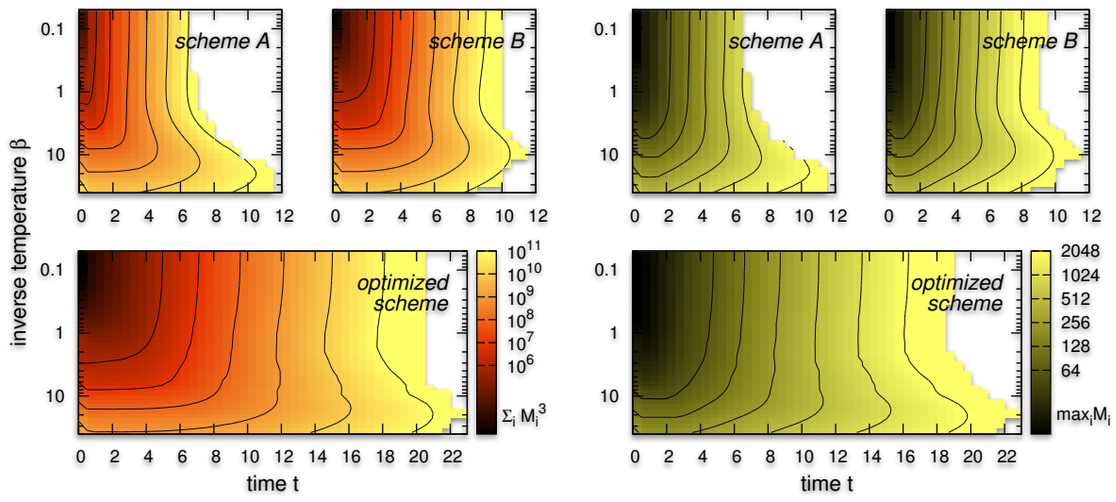
$$\mathrm{e}^{-\beta\hat{H}} = \mathrm{e}^{-\beta\hat{H}/2}\cdot\hat{I}_P\cdot\mathrm{e}^{-\beta\hat{H}/2} = \mathrm{tr}_Q\mathrm{e}^{-\beta\hat{H}/2}|\rho_0\rangle_{PQ}\ {}_{PQ}\langle\rho_0|\mathrm{e}^{-\beta\hat{H}/2}$$

purification of infinite-T state: product of local totally mixed states

gauge degree of freedom: arbitrary unitary evolution on Q

lots of room for improvement:

build MPOs and compress them:



$$\langle\hat{B}(2t)\hat{A}\rangle_\beta = Z(\beta)^{-1}\mathrm{tr}\left(\left[\mathrm{e}^{\mathrm{i}\hat{H}t}\mathrm{e}^{-\beta\hat{H}/2}\hat{B}\mathrm{e}^{-\mathrm{i}\hat{H}t}\right]\left[\mathrm{e}^{-\mathrm{i}\hat{H}t}\hat{A}\mathrm{e}^{-\beta\hat{H}/2}\mathrm{e}^{\mathrm{i}\hat{H}t}\right]\right)$$

linear prediction

(Barthel, Schollwöck, White, PRB 79, 245101 (2009))

- ansatz: data is linear combination of *p* previous data points

prediction calculation

$$\tilde{x}_n = -\sum_{i=1}^{p} a_i x_{n-i}$$

index labels time: time series

- find prediction coefficients by minimising error for available data

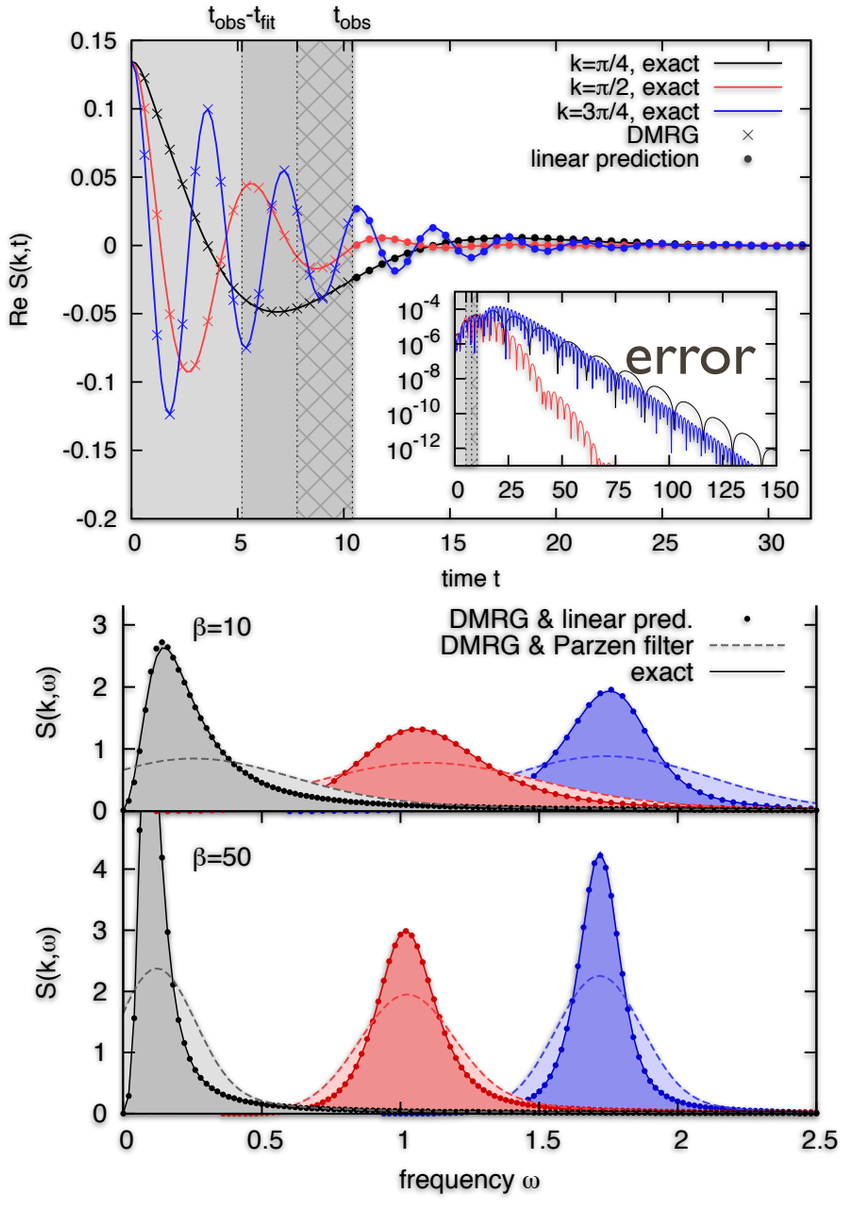
$$E = \sum_n \frac{|\tilde{x}_n - x_n|^2}{w_n}$$

error estimate

- iteratively continue time series from data using ansatz

some results of linear prediction

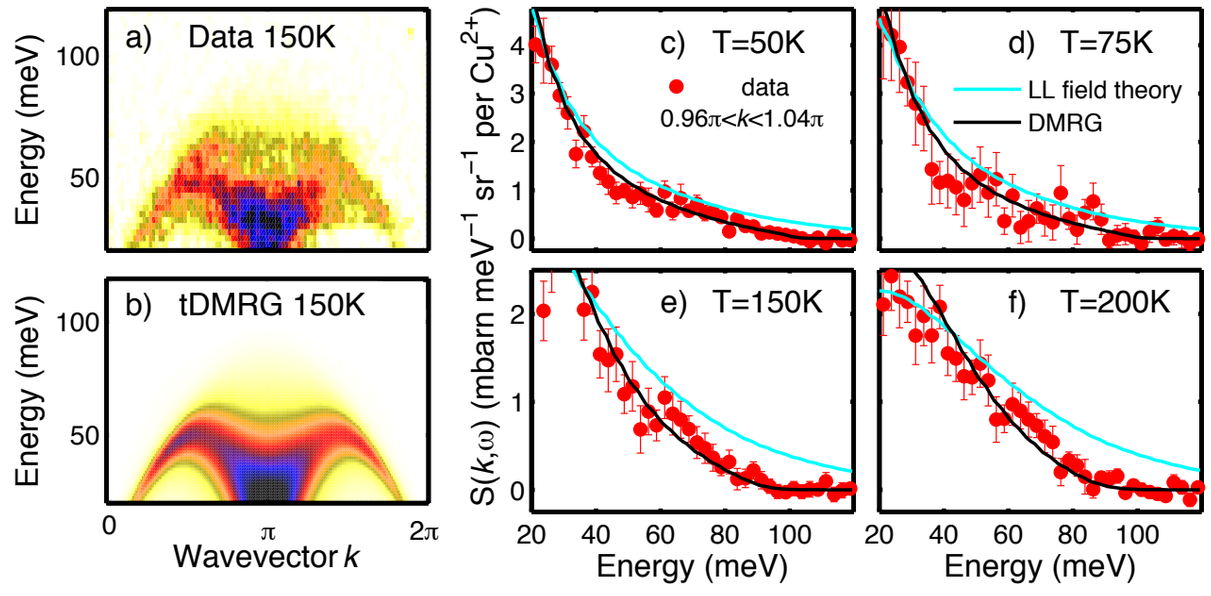
- transverse Ising model: prediction of *S(k,t)*



extends time domain 10x

Barthel, US, White (2009)

- spinons in spin-1/2 chain: experiment vs. numerics



perfect agreement with high-precision neutron scattering

Lake, … Barthel, US, …
PRL 111, 137 (2013)

when does it work?

- why do we predict *S(k,t)* in time and not e.g. *G(x,t)* (and Fourier transform to momentum space later)?

  linear prediction works best for special time series

- superposition of exponential decays

$$x_{n+m} = \sum_{\nu=1}^{p} c_\nu e^{i(\omega_\nu - \eta_\nu)m} x_n$$

- cf. pole structure of momentum-space of Green's functions

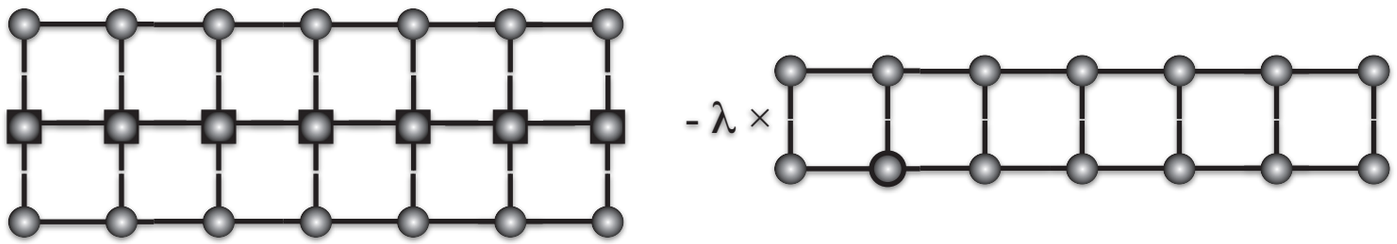
$$G(k,\omega) = \frac{1}{\omega - \epsilon_k - \Sigma(k,\omega)} \qquad G(k,t) = a_1 e^{-i\omega_1 t - \eta_1 t}$$

variational ground state search: DMRG

problem: find MPS (of a given dimension) that minimizes energy

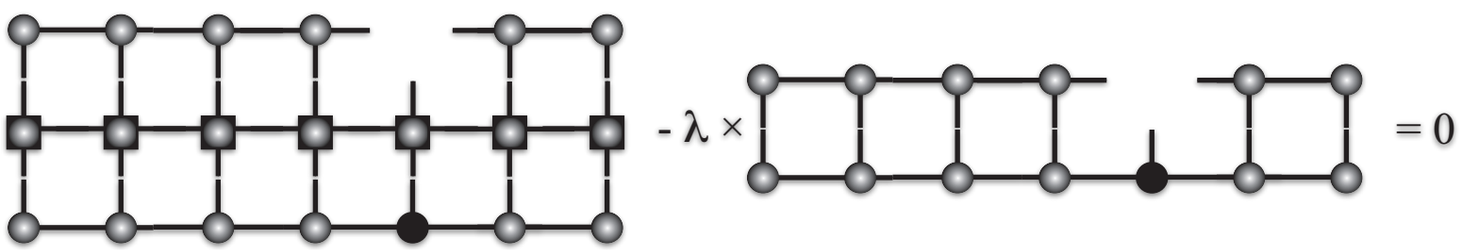
$$\min \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle} \quad \Leftrightarrow \quad \min \Big(\langle\psi|\hat{H}|\psi\rangle - \lambda \langle\psi|\psi\rangle \Big)$$

graphical representation of expression to be minimized:

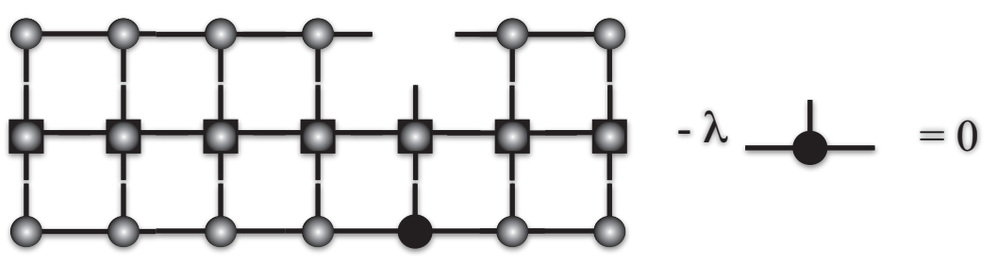


multilinear :-(

variational minimization with respect to one matrix:



unnormalized MPS:
generalized EV problem



mixed normalization MPS:
eigenvalue problem

ground state DMRG

analytical representation of variational problem:

$$\frac{\partial}{\partial M^{\sigma_i *}} \left(\langle \psi | \hat{H} | \psi \rangle - \lambda \langle \psi | \psi \rangle \right) \stackrel{!}{=} 0$$

$$\sum_{\sigma_i' a_{i-1}' a_i'} H_{\sigma_i a_{i-1} a_i, \sigma_i' a_{i-1}' a_i'} M_{\sigma_i' a_{i-1}' a_i'} = \sum_{\sigma_i' a_{i-1}' a_i'} N_{a_{i-1} a_i, a_{i-1}' a_i'} \delta_{\sigma_i, \sigma_i'} M_{\sigma_i' a_{i-1}' a_i'} \equiv \sum_{\sigma_i' a_{i-1}' a_i'} N_{\sigma_i a_{i-1} a_i, \sigma_i' a_{i-1}' a_i'} M_{\sigma_i' a_{i-1}' a_i'}$$

$$H\mathbf{m} = \lambda N \mathbf{m}$$

DMRG algorithm:

- start with random or guess initial MPS
- maintaining mixed normalization, sweep „hot site“ forth and back
- at each step, optimize local matrices by solving eigenvalue problem

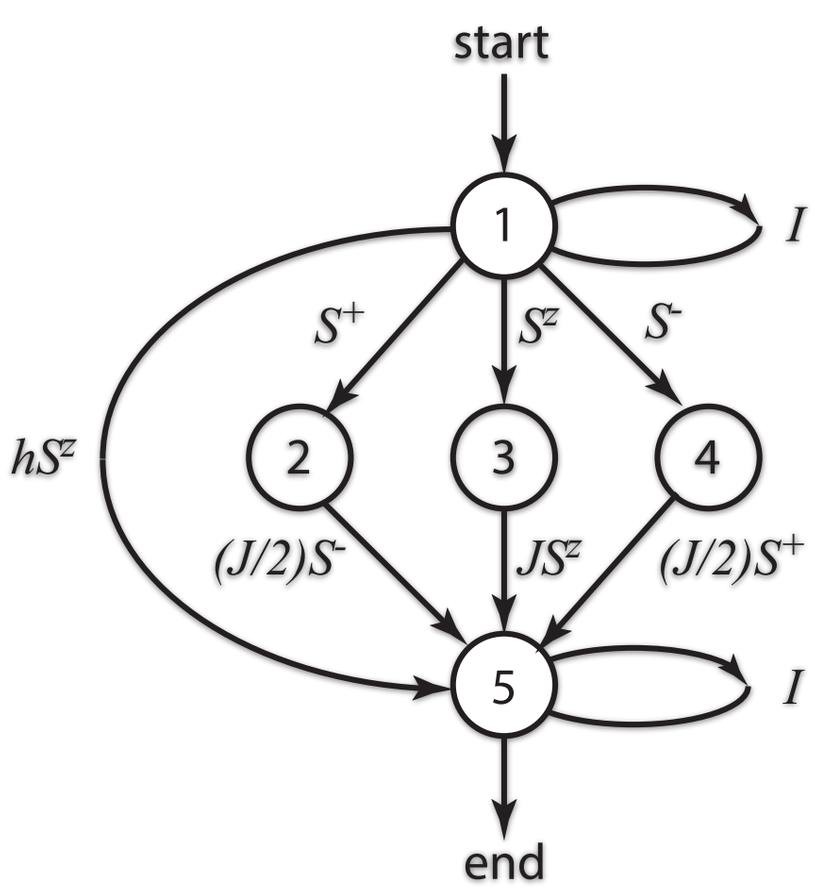
convergence: monitor $\langle \psi | \hat{H}^2 | \psi \rangle - (\langle \psi | \hat{H} | \psi \rangle)^2$

Hamiltonians in MPO form

construct Hamiltonian as automaton that moves through chain (e.g. from right to left) building Hamiltonian

$$\hat{H} = \hat{M}^{[1]}\hat{M}^{[2]}\dots\hat{M}^{[L]} \qquad \hat{M}^{[i]} = \sum_{\sigma_i,\sigma_i'} M^{\sigma_i,\sigma_i'}|\sigma_i\rangle\langle\sigma_i'|$$

$$\hat{H} = J\sum_{i=1}^{L-1}\frac{1}{2}(\hat{S}_i^+\hat{S}_{i+1}^- + \hat{S}_i^-\hat{S}_{i+1}^+) + \hat{S}_i^z\hat{S}_{i+1}^z + h\sum_{i=1}^{L}\hat{S}_i^z$$



Hamiltonians in MPO form II

short ranged Hamiltonians find very compact, exact representation!

$$\hat{M}^{[i]} = \begin{bmatrix} \hat{I} & 0 & 0 & 0 & 0 \\ \hat{S}^+ & 0 & 0 & 0 & 0 \\ \hat{S}^z & 0 & 0 & 0 & 0 \\ \hat{S}^- & 0 & 0 & 0 & 0 \\ h\hat{S}^z & (J/2)\hat{S}^- & J^z\hat{S}^z & (J/2)\hat{S}^+ & \hat{I} \end{bmatrix}$$

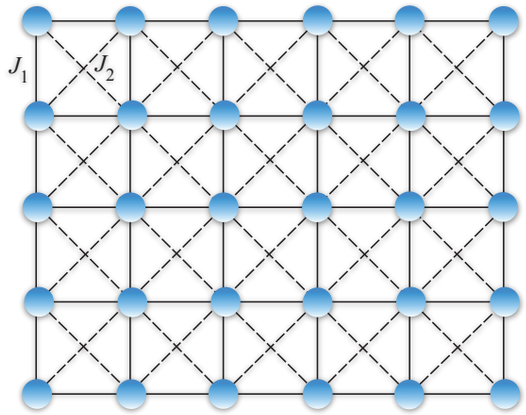
$$\hat{M}^{[1]} = \begin{bmatrix} h\hat{S}^z & (J/2)\hat{S}^- & J^z\hat{S}^z & (J/2)\hat{S}^+ & \hat{I} \end{bmatrix} \qquad \hat{M}^{[L]} = \begin{bmatrix} \hat{I} \\ \hat{S}^+ \\ \hat{S}^z \\ \hat{S}^- \\ h\hat{S}^z \end{bmatrix}$$

frustrated magnetism in 2D

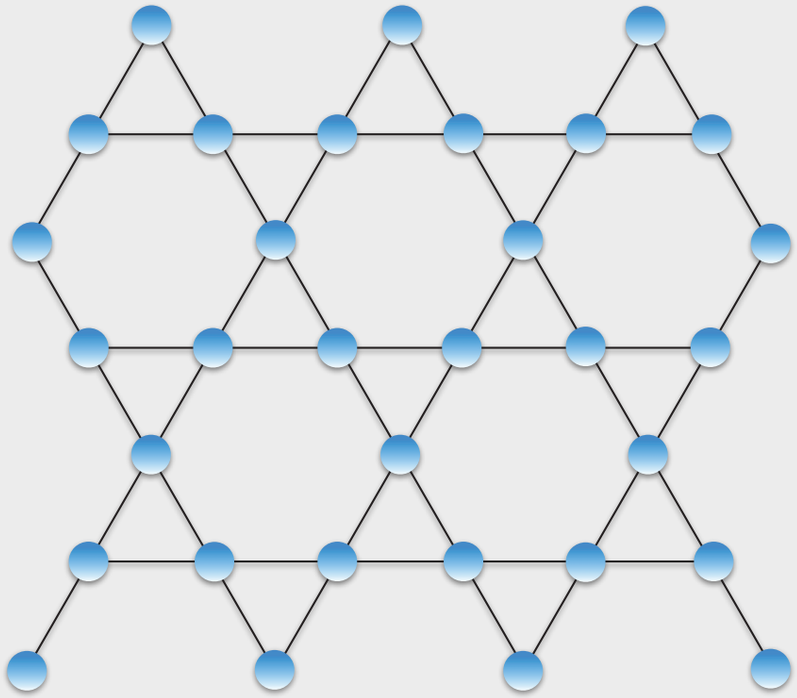
- „classic“ candidates (spin length 1/2):

Yan et al, Science (2011)
Depenbrock et al, PRL (2012)

J_1-J_2 model on a square lattice

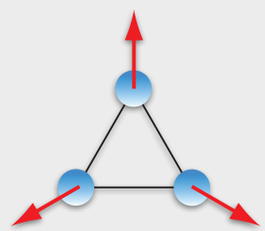


kagome lattice



herbertsmithite
$ZnCu_3(OH)_6Cl_2$

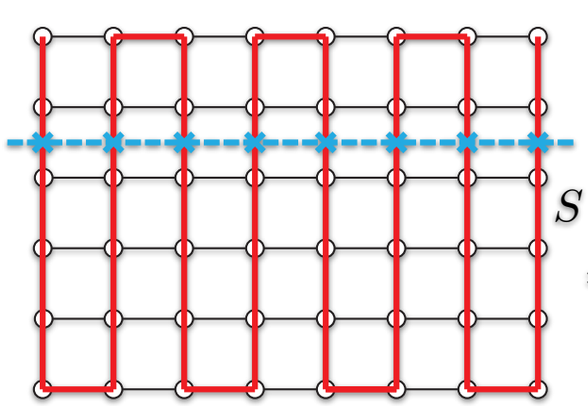
- classical model
  - order only locally coplanar
  - extensive T=0 entropy



- agreement: no magnetic order for S=1/2

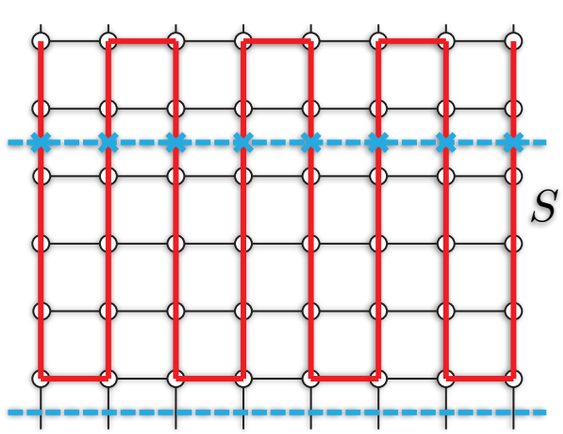
DMRG in two dimensions

- map 2D lattice to 1D (vertical) „snake“ with long-ranged interactions



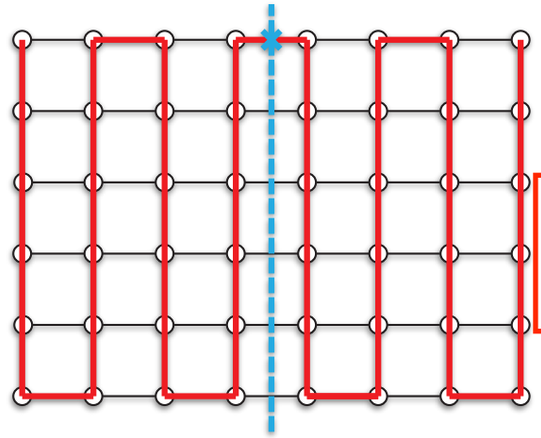
$S \sim \log_2 M^L$
$= L \log_2 M$

vertically OBC



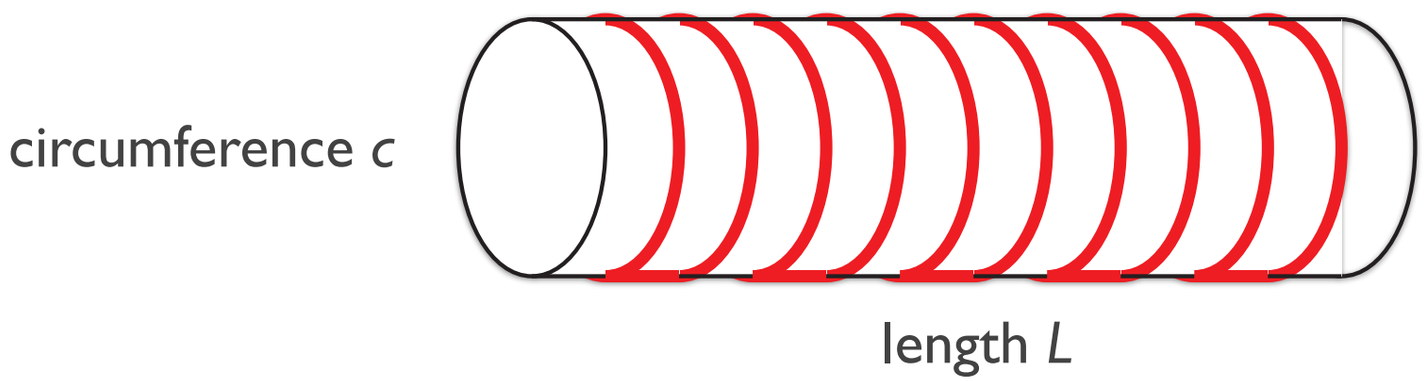
$S \sim \log_2 (M^2)^L$
$= 2L \log_2 M$

vertically PBC: extra cost!



