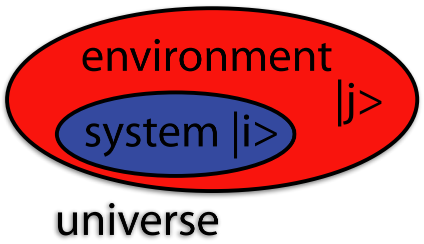
when does it work?

- measuring bipartite entanglement *S*: reduced density matrix



$$|\psi\rangle = \sum_{ij} \psi_{ij} |i\rangle |j\rangle \qquad \hat{\rho} = |\psi\rangle\langle\psi| \rightarrow \hat{\rho}_A = \mathrm{tr}_B \hat{\rho}$$

$$S = -\mathrm{tr}\, \hat{\rho}_A \ln \hat{\rho}_A = -\sum_{\alpha} w_\alpha \ln w_\alpha$$

- arbitrary bipartition of MPS:

AAAAAAAA BBBBBBBBBBBBBBBBB

$$|\psi\rangle = \sum_{\alpha}^{D} \sqrt{w_\alpha} |\alpha_A\rangle |\alpha_B\rangle$$

use Schmidt decomposition

- reduced density matrix and bipartite entanglement

$$\hat{\rho}_A = \sum_{\alpha} w_\alpha |\alpha_A\rangle\langle\alpha_A|$$

$$\boxed{S = -\sum_{\alpha}^{D} w_\alpha \ln w_\alpha \leq \ln D}$$

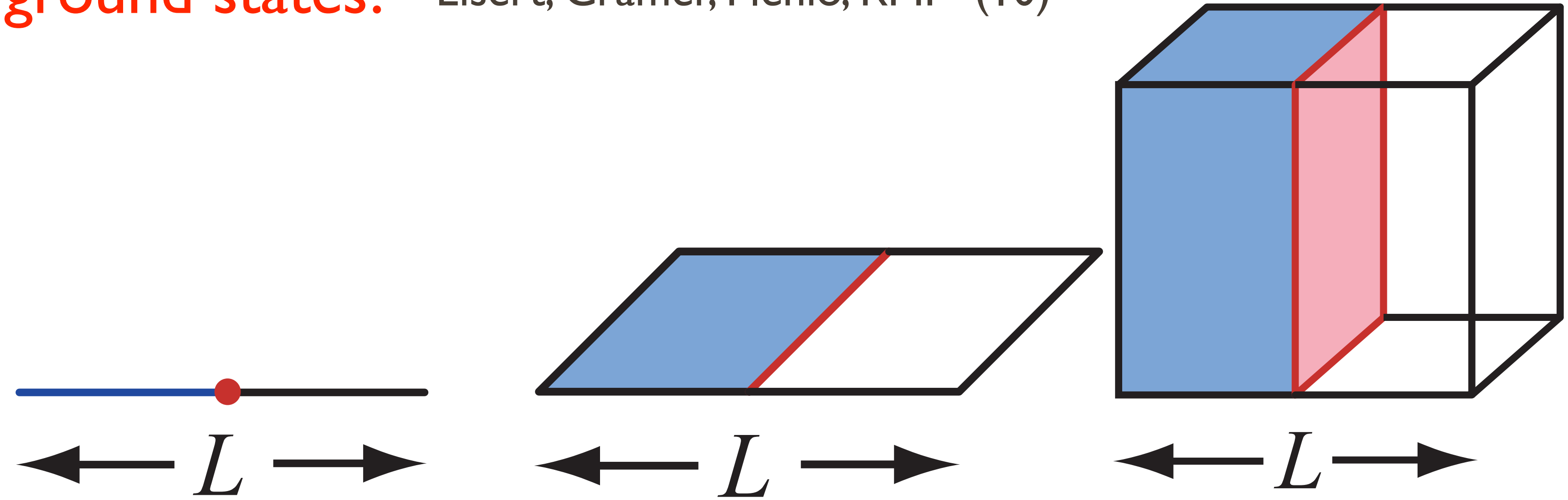
codable maximum

why DMRG loves one dimension

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



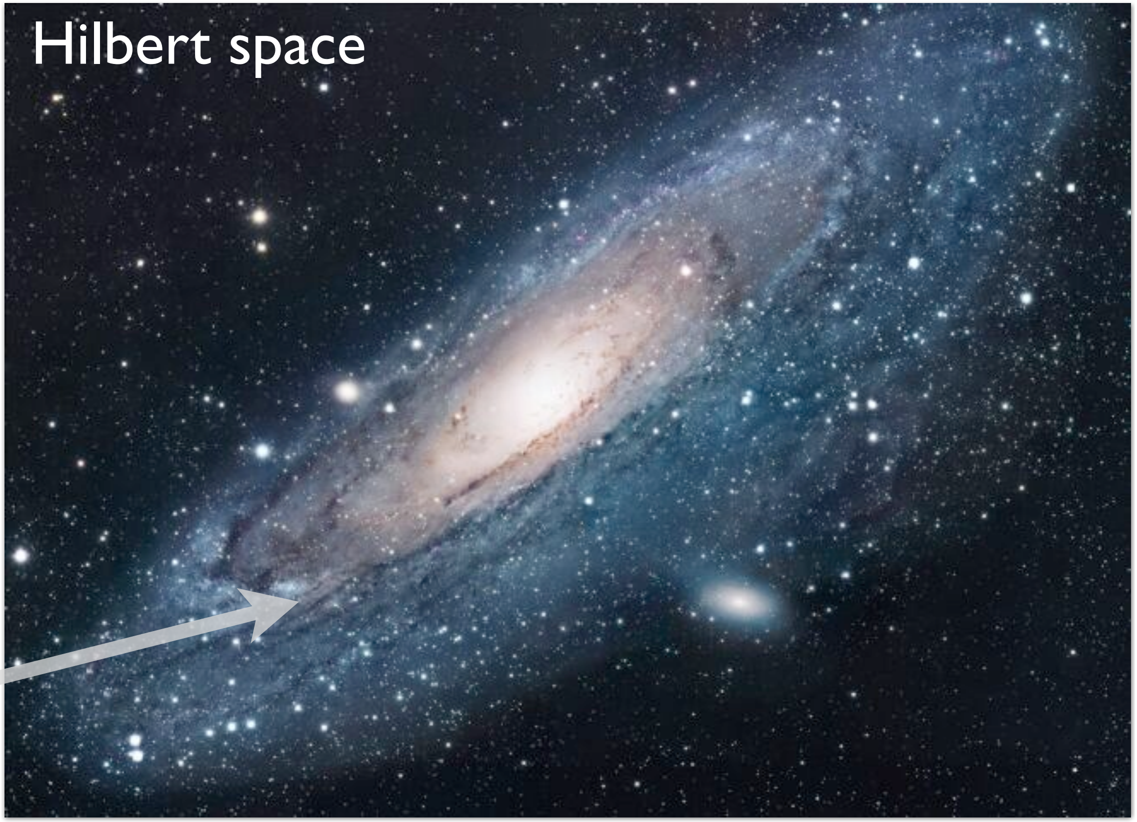
gapped $S(L) \sim \mathrm{cst.}$ $S(L) \sim L$ $S(L) \sim L^2$ black hole

$$\boxed{S \leq \ln D \Rightarrow D \geq \mathrm{e}^S}$$

dimension $D \sim \mathrm{e}^{\mathrm{cst.}}$ $D > \mathrm{e}^L$ $D > \mathrm{e}^{L^2}$

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
- but contain ground states!
- MPS parametrize low-entanglement states efficiently!



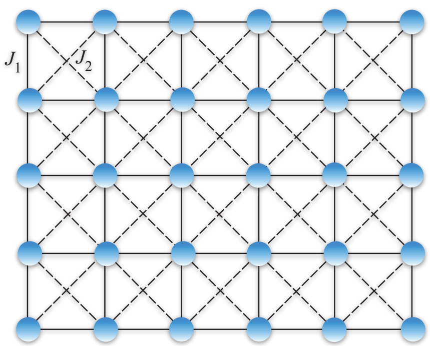
ground states are here!

frustrated magnetism in 2D

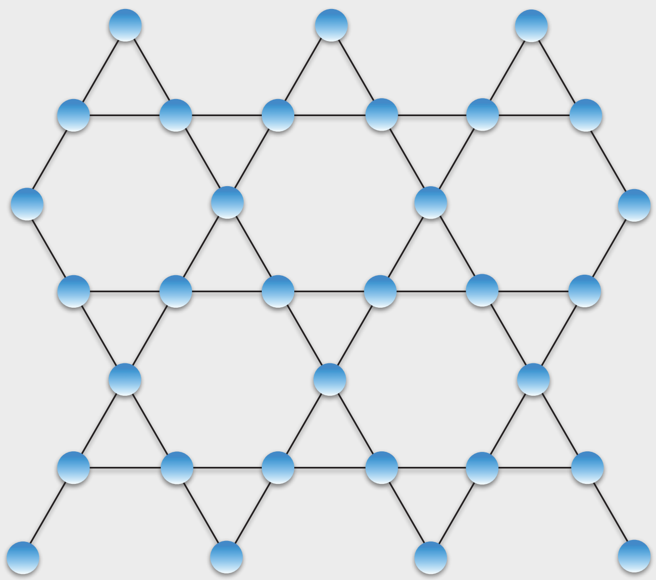
- „classic“ candidates (spin length 1/2):

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

J_1-J_2 model on a square lattice

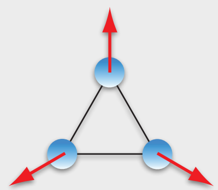


kagome lattice



herbertsmithite
$ZnCu_3(OH)_6Cl_2$

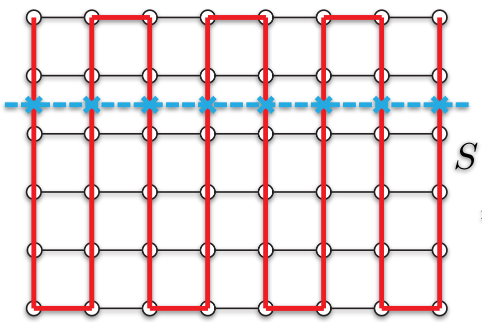
- classical model
  - order only locally coplanar
  - extensive T=0 entropy



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

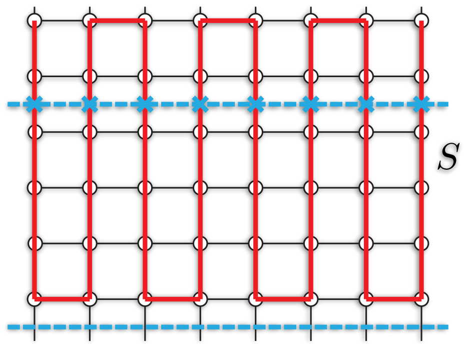
DMRG in two dimensions

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



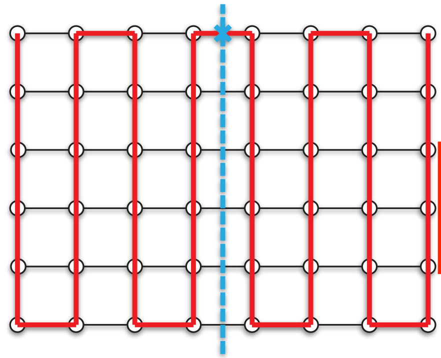
$S \sim \log_2 M^L$
$= L \log_2 M$

vertically OBC



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

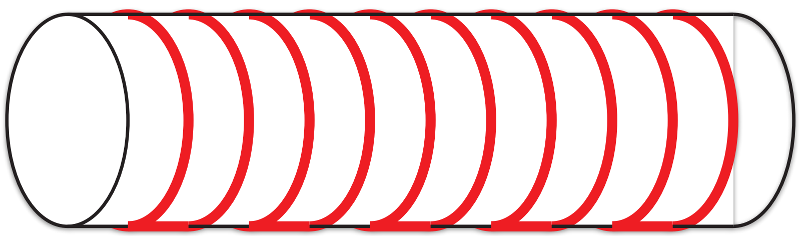
vertically PBC: extra cost!



$\boxed{S \sim \log_2 M \\ \to M \sim 2^L}$

- 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

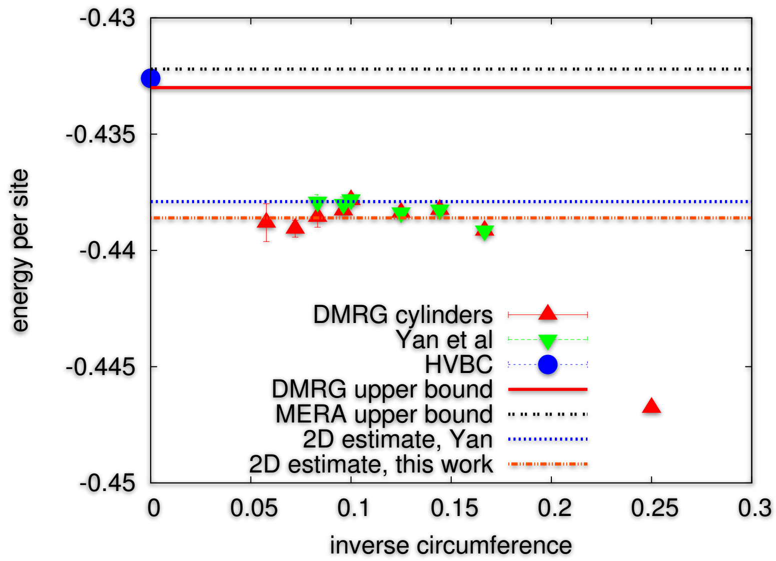
circumference c



length L

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

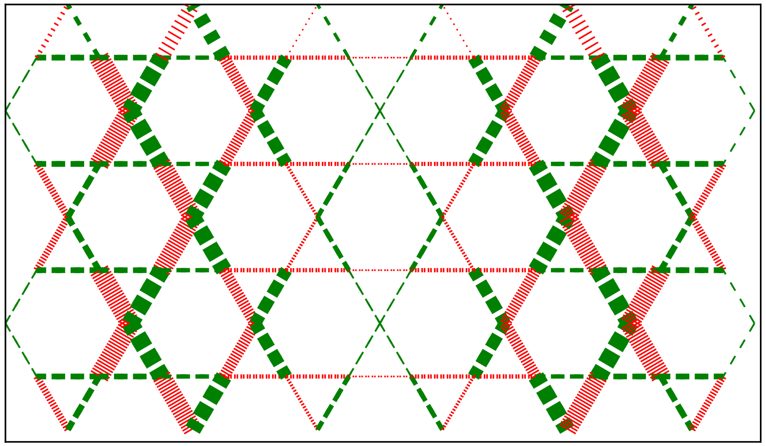


- TD limit energy estimate: -0.4386(5)
- iDMRG (infinite cylinder) upper bounds below HVBC; YC8: -0.4379

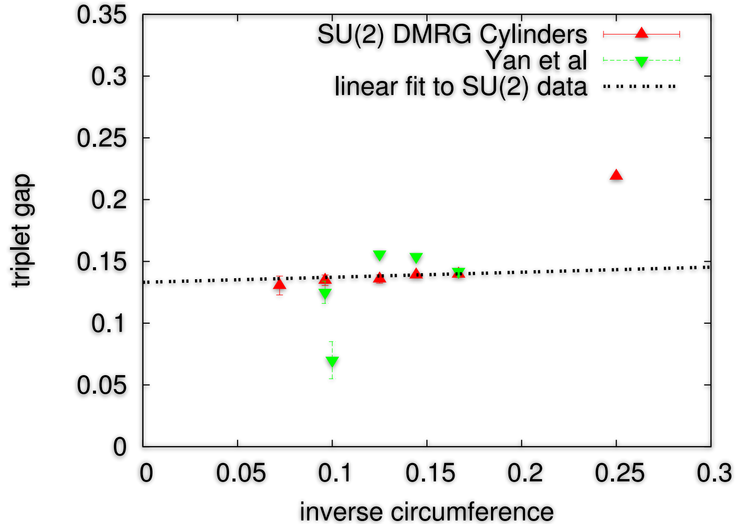
iDMRG: I.P. McCulloch, arXiv:0804.2509

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

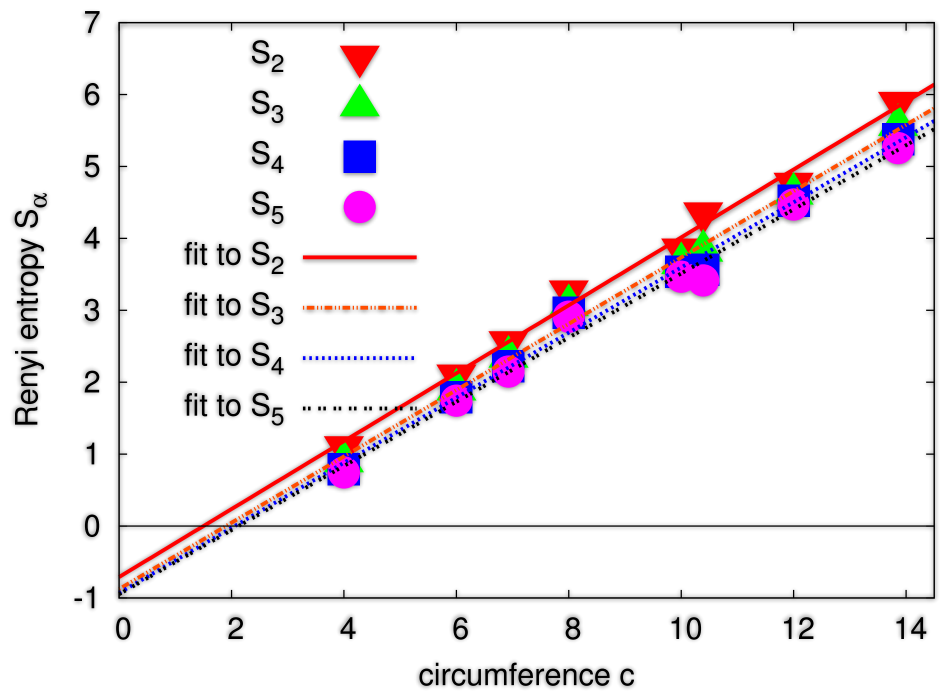
- bulk excitation
- much smoother gap curve
- triplet gap estimate: 0.13(1)

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)

time evolution

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

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

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

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

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:

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

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

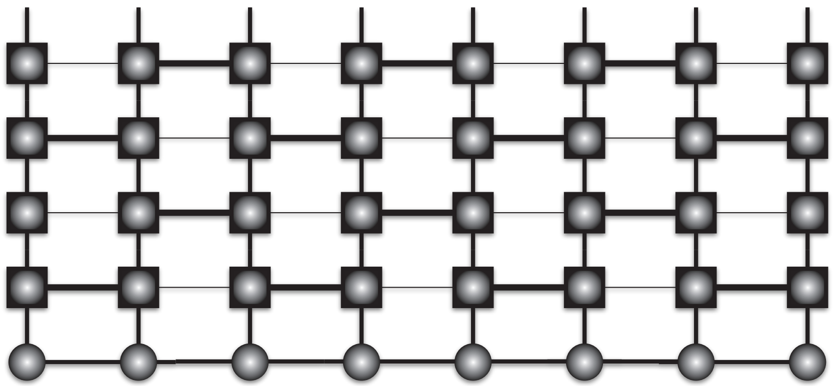
tDMRG, tMPS, TEBD

bring local evolution operator into MPO form:

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

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

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



even bonds

odd bonds

initial state

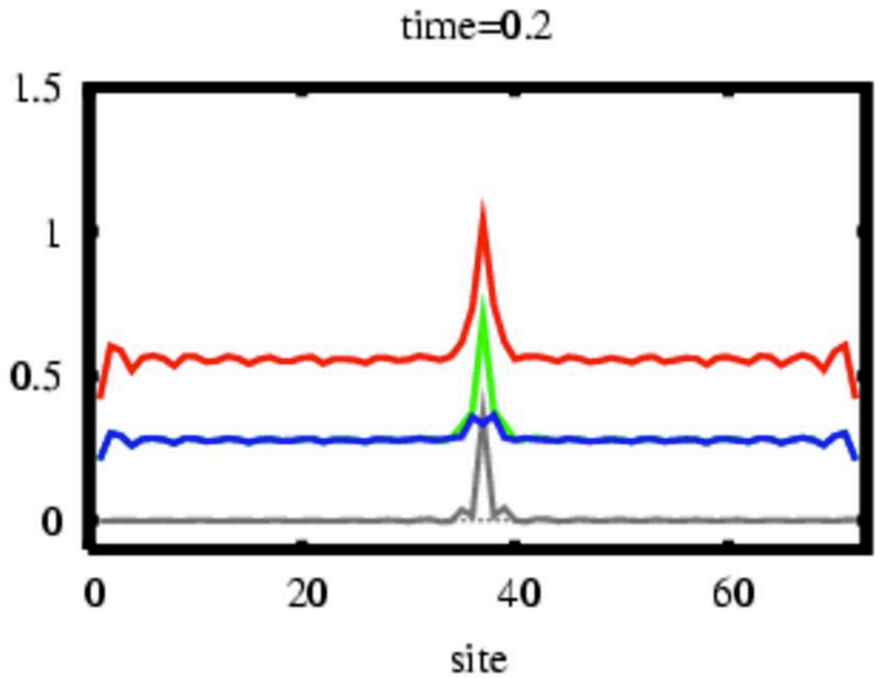
one time step: dimension grows as d^2

- 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 ...

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

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

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

real time evolution limited by entanglement growth:

$$S(t) \leq S(0) + \nu t \qquad D \sim \mathrm{e}^{S} \sim \mathrm{e}^{\nu t}$$

in the worst case, matrix dimensions grow exponentially!

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

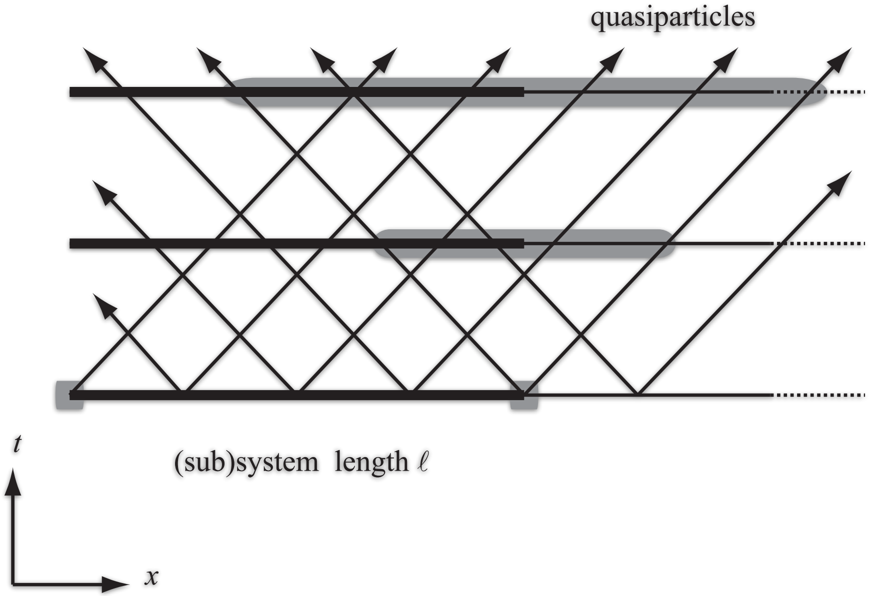
Lieb-Robinson theorem (CMP, 1972)

- entanglement bound:

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

linear in time

exponential resources



out-of-equilibrium cartoon:

quasiparticles entangle in „light“ cone

Calabrese, Cardy (since 2004) and others

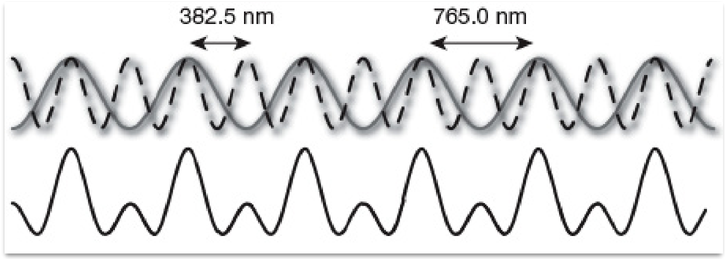
dynamical quantum simulator

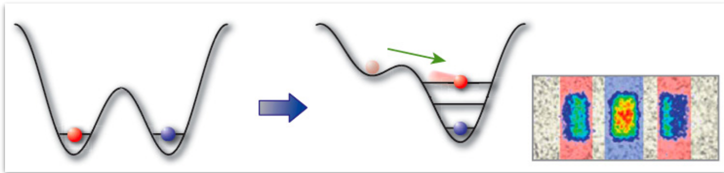
coherent dynamics! controlled preparation? local measurements?

first experiments:

period-2 superlattice

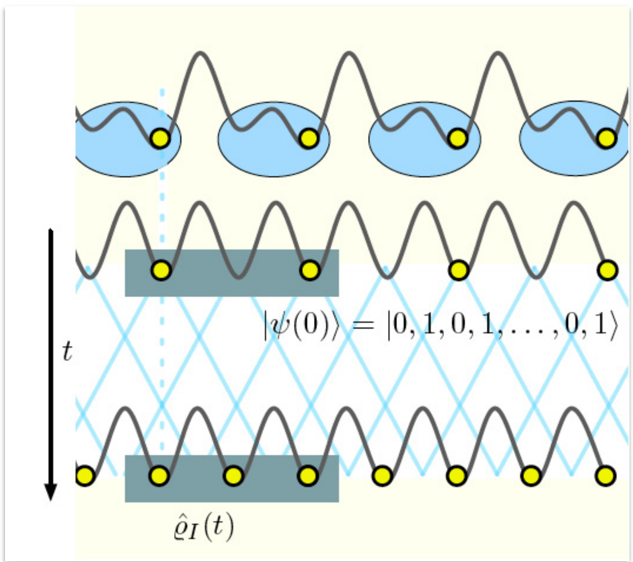
- double-well formation
- staggered potential bias





- pattern loading
- odd/even resolved measurement

(Fölling *et al.* (2007))

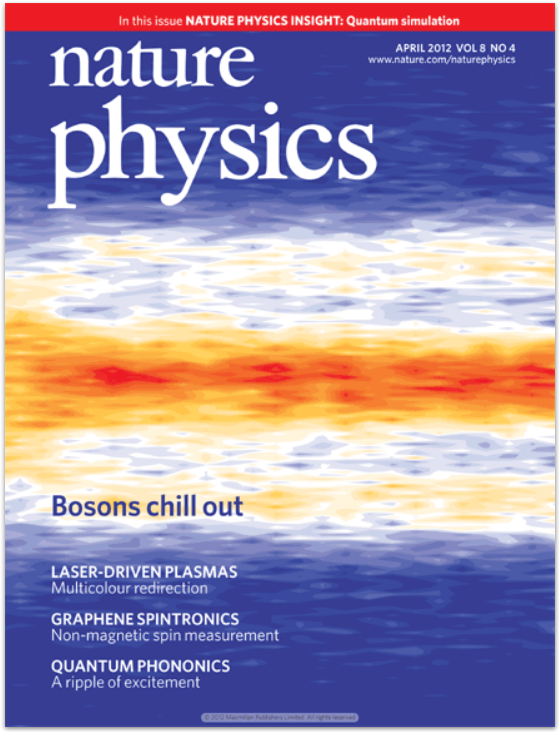


first theory proposals:

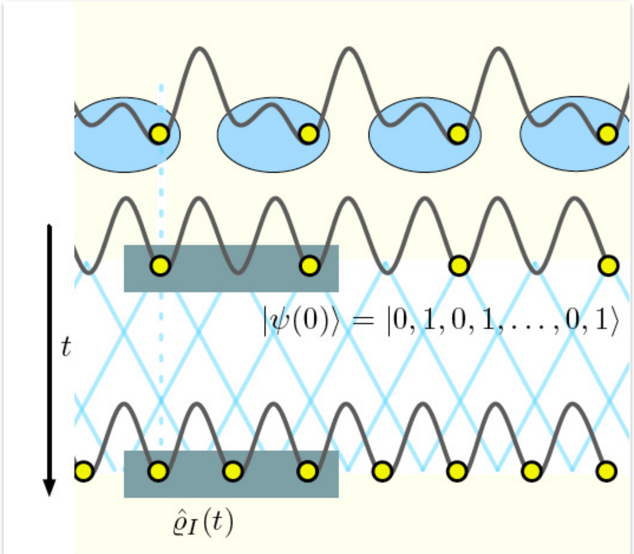
- prepare $|\psi\rangle = |1,0,1,0,1,0,\ldots\rangle$
- switch off superlattice
- observe Bose-Hubbard dynamics