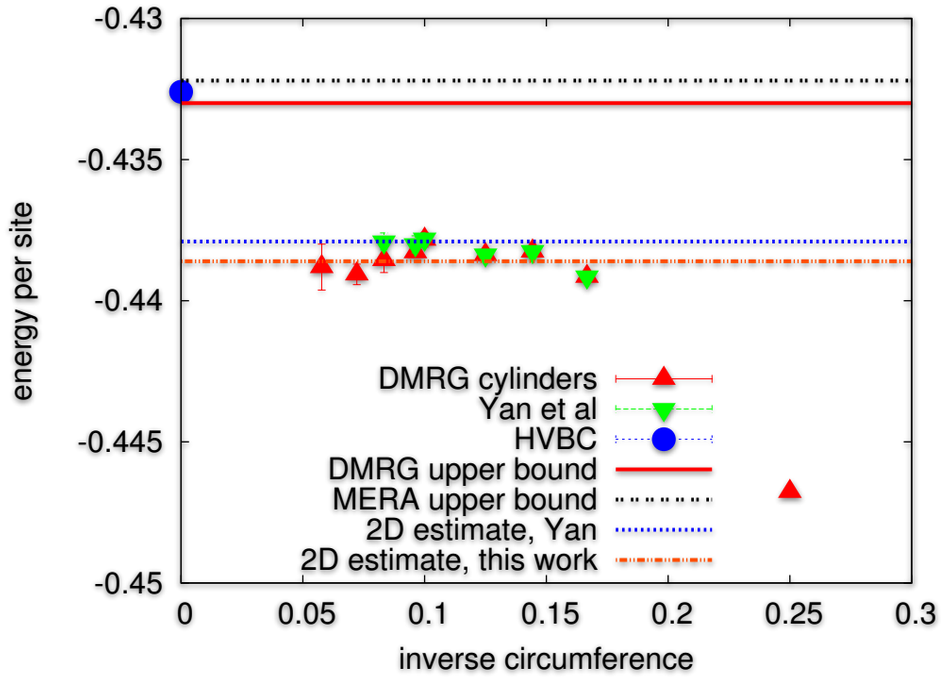
$S \sim \log_2 M$
$\rightarrow M \sim 2^L$

- horizontally: ansatz obeys area law: easy axis, long at linear cost
- vertically: ansatz violates area law: hard axis, long at exponential cost
- consider long cylinders of small circumference *c*: mixed BC



ground state energies

- fully *SU(2)* invariant DMRG code
- up to 3,800 representatives (16,000 *U(1)* DMRG states) — 100% increase
- cylinders up to circumference c=17.3, N=726 — 50% increase
- tori up to N=(6x6)x3=108 sites — ED: 48 sites

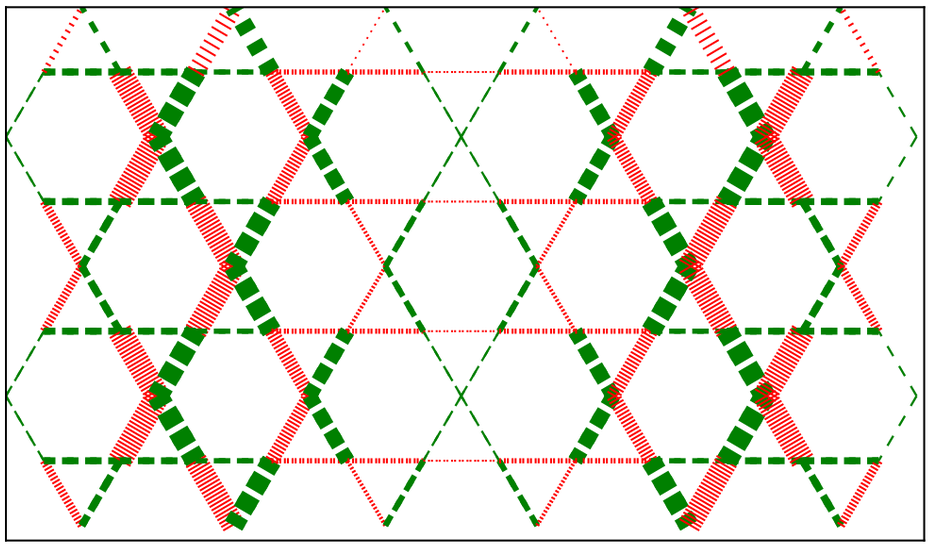


- TD limit energy estimate: -0.4386(5)
- iDMRG (infinite cylinder) upper bounds below HVBC; YC8: -0.4379

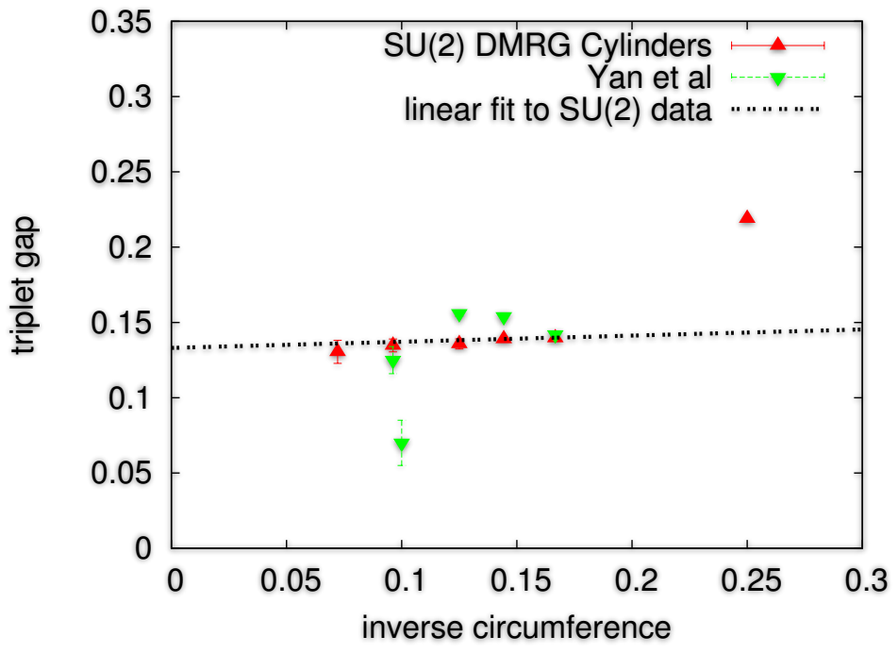
  iDMRG: I.P. McCulloch, arXiv:0804.2509

triplet gap

- fully *SU(2)* invariant DMRG code
- eliminates need for special edge manipulations of *U(1)* DMRG: ground state of *S*=1 sector



bond energy deviations from mean



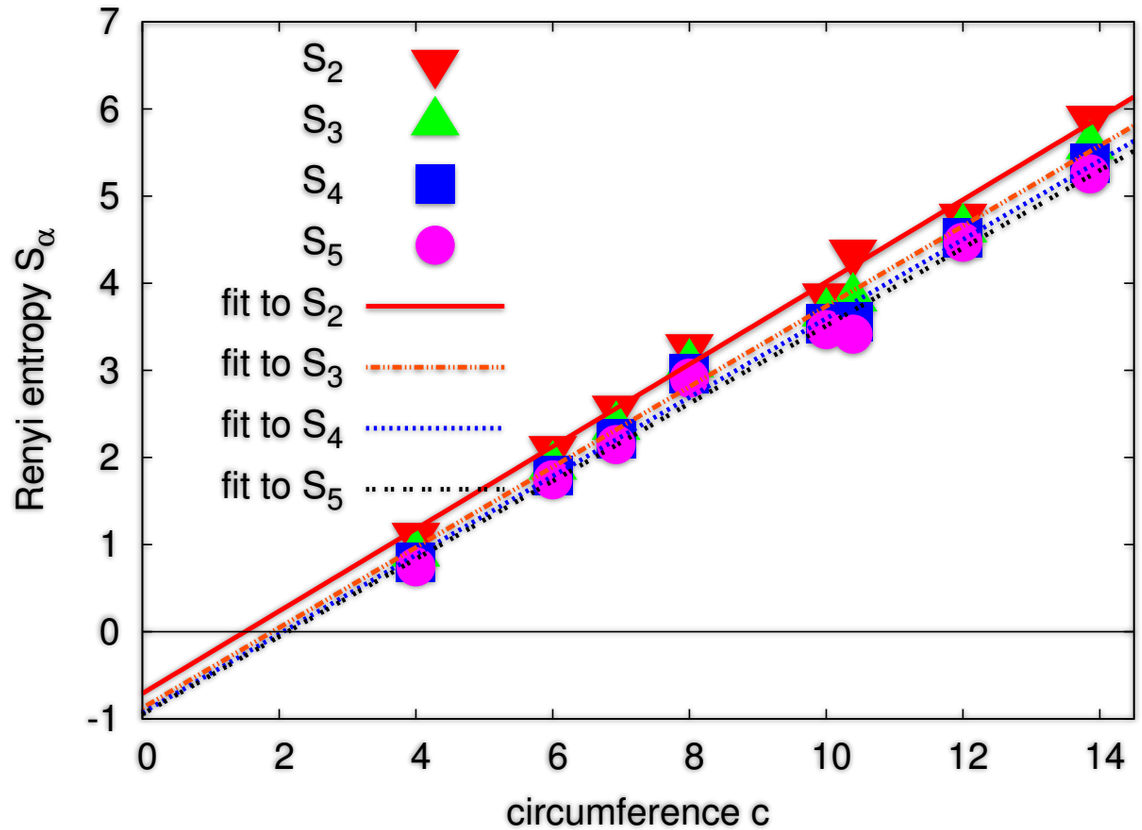
triplet gap for infinitely long cylinders

- bulk excitation
- much smoother gap curve
- triplet gap estimate: 0.13(1)

singlet gap estimate: approx 0.05
(Yan *et al.* (2011))

TEE in the kagome lattice

- extrapolate Renyi entropies to circumference c=0
- negative intercept is TEE
- find topological order!



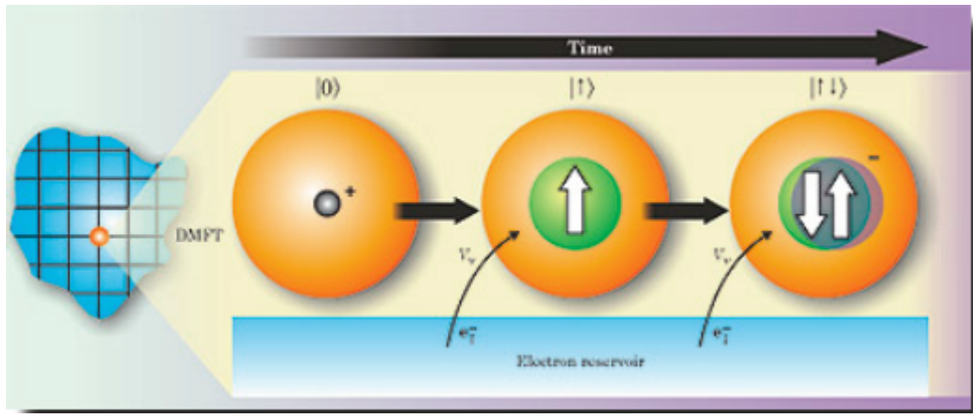
$$\gamma \approx 0.94 \qquad D \approx 2$$

- TEE extracted from random state in GS manifold lower bound
- true value for so-called minimum entropy state
- DMRG seems to systematically pick those

Zhang, Grover, Turner, Oshikawa, Vishvanath, PRB (2012)

DMFT primer

- dynamical mean field theory (DMFT):
  - Hubbard model replaced by single impurity embedded in non-interacting effective bath
  - impurity dynamically exchanges electrons with bath: beyond static mean-field theory
  - self-consistency condition:
    local lattice self-energy = self-energy of effective impurity model etc.