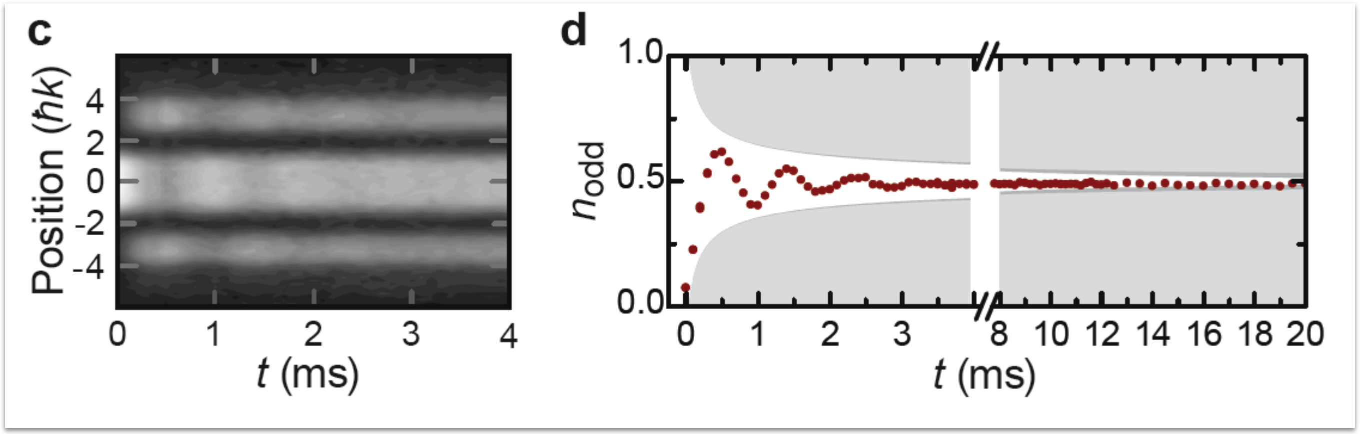
Cramer *et al.*, PRL 101, 063001 (2008)
Flesch *et al.*, PRA 78, 033608 (2008)

dynamical quantum simulator



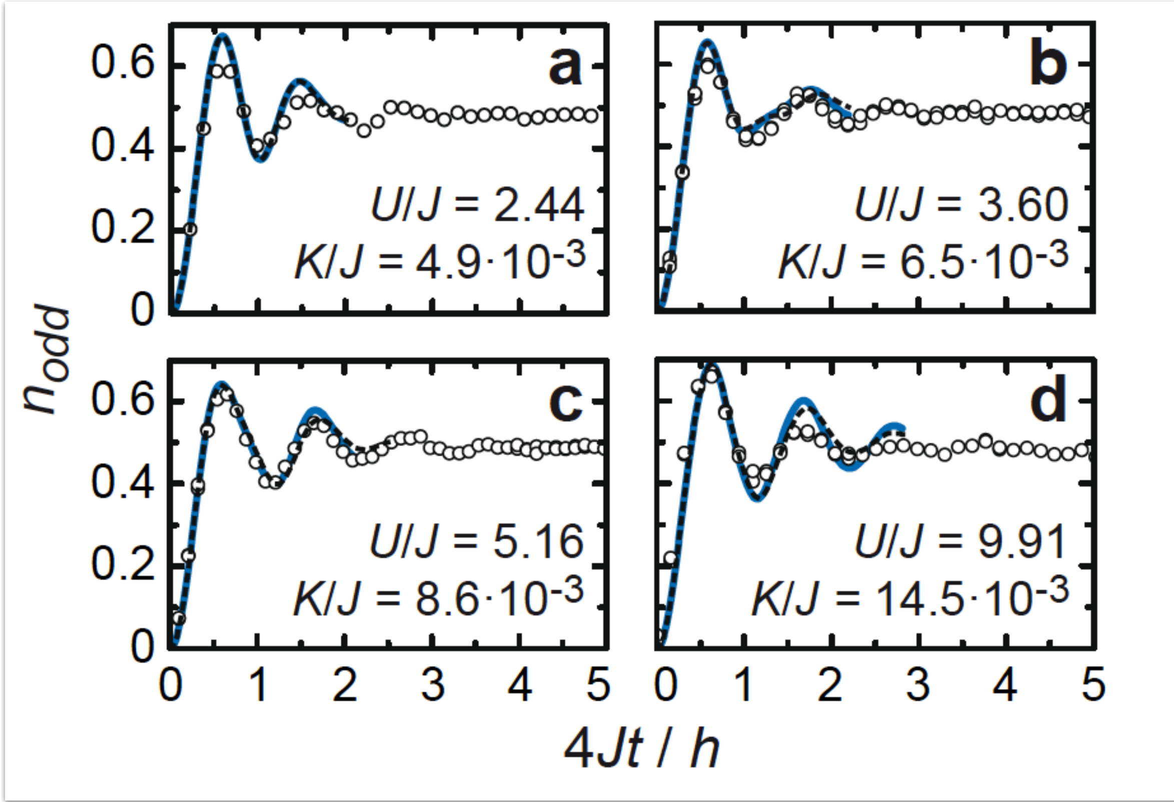
Trotzky *et al.*, Nat. Phys. 8, 325(2012)





45,000 atoms,
U=5.2
momentum
distribution

densities: relaxing to n=0.5



no free fit parameters!

fully controlled relaxation in closed quantum system!

*validation of **dynamical** quantum simulator*

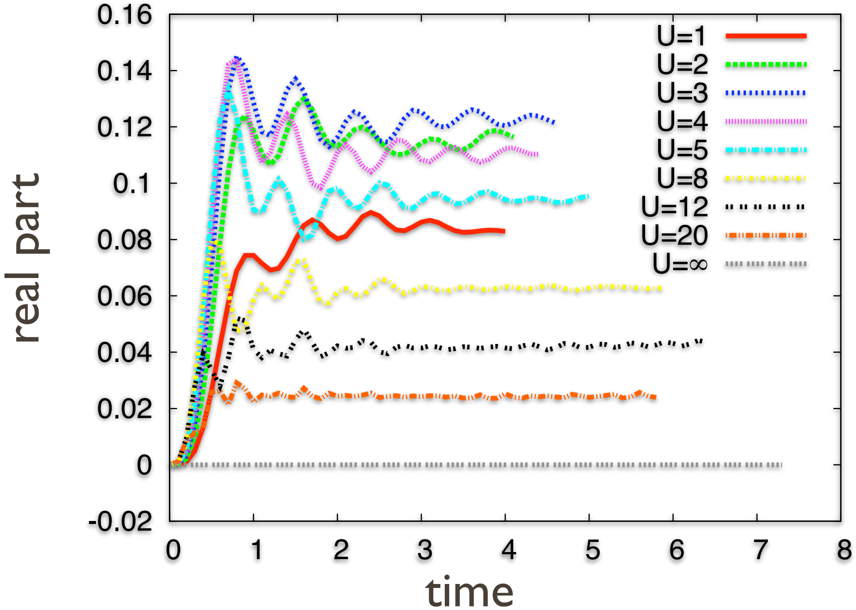
time range of experiment > 10 x time range of theory

real „analog computer“ that goes beyond theory

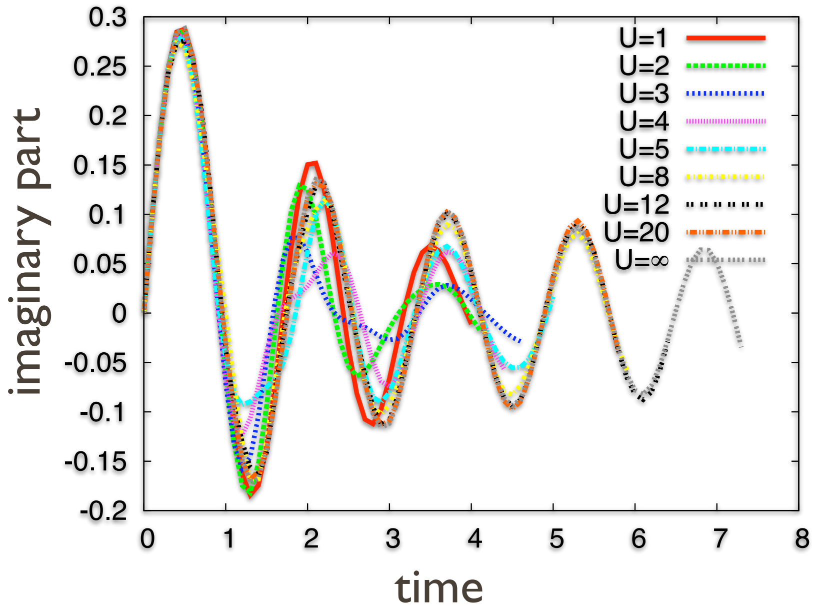
nearest-neighbour correlators

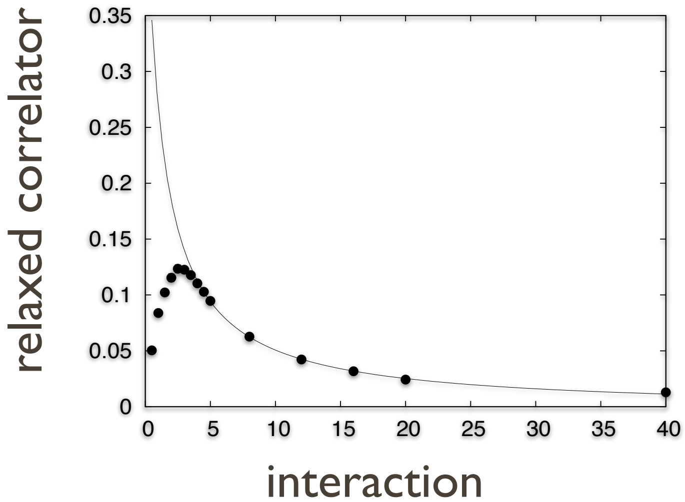
$$\langle \hat{b}_n^\dagger(t)\hat{b}_{n+1}(t)\rangle$$