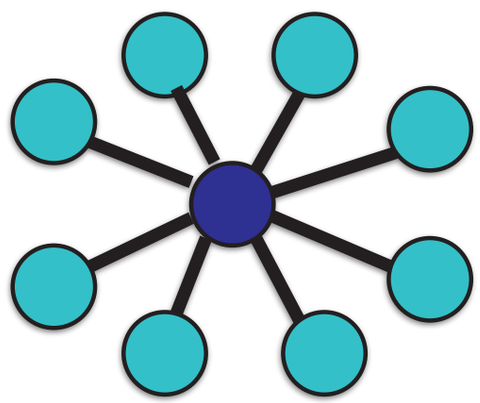


- exact in the limit of infinite coordination number (dimension)
- many applications also in more material-oriented simulations
- impurity solver needed to calculate spectral functions
  place of methodological progress!!!

Metzner, Vollhardt, PRL (1989)
Georges *et al.*, RMP (1996)
Kotliar *et al.*, RMP (2006)

spectral functions in DMFT (T=0)

- star geometry



hopping impurity - bath sites

- calculate in frequency space

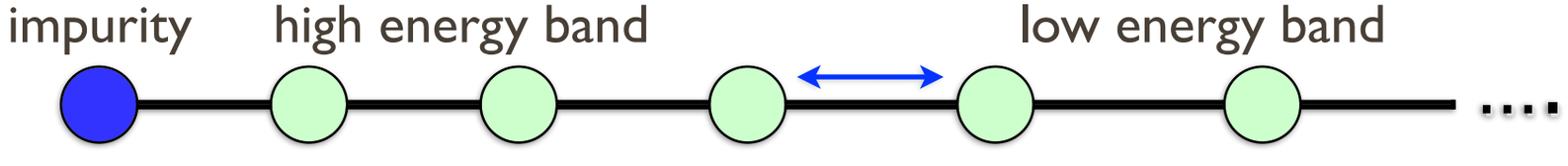
$$C_\eta(\omega) = \langle 0|d\frac{1}{H-\omega-E_0+\mathrm{i}\eta}d^\dagger|0\rangle$$

- calculate in real-time space: superior

$$C(t) = \langle 0|\mathrm{e}^{\mathrm{i}(H-E_0)t}d\mathrm{e}^{-\mathrm{i}(H-E_0)t}d^\dagger|0\rangle$$

FT trafo to frequency space
damping with eta
limit: reachable times

- bath often mapped to one-dimensional chain



why DMRG as DMFT solver?

- there are many impurity solvers:
  - exact diagonalization (ED)
  - numerical renormalization group (NRG)
  - continuous quantum Monte Carlo (QMC; in various incarnations)
- what advantages of DMRG/MPS solver were hoped for:
  - larger bath sizes (compared to ED)
  - homogeneous energy resolution (compared to NRG)
  - no analytic continuation from imaginary axis (compared to QMC)
  - no sign problem for complex problems (compared to QMC)
- previous attempts: single-band DMFT (C=1)
  stuck for about 10 years!

Hallberg *et al.* (since 2004)
Nishimoto, Jeckelmann
Karski, Raas, Uhrig

Our Method

$$G_{loc}(i\omega_n) = \int dk \frac{1}{i\omega_n + \mu - \epsilon_k - \Sigma_{latt}(i\omega_n)}$$

$$G_{imp}(i\omega_n) = \frac{1}{i\omega_n + \mu - \Lambda(i\omega_n) - \Sigma_{imp}(i\omega_n)}$$

$G_{loc} = G_{imp}$

$\Sigma_{latt} = \Sigma_{imp}$

$G_{loc} = G_{imp}$

$\Sigma_{latt} = \Sigma_{imp}$

$\Lambda(i\omega_n)$

$$\chi = \frac{1}{N}\sum_{n=1}^{N} |\Lambda(i\omega_n) - \Lambda_{Discr}(i\omega_n)|^2$$

$$\Lambda_{Discr}(i\omega_n) = \sum_{l=1}^{L_b} \frac{V_l^2}{i\omega_n - \varepsilon_l}$$

ε_k, V_k

$|\psi_{GS}\rangle$

$$G^p(\tau) = \langle\Psi|ce^{-(H-E)\tau}c^\dagger|\Psi\rangle$$

$$G^h(\tau) = \langle\Psi|c^\dagger e^{-(H-E)\tau}c|\Psi\rangle$$

$$G^p(t) = \langle\Psi|ce^{-iHt}c^\dagger|\Psi\rangle$$

$$G^h(t) = \langle\Psi|c^\dagger e^{-iHt}c|\Psi\rangle$$

$$G_\eta^{ret}(\omega) = -i\int_0^\infty dt[G^p(t) + G^h(t)]e^{i\omega t}e^{-\frac{\eta^2 t^2}{2}}$$

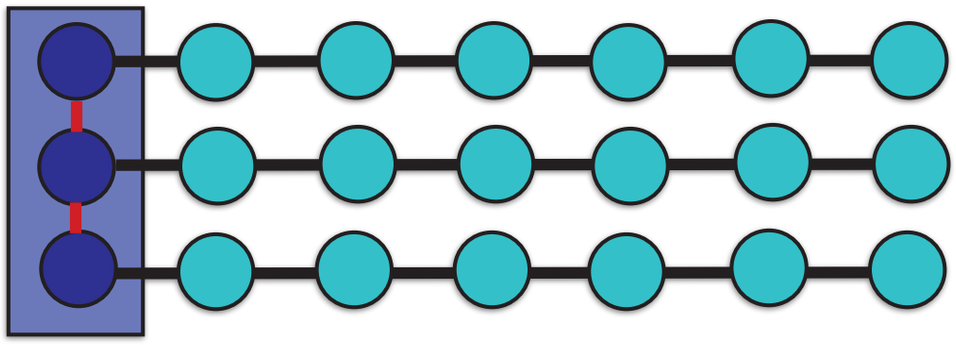
$$G(i\omega_n) = \int_{-\infty}^{\infty} d\tau e^{-i\omega_n\tau}[-\theta(\tau)G^p(\tau) + \theta(\tau)G^h(\tau)]$$

$\Sigma_{imp}(i\omega_n) = G^{-1}_{imp,0}(i\omega_n) - G^{-1}_{imp}(i\omega_n)$

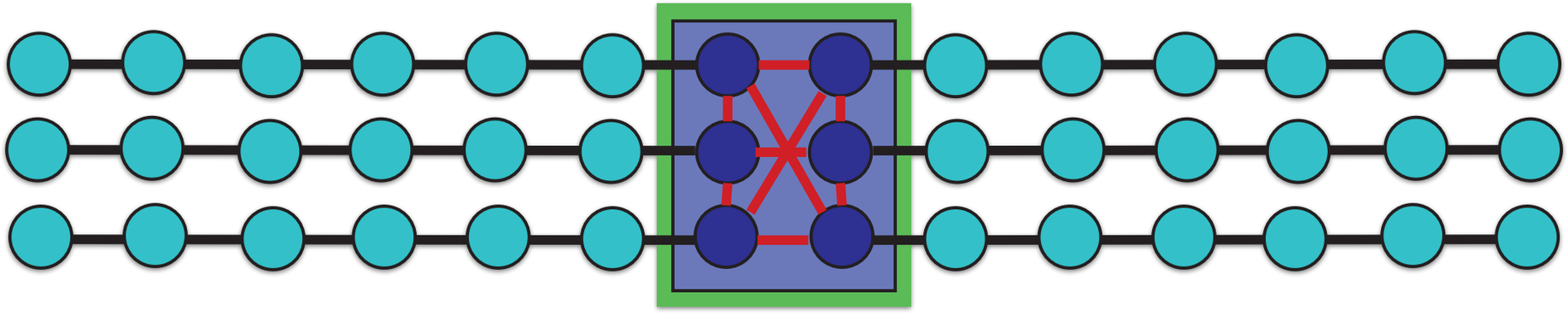
towards realistic DMFT

- originally a single impurity and a single valence band:

- in real substances, often multiple valence bands (orbitals):



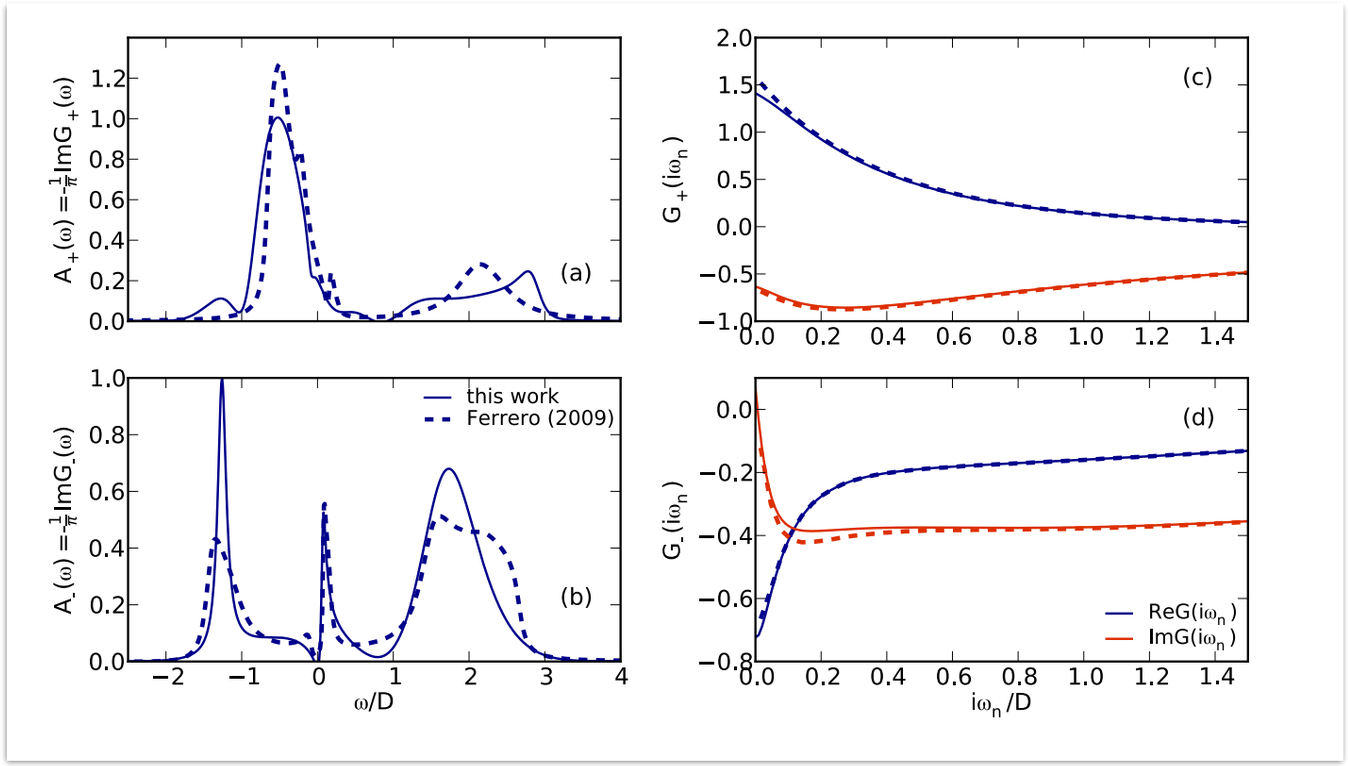
- improve realism by multiple sites (DCA) - bands from DFT



- figure of merit *C*: sites times orbitals; here 1 - 3 - 6

DMFT: two-site cluster DCA

- hole-doped Hubbard model on square lattice, 4% doping, U=10



- calculation time: ca. 50 hs for spectral function (Chebyshev 2011)

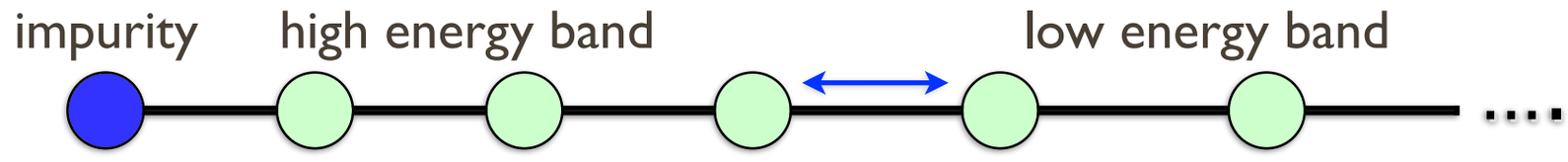
CT-QMC: Ferrero, Cornaglia, De Leo, Parcollet, Kotliar, Georges, PRB (2009)
DMRG/MPS: Wolf, McCulloch, Parcollet, Schollwöck, PRB (2014)

no doping: see also Ganahl et al, PRB (2014)

which bath geometry?

Wolf, McCulloch, Schollwöck, PRB 90, 235131 (2014)

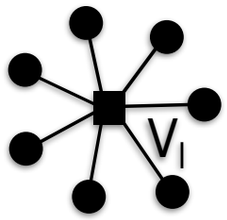
- bath modeled by chain geometry in DMRG, MPS, NRG

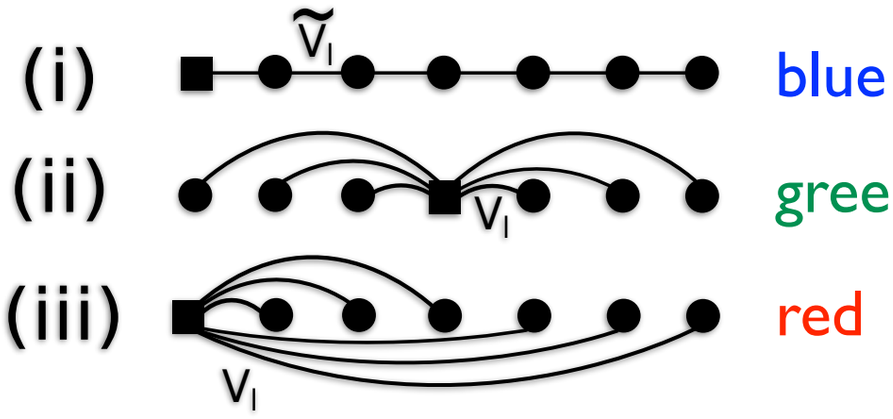


- only restriction: deliver self-consistent hybridization function
- star geometry emerges more naturally
- so why chain geometry?
  - Wilson NRG: separation of energy scales — Wilson, RMP (1975)
  - DMRG, MPS: star must be arranged as chain (short-ranged hopping), star generates undesirable long-range entanglement (conventional wisdom)
- is this so?

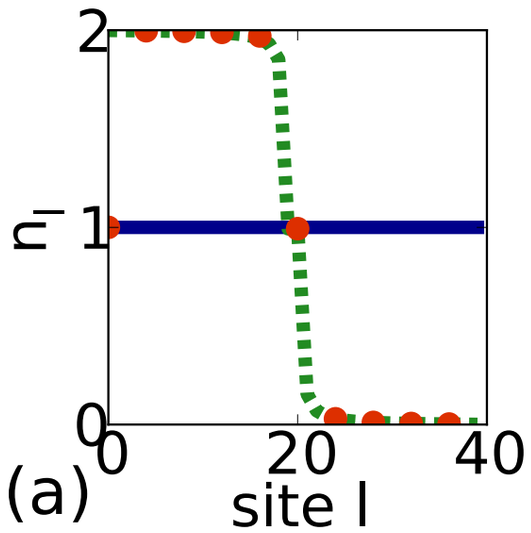
star geometry is better!

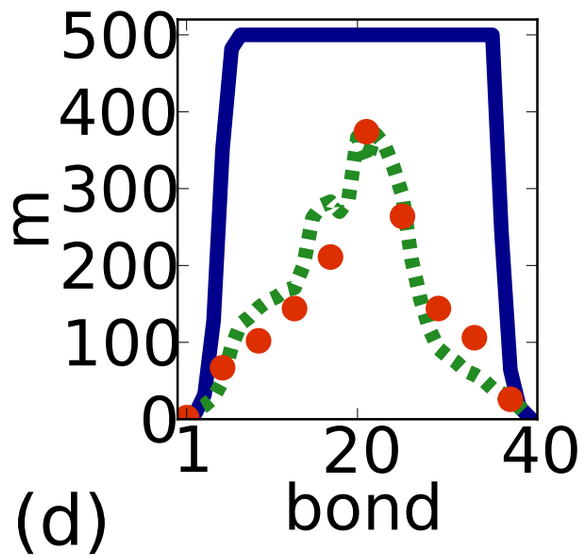
lower entanglement: star or chain geometry?

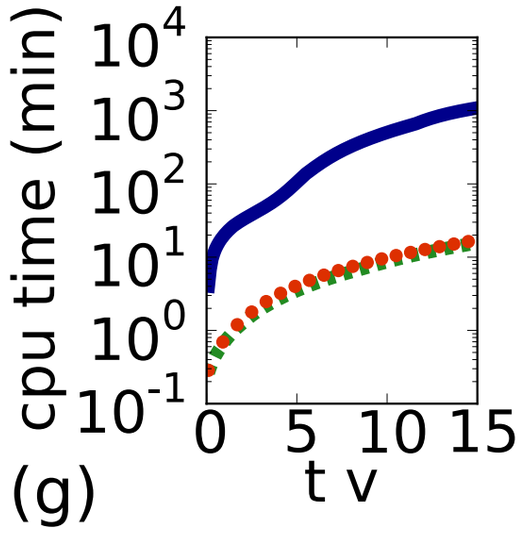




strongly different growth of MPS bond dimensions





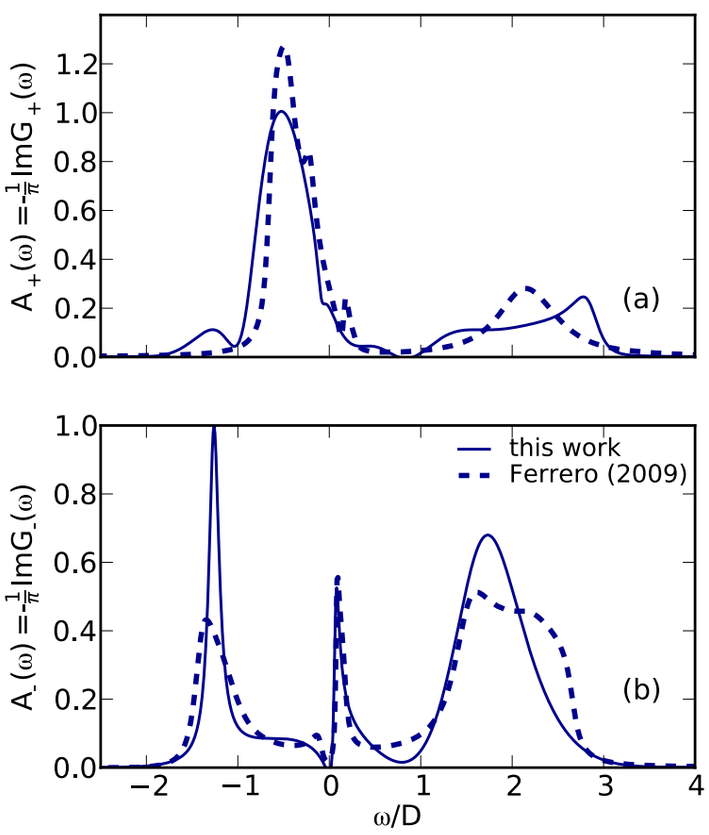


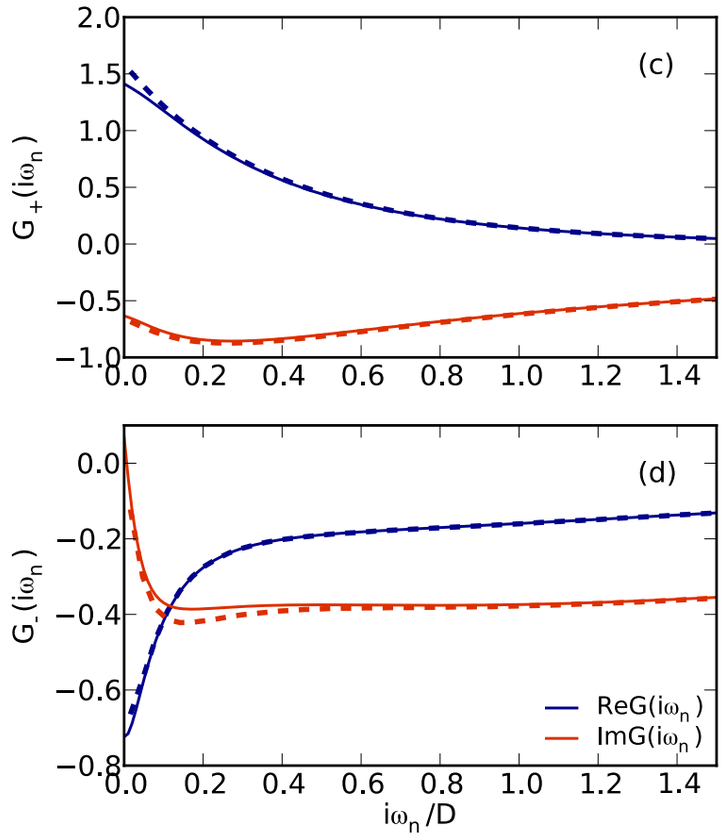
Wolf *et al.*, PRB (2014)

2-site cluster DCA in k-space

DMRG/MPS: Wolf, McCulloch, Parcollet, Schollwöck, PRB (2014)

- model: hole-doped (4%) Hubbard model on 2d square lattice
- spectral function: time evolution, linear prediction
- bath discretization: linear; L_b/L_c = 30 … 40; geometry: star
- CPU time: 60 min ground state; 40 min spectral (down from several days!)





U=2D

C=2

where do we do the spectral function?

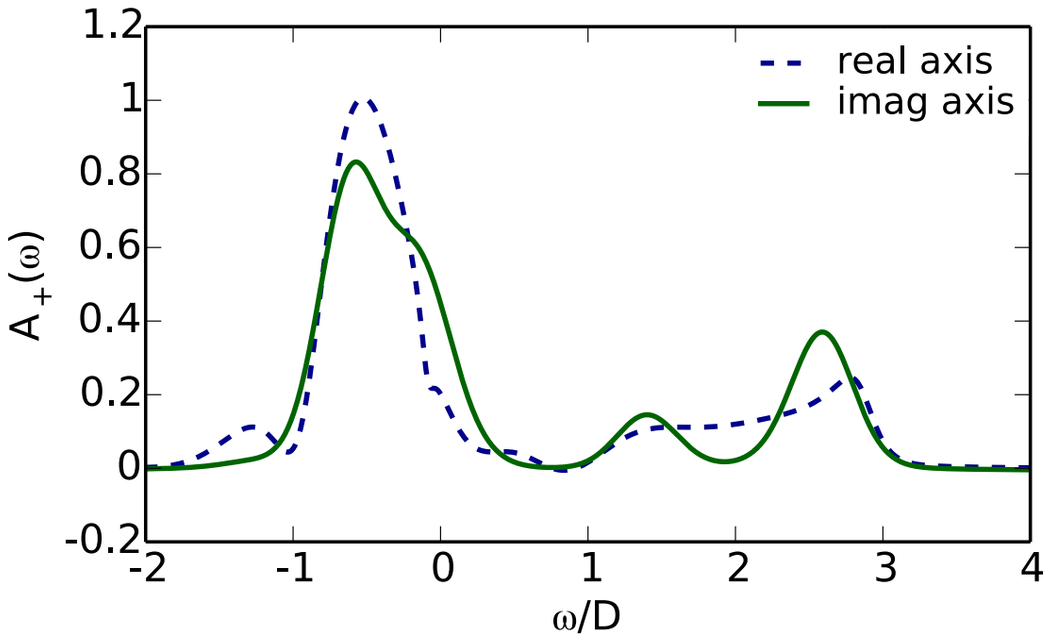
Wolf, Go, McCulloch, Millis, Schollwöck, PRX 5, 041032 (2015)