correlator



current



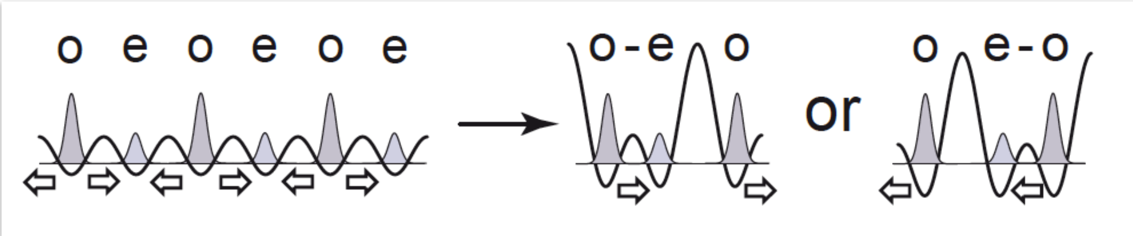


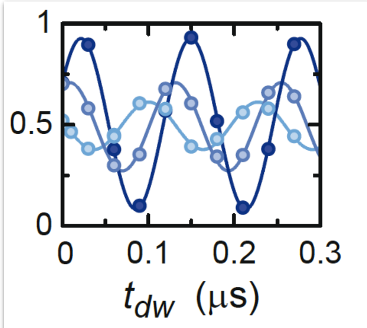
- again three regimes
- *U*≈3: crossover regime

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

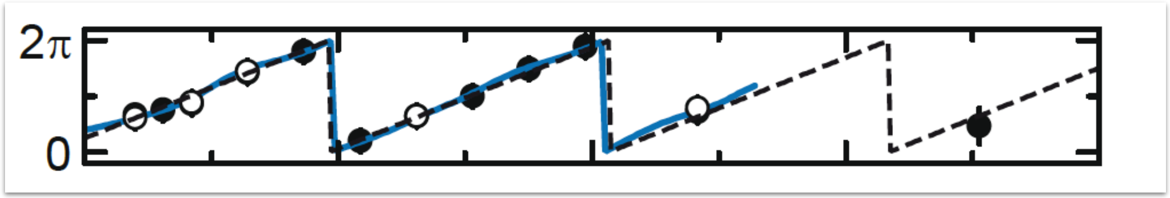
currents

measurement: split in double wells, measure well oscillations



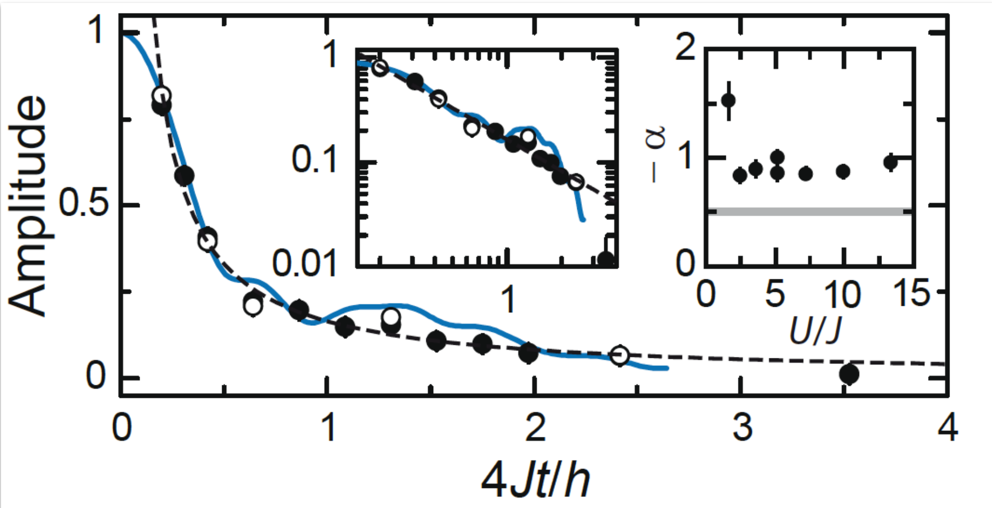


phase and amplitude



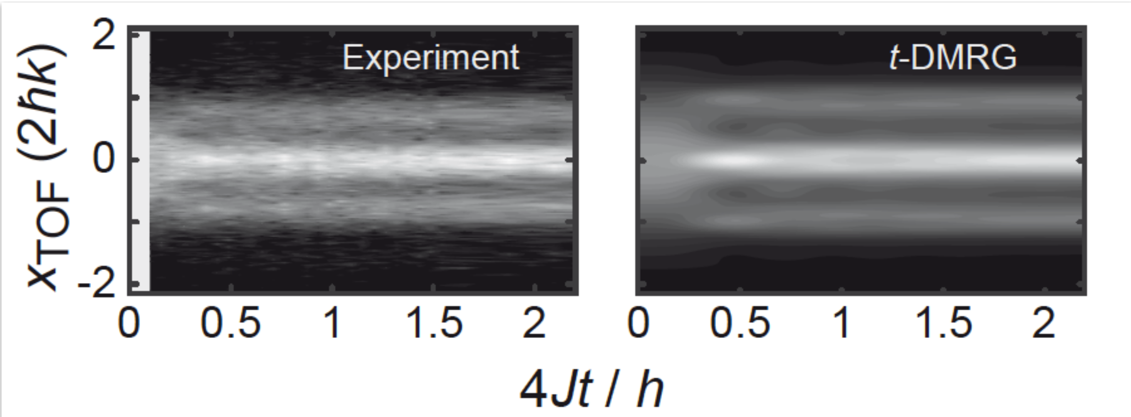
sloshing;

no c.m. motion



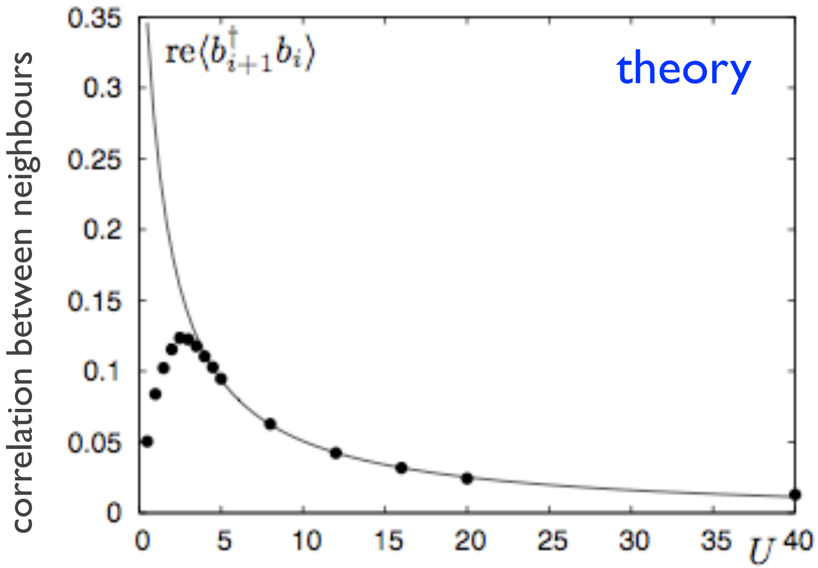
current decay as power law?