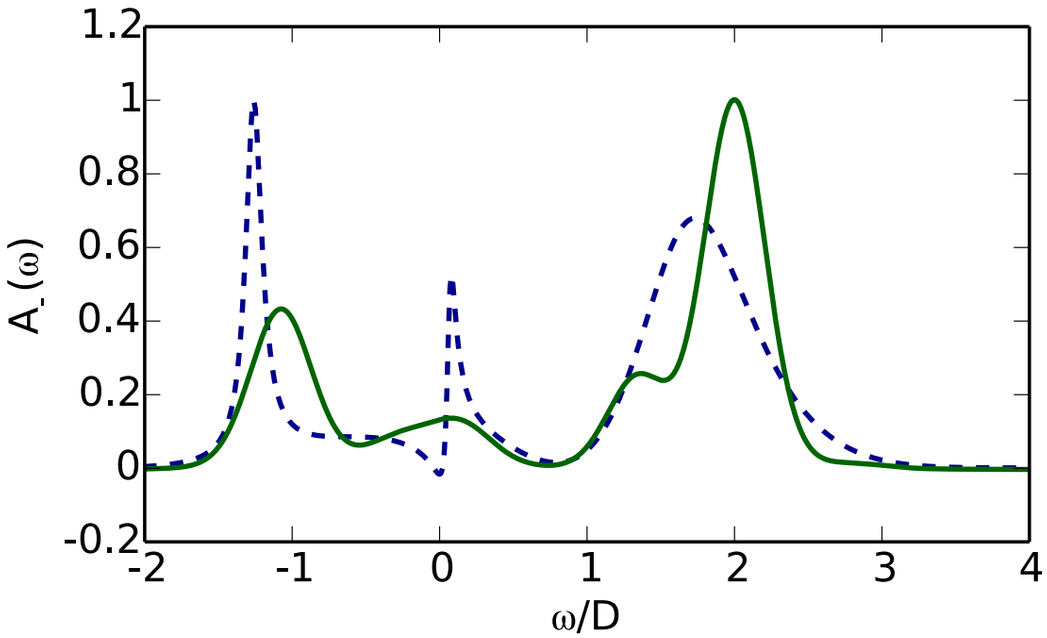
- spectral function can be calculated anywhere in complex plane
- Quantum Monte Carlo: imaginary axis only;
  ill-conditioned analytic continuation to real axis for freq. info
- advantage: DMRG/MPS on real axis! but cumbersome!
- now switch to imaginary axis:
  - much smaller bath sizes possible
  - essentially no entanglement growth
  - much larger no of sites/orbitals (up to C=20) where QMC fails totally
  - no analytic continuation: spectral function from converged DMFT
  - prize to pay: partial loss of detailed information

2-site cluster DCA in k-space

- model: hole-doped (4%) Hubbard model on 2d square lattice
- Matsubara Green's function: imaginary time evolution
- bath discretization: fitting; $L_b/L_c = 3$; geometry: star
- CPU time: 1 min ground state; 4 min spectral

$U=2D$ **C=2**

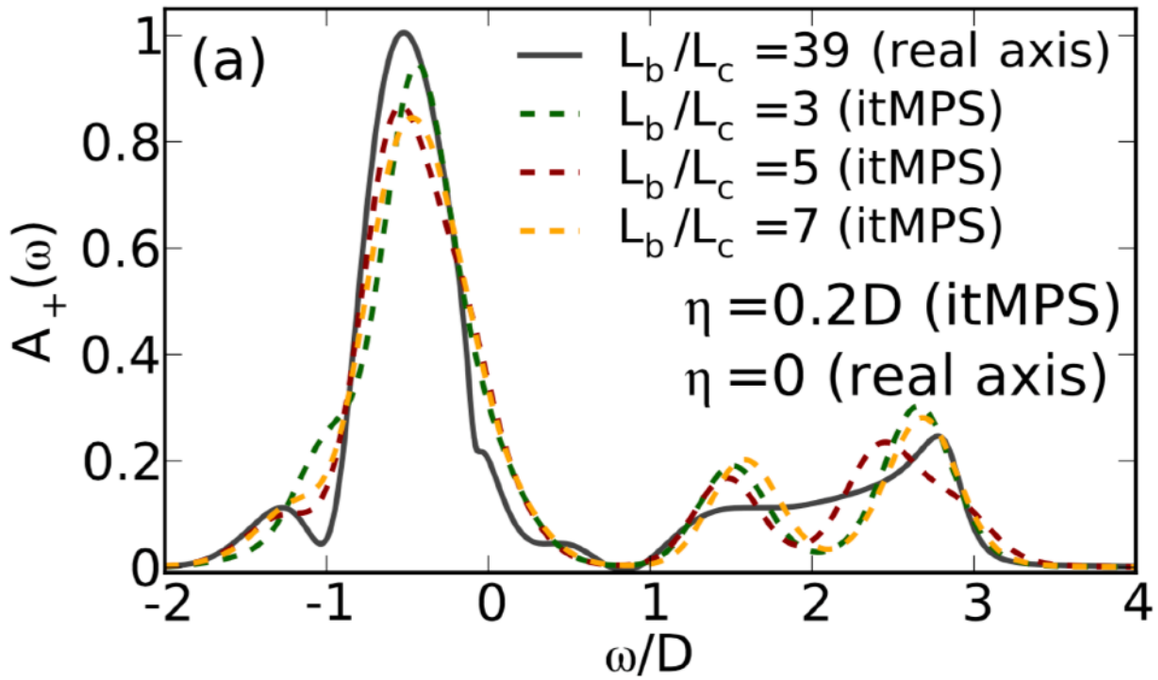


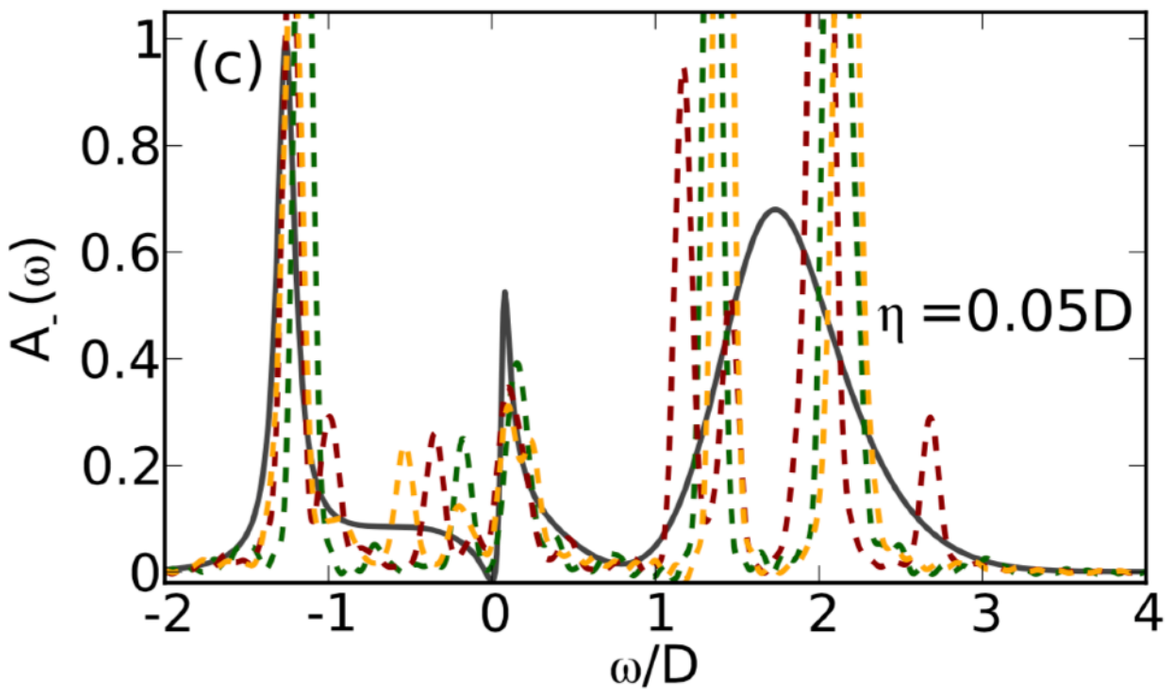


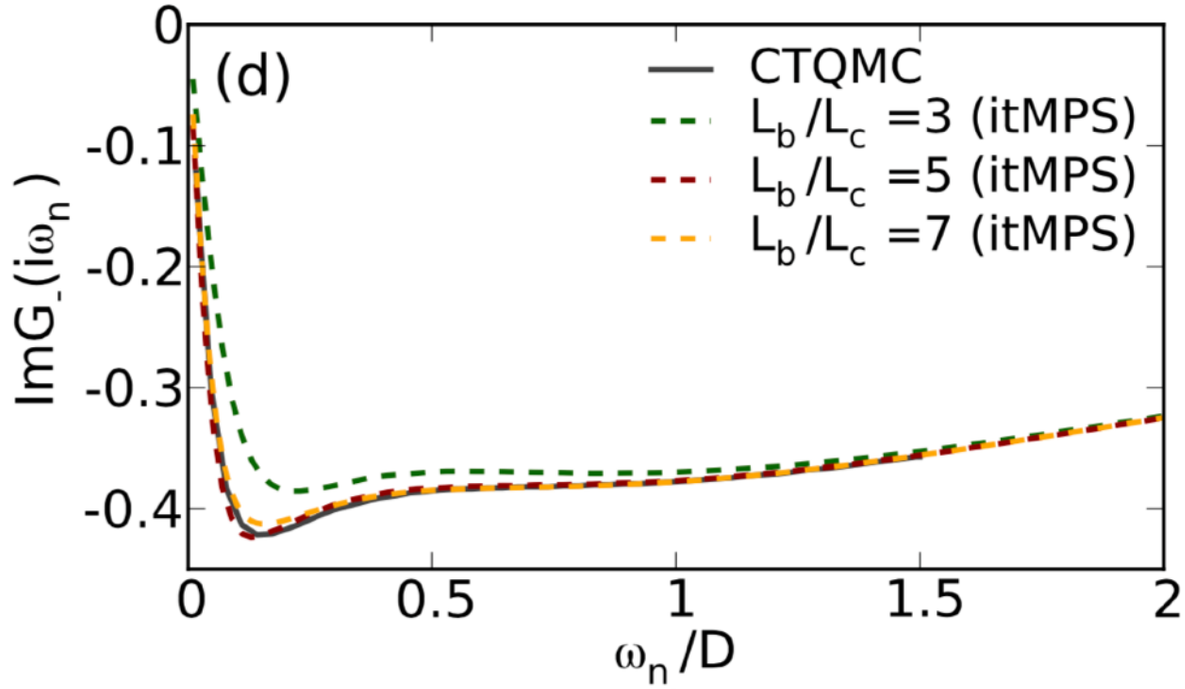
pseudogap not reproduced, other features represented!

more details

- 1 band Hubbard model
- good agreement on the + Patch but not for - Patch on real axis
- broadening and finite size effects
- on imaginary axis good

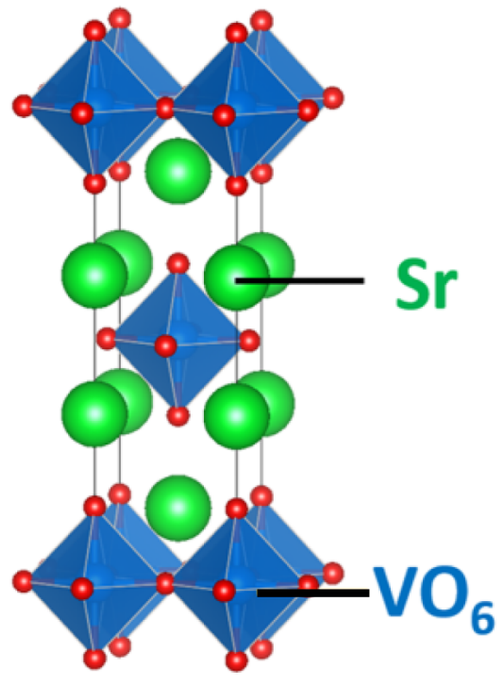


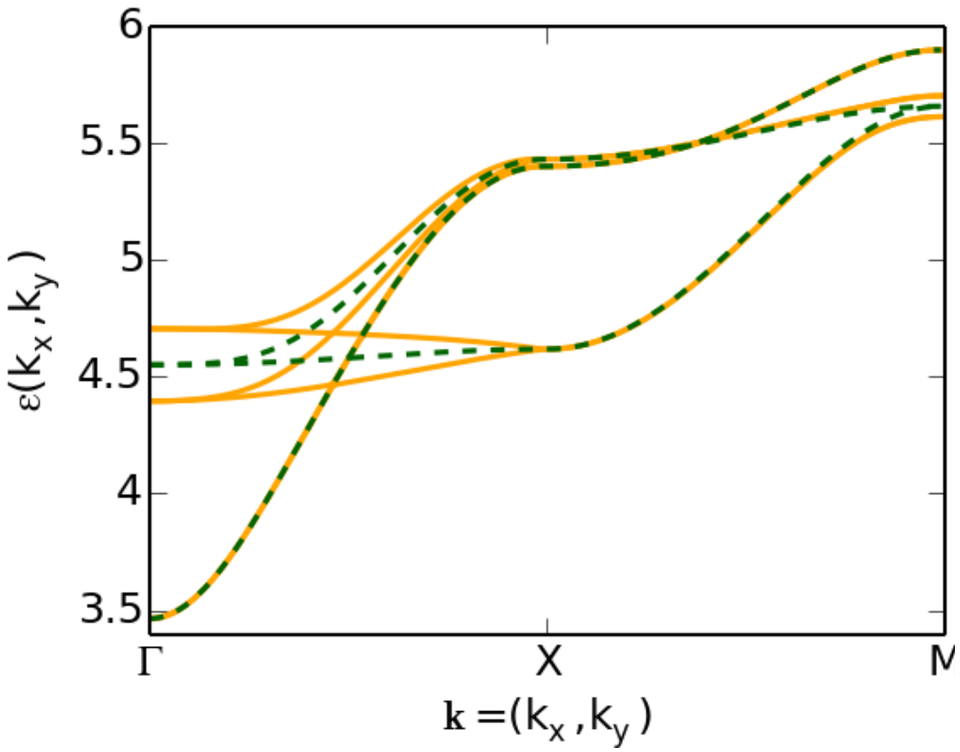


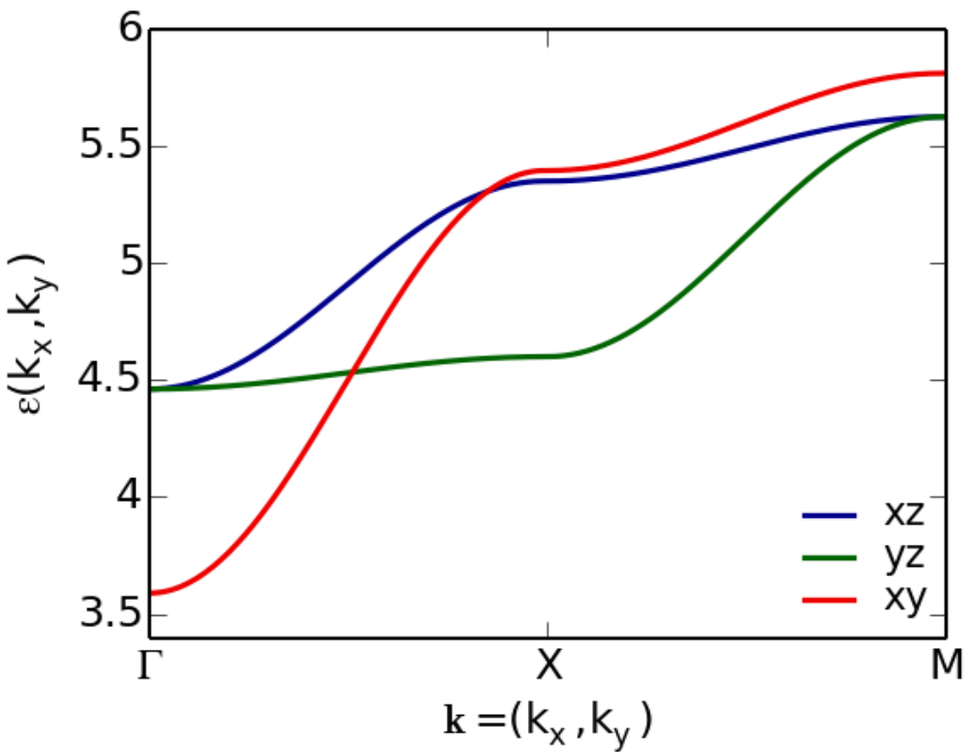


the model - vanadate

- Real material Sr_2VO_4: insulator
  - DMFT overestimates U_c by a factor 2
- Dispersion relation from DFT
  - 6 bands and no k_z-dependence
- Neglect coupling between Sr atoms -> 3 bands
- Hund's coupling







three-band Hubbard-Kanamori model

(Wolf, Go, McCulloch, Millis, Schollwöck, PRX (2015))

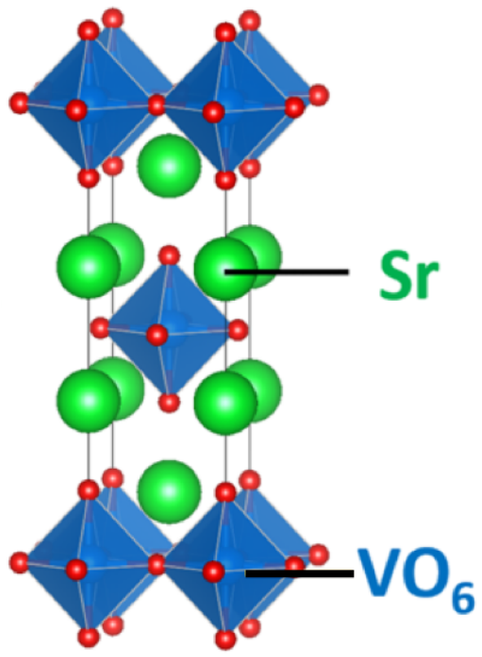
$$H = H_{\mathrm{loc}} + H_{\mathrm{coupl}} + H_{\mathrm{bath}}$$

$$H_{\mathrm{loc}} = \sum_a U n_{a,\uparrow} n_{a,\downarrow} + \sum_{a>b,\sigma} \left[U' n_{a,\sigma} n_{b,-\sigma} + (U' - J) n_{a,\sigma} n_{b,\sigma} \right]$$
$$- \sum_{a \neq b} J (d^\dagger_{a,\downarrow} d^\dagger_{b,\uparrow} d_{b,\downarrow} d_{a,\uparrow} + d^\dagger_{b,\uparrow} d^\dagger_{b,\downarrow} d_{a,\uparrow} d_{a,\downarrow} + h.c.)$$

$$H_{\mathrm{coupl}} = \sum_{k,a,\sigma} V_{k,a,\sigma} \; d^\dagger_{a,\sigma} c_{k,a,\sigma} + h.c.$$

$$H_{\mathrm{bath}} = \sum_{k,a,\sigma} \varepsilon_{k,a} \; c^\dagger_{k,a,\sigma} c_{k,a,\sigma}$$

strontium vanadate(s)

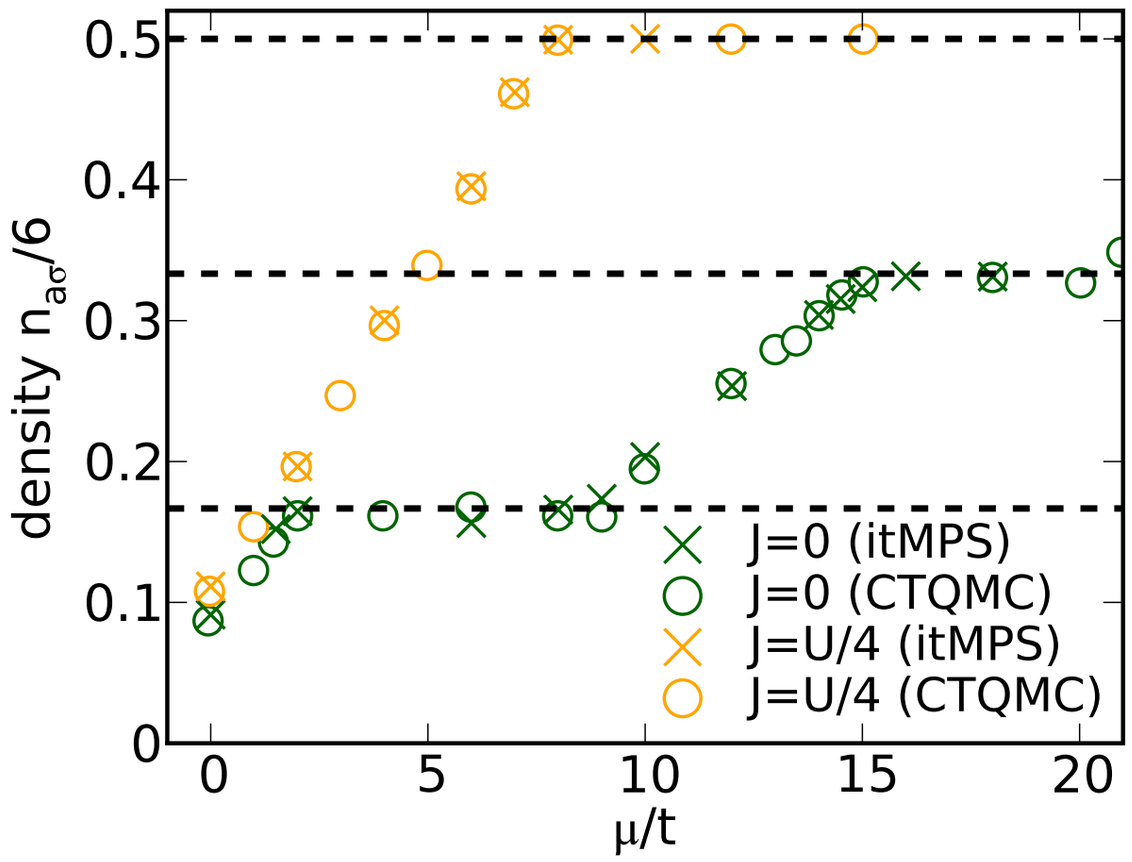


- bath discretization using numerical optimization on the imaginary axis (Caffarel & Krauth, PRL (1994))

three bands: reproducing CTQMC

(CTQMC by Werner *et al.*, PRL 101 (2008), Werner *et al.*, PRB (2009))

- using only 3 bath states per correlated state (total size L=12)
- quantitatively reproduce Mott transition (DMFT loop mins/hrs)