nearest neighbour correlations

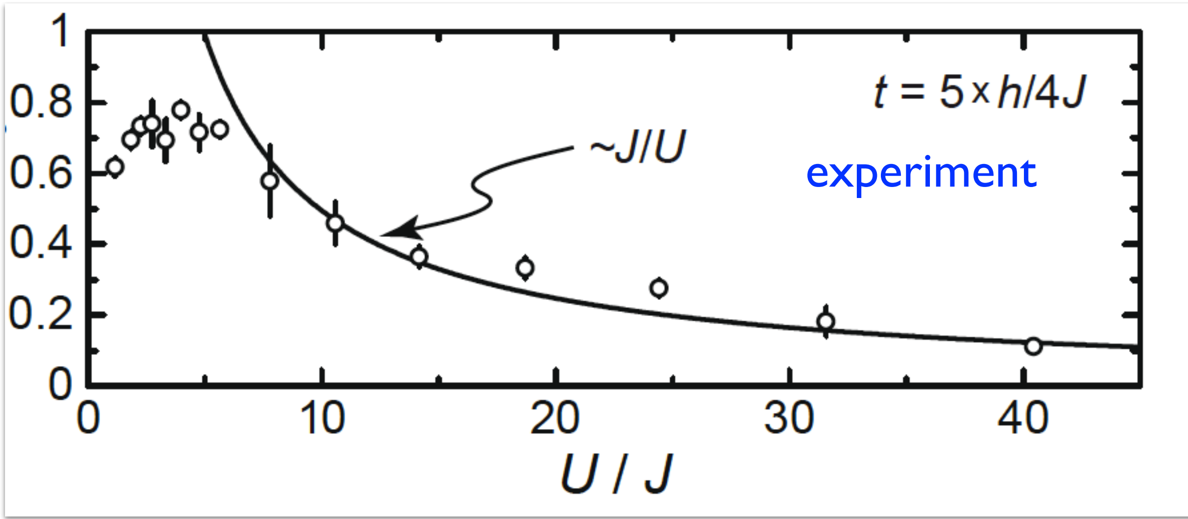


momentum distribution

visibility proportional to nearest neighbour correlations



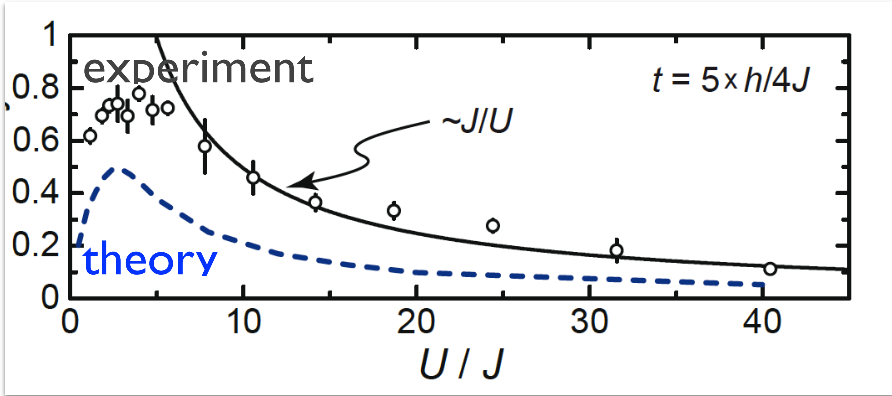
interaction strength



build-up of quantum coherence

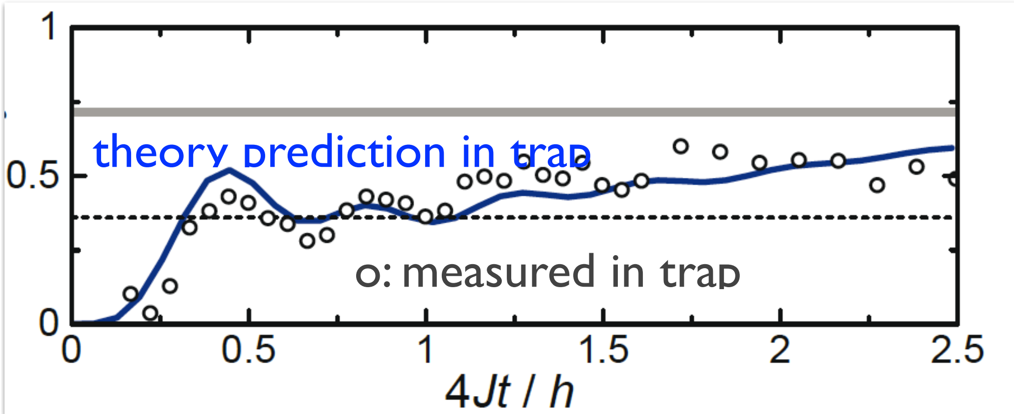
general trend, 1/U correct!

build-up of quantum coherence



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

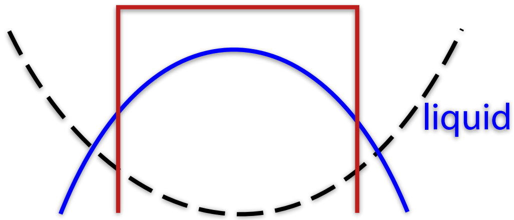
discrepancy because original theory ignored trap:



measurement at „long time“

old theory prediction for long times without trap

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



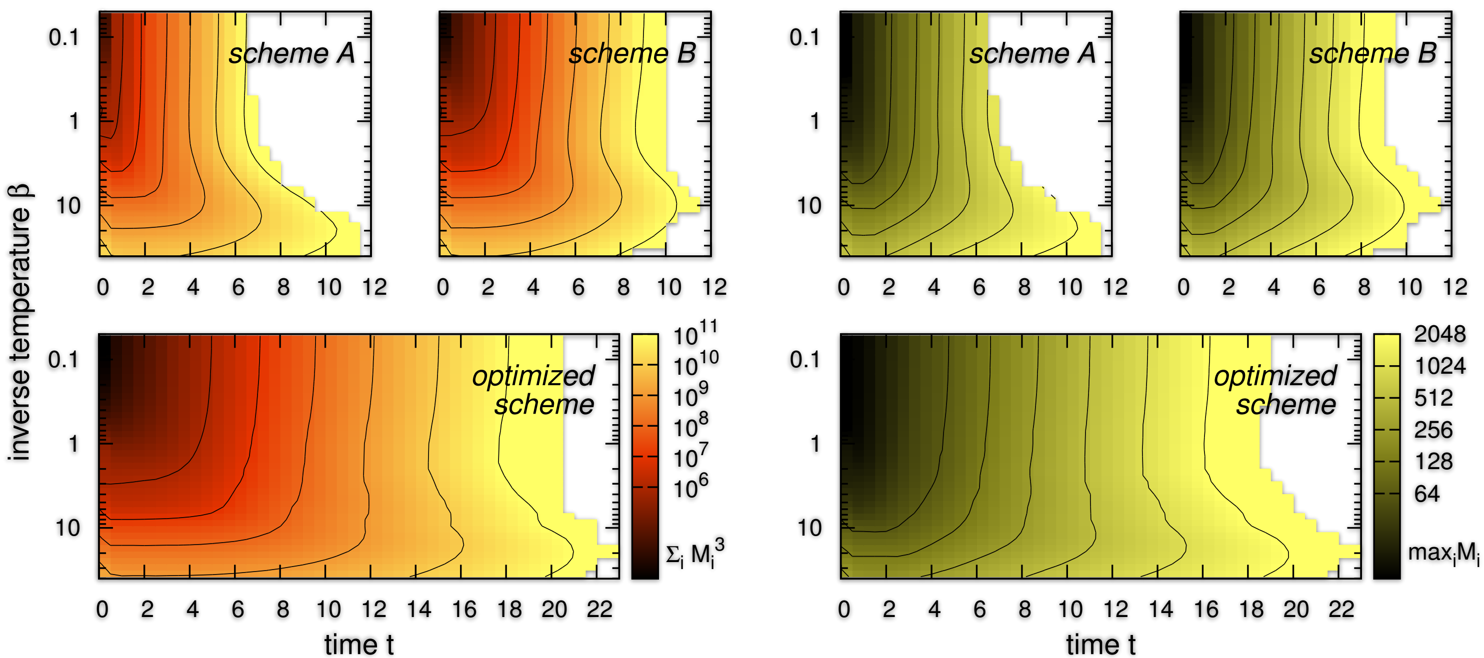
$$E_{kin} = -J\langle b_i^\dagger b_{i+1} + b_{i+1}^\dagger b_i \rangle$$

new: we do even better!

Barthel, US, Sachdev, 1212.3570 (2012); Barthel, 1301.2246 (2013)

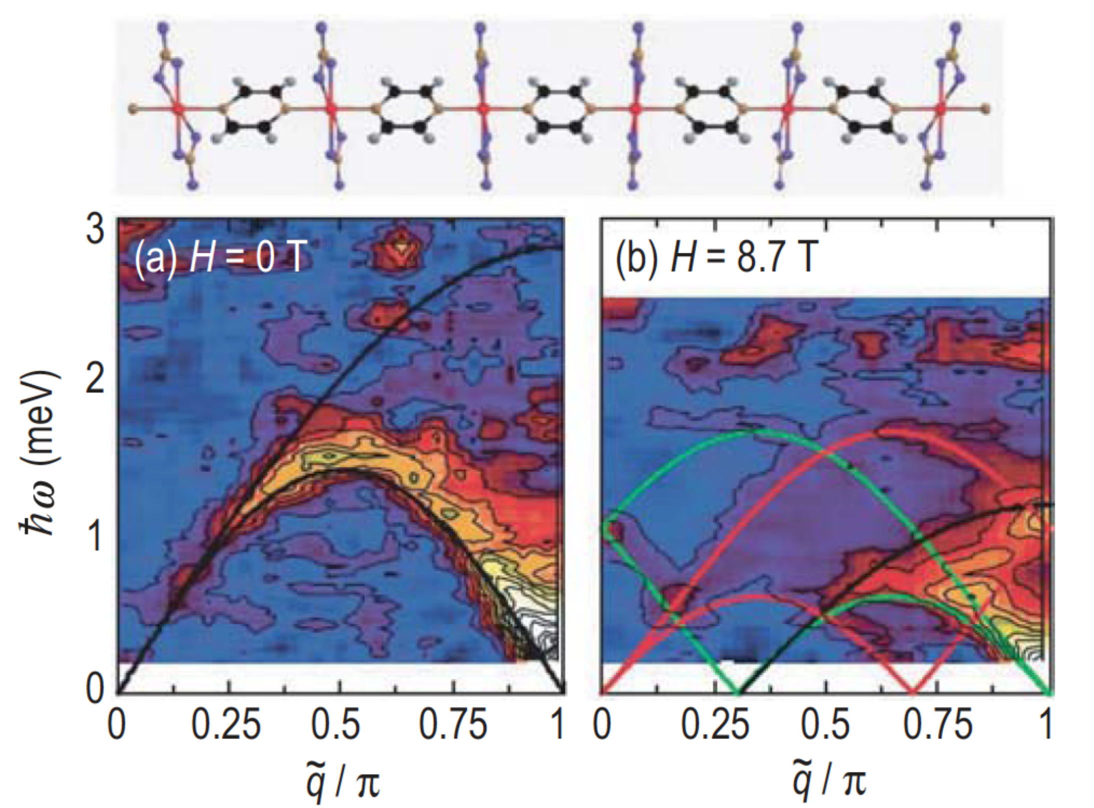
$$\langle \hat{B}(2t)\hat{A}\rangle_\beta = Z(\beta)^{-1}\mathrm{Tr}\left(\left[\mathrm{e}^{\mathrm{i}\hat{H}t}\mathrm{e}^{-\beta\hat{H}/2}\hat{B}\mathrm{e}^{-\mathrm{i}\hat{H}t}\right]\left[\mathrm{e}^{-\mathrm{i}\hat{H}t}\hat{A}\mathrm{e}^{-\beta\hat{H}/2}\mathrm{e}^{\mathrm{i}\hat{H}t}\right]\right)$$