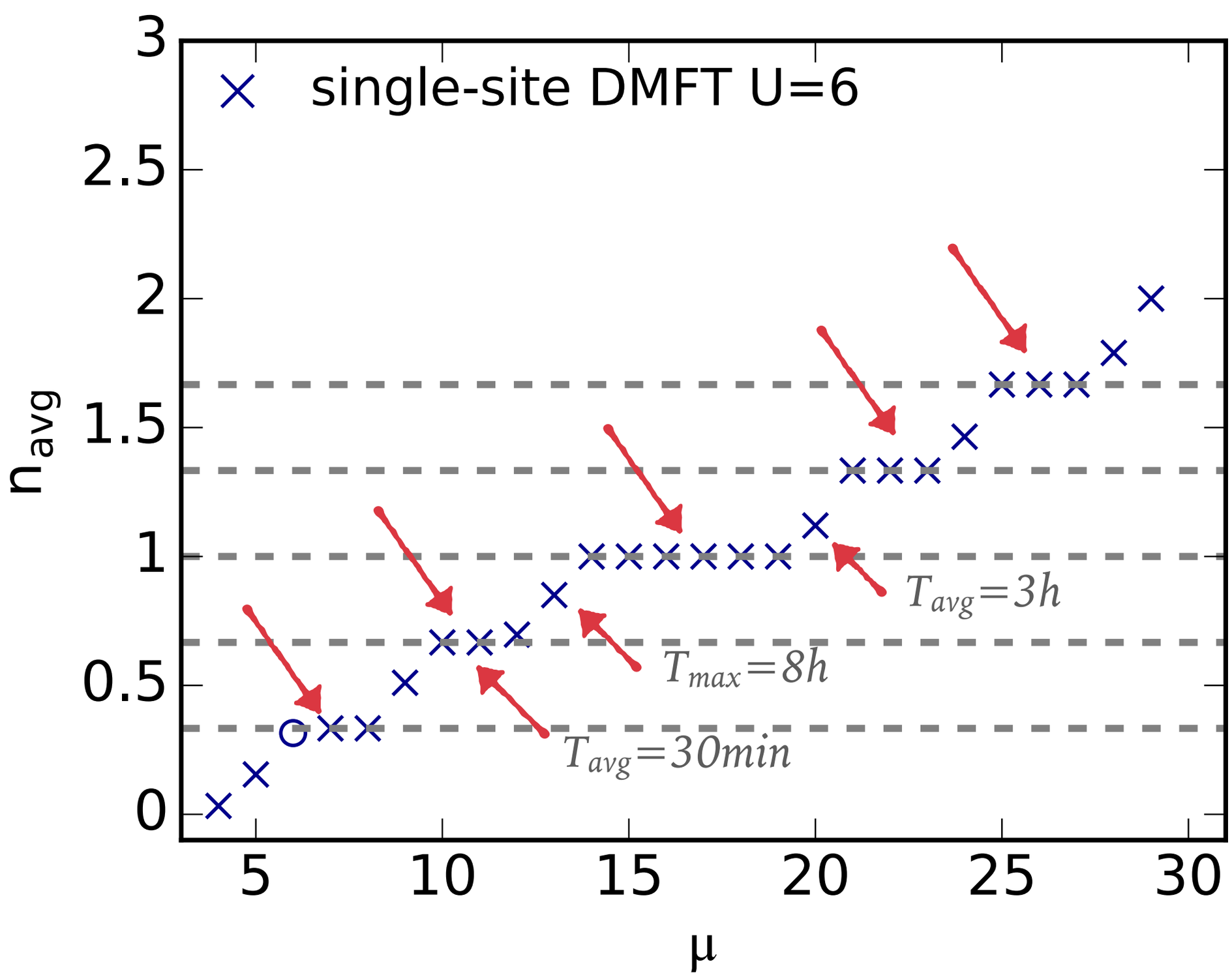


C=3

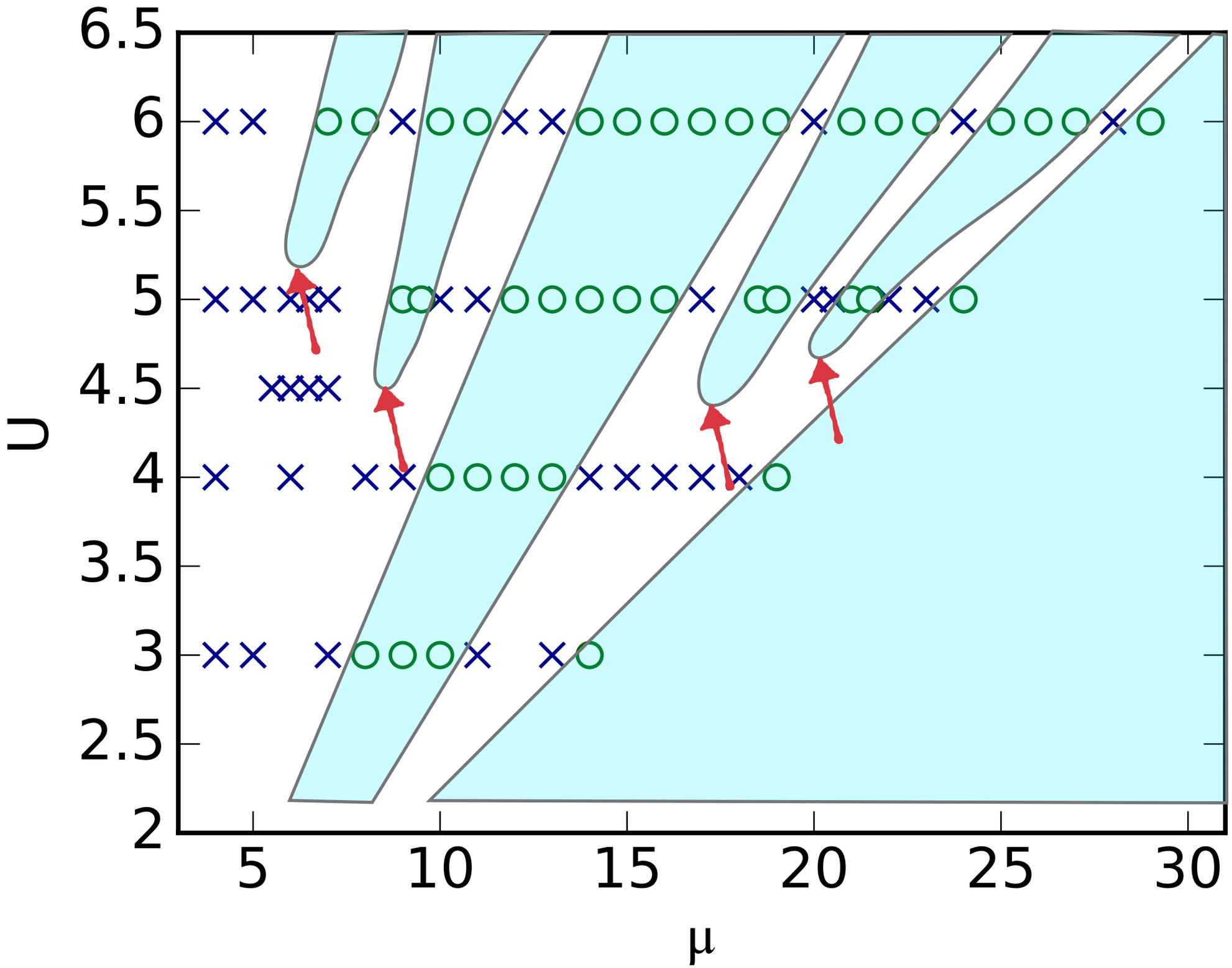
U=2D

U'=U-2J

The First Results: J=0.7

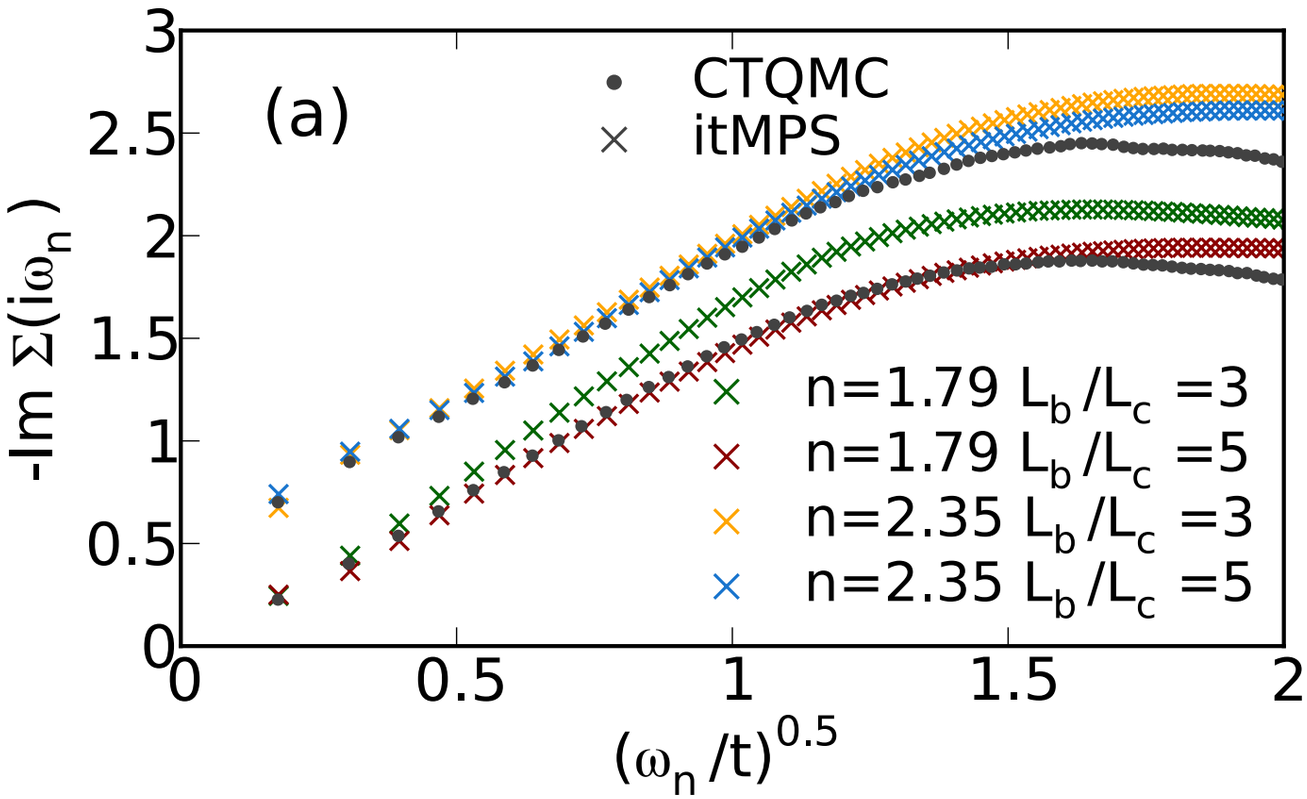


phase diagram: J=0.7



three-bands: reproducing CTQMC

- reproduce anomalous low-frequency behavior of self-energy



***C*=3**

U=2D

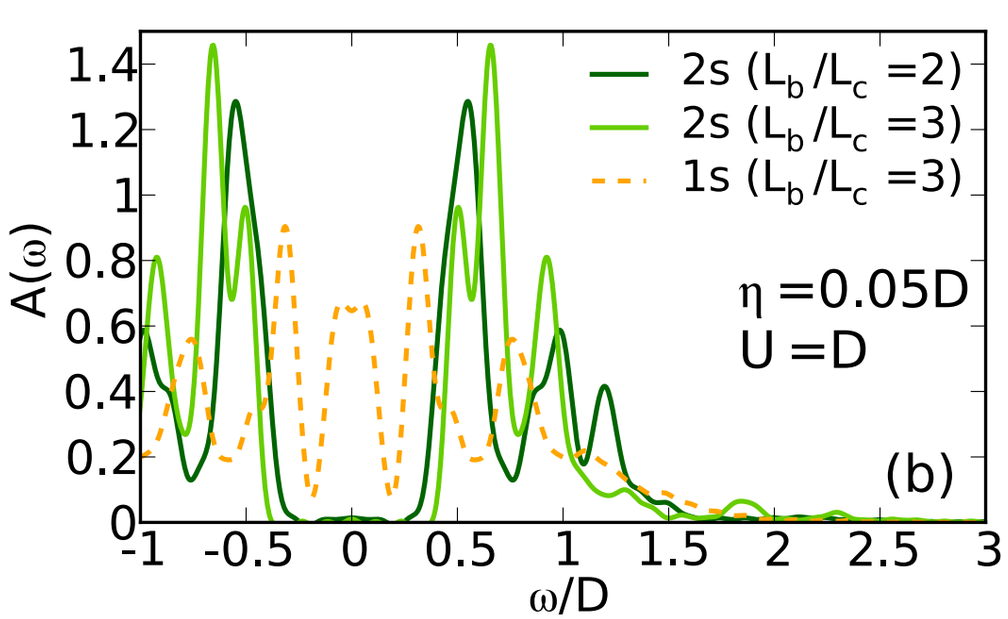
U'=U-2J

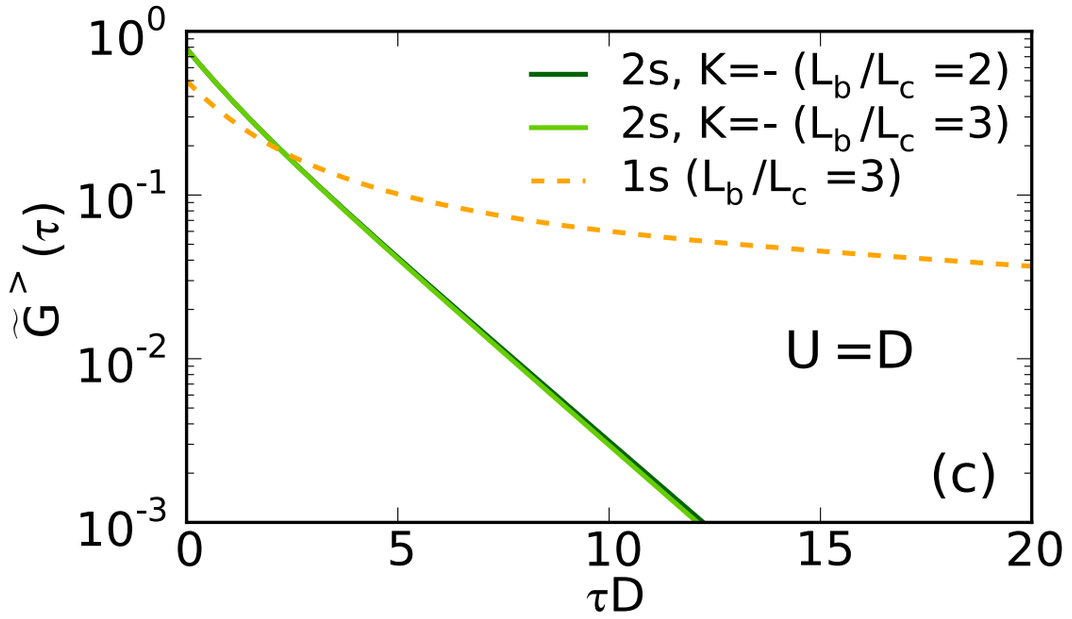
- one site, three bands (*C*=3) is as far as QMC can go here!!! (unless temperature is quite high!)

- explore the unknown …

2 sites & 3 bands: beyond CTQMC

- move to 2 sites (patches) with 3 bands: physics changes!





C=6

- drastic shift of position of Mott insulator transition
- *U=D*: conductor in 1 site, very good insulator in 2 site approx
- physical reason: 1 site approximation misses interaction energy cost of hopping to neighboring sites!
  in reality: charge fluctuations frozen out; insulator favored

conclusions

- 1D: DMRG/MPS currently most powerful method
  - ground states
  - time-evolution, also at non-zero temperature
  - limitation: exponential growth of resources; entanglement growth
- 2D: DMRG/MPS starts making very interesting forays
  - long cylinders
  - suboptimal ansatz, but numerically extremely stable
- barring new ideas, key challenges for powerful codes:
  - parallelization
  - (non-)Abelian quantum numbers
  - non-trivial geometries (impurity solvers, quantum chemistry)
  - convergence of ground states