- one calculation if $\hat{B}^\dagger = \hat{A}$
- doubles reachable time for same effort as in Karrasch scheme



same colors: same effort

neutron scattering at T>0



structure function
by neutron scattering
(Broholm group)

high flux

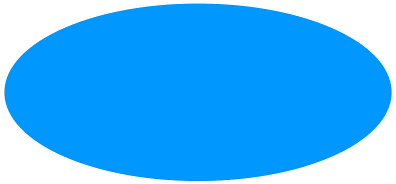
precise lineshapes

- 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

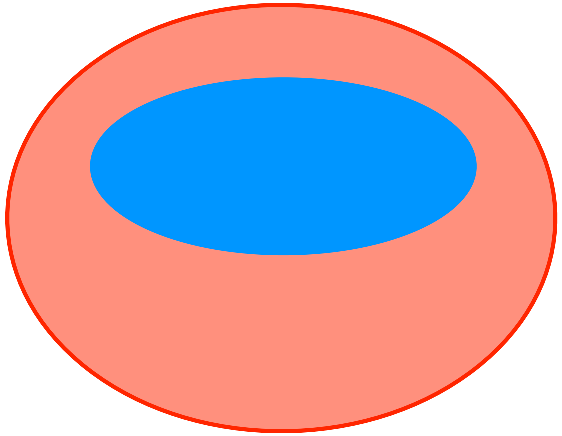
finite-temperature dynamics

- 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)

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

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

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

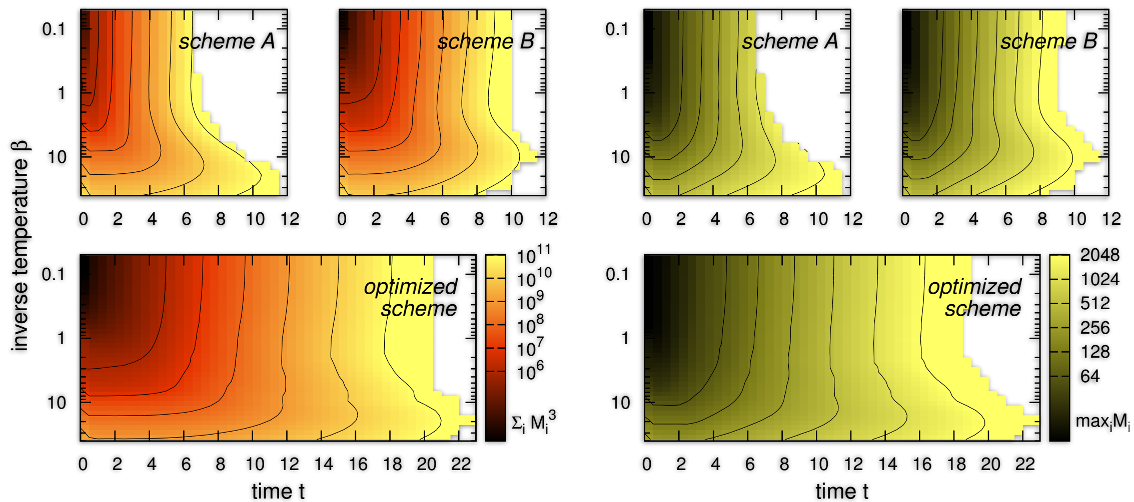
thermal states: easy way out by imaginary *t*-evolution

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

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:
see further slides!!



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

linear prediction

(Barthel, US, 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

- find prediction coefficients by minimising error for available data

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

error estimate

$$0 = \sum_j a_j \sum_{n \in \mathcal{N}_{fit}} \frac{x^*_{n-k} x_{n-j}}{w_n} + \sum_{n \in \mathcal{N}_{fit}} \frac{x^*_{n-k} x_n}{w_n}$$

linear prediction II

- solving for the coefficients: matrix equation

$$\mathbf{R} \cdot \mathbf{a} = -\mathbf{r}$$

$$\mathbf{a} = -\mathbf{R}^{-1} \cdot \mathbf{r}$$

$$R_{ij} = \sum_{n \in \mathcal{N}_{fit}} \frac{x^*_{n-i} x_{n-j}}{w_n}$$

$$r_i = \sum_{n \in \mathcal{N}_{fit}} \frac{x^*_{n-i} x_n}{w_n}$$

attention: close to singular!

- iterating the solution towards the future

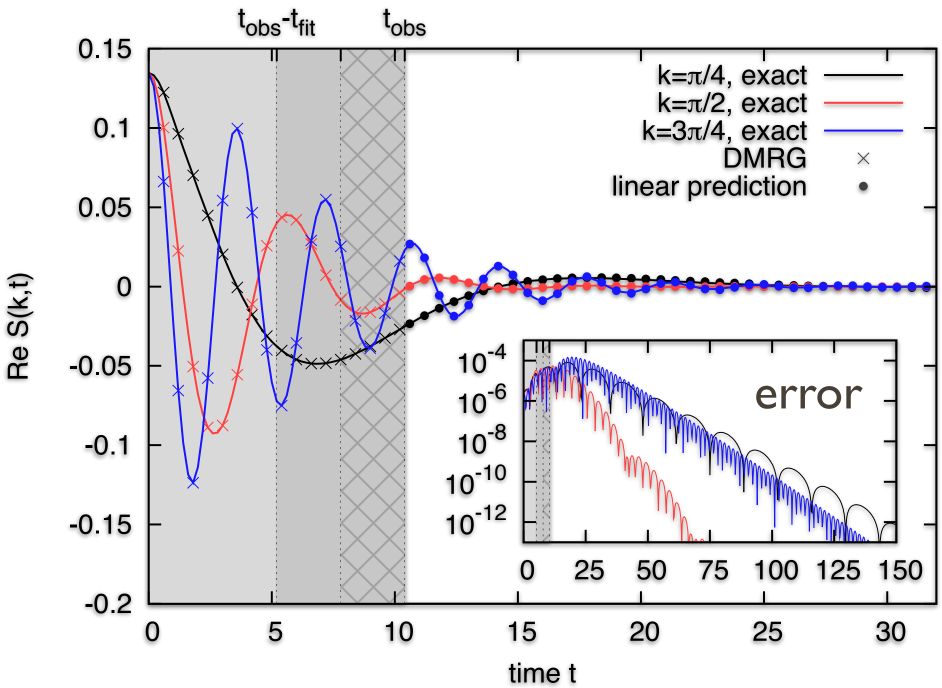
$$\mathbf{x}_n = [x_{n-1} \ldots x_{n_p}]^T$$

$$\mathbf{x}_{n+1} = \mathbf{A} \cdot \mathbf{x}_n$$

$$\mathbf{A} = \begin{bmatrix} -a_1 & -a_2 & \ldots & -a_P \\ 1 & 0 & & \\ 0 & 1 & \ddots & \\ & \ddots & \ddots & 0 \\ & & 0 & 1 \end{bmatrix}$$

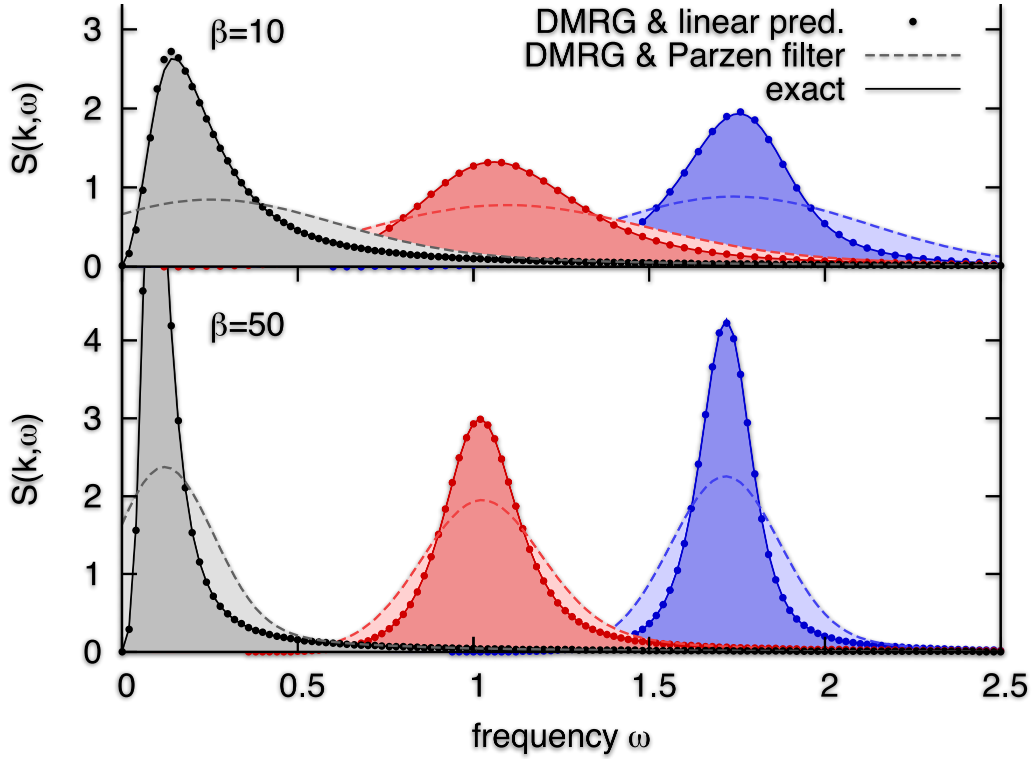
transverse Ising model

- cuts in momentum space: time domain



extends time domain 10x

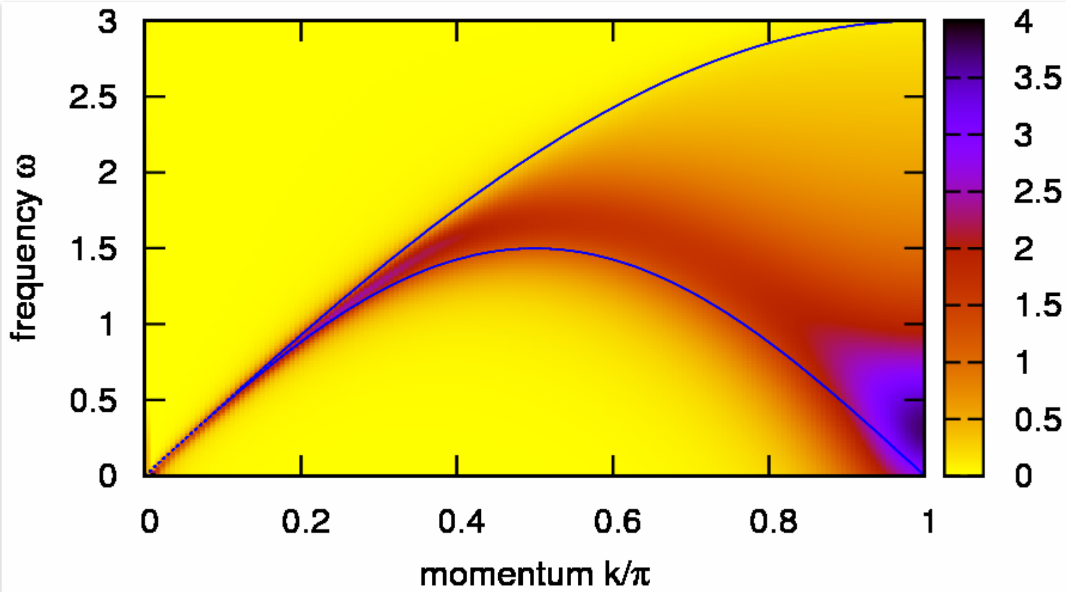
- cuts in momentum space: frequency domain

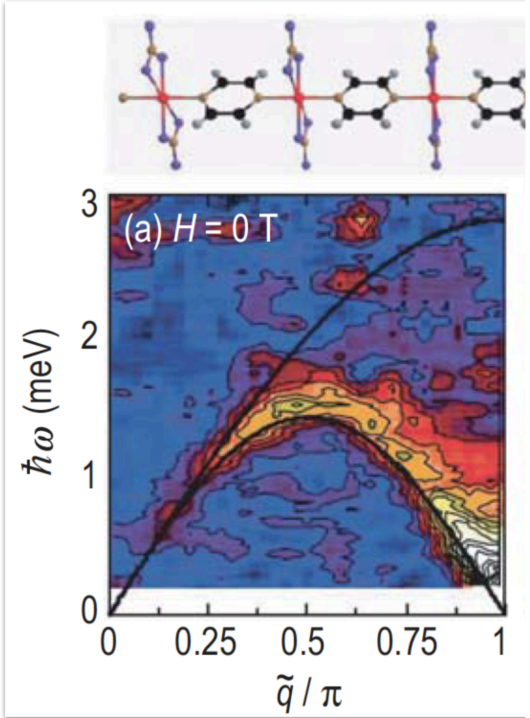


k=pi/4 k=pi/2 k=3pi/4

spin-1/2 Heisenberg chain

- structure function at finite T in real space and time



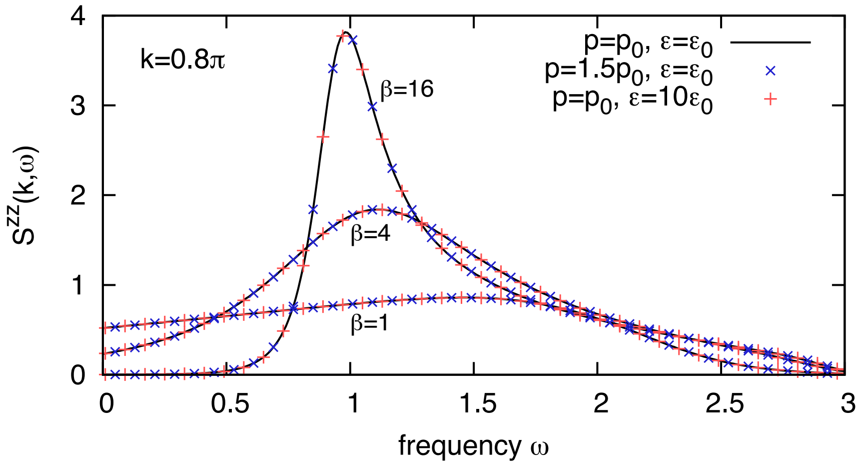


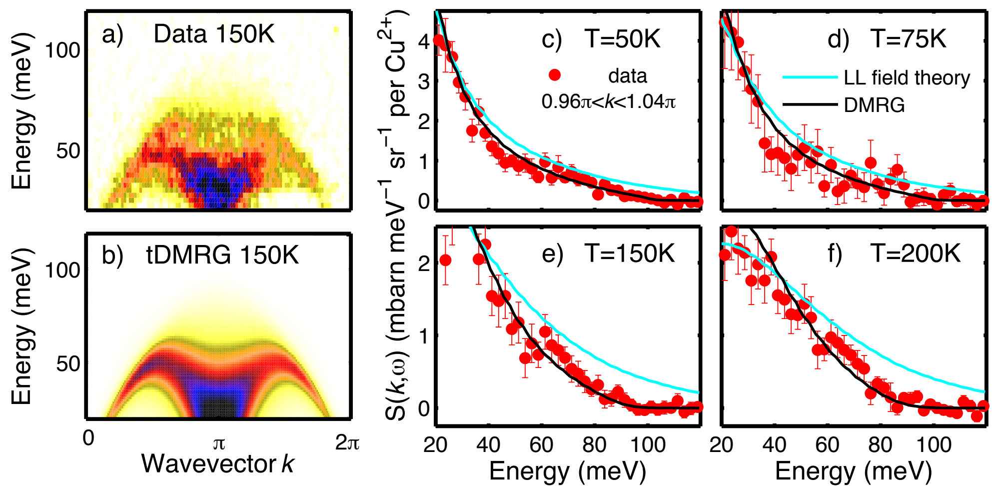
- spinonic continuum of excitations: much harder!?

$(\pi/2)|\sin k| \leq \omega(k) \leq \pi \sin k/2$ at T=0

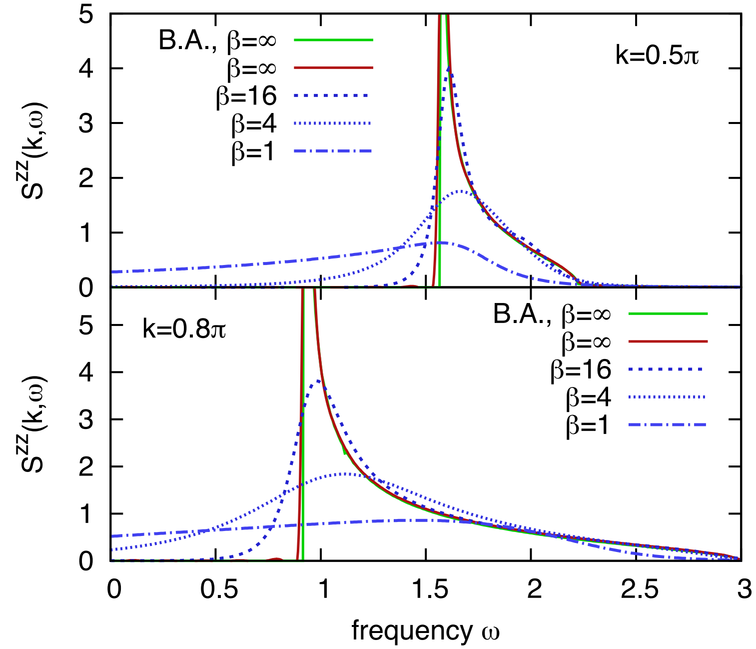
spin-1/2 Heisenberg chain II

- dependence on prediction parameters negligible





- excellent convergence to Bethe ansatz (98%)



(Bethe data: J.S. Caux)

- perfect agreement with experiment

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

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

evolution of the auxiliary system

- problem: sometimes results are not good enough even using prediction
- solution: degree of freedom: „time evolution“ of auxiliary system Q

$$\langle \hat{B}_P(t)\hat{A}_P\rangle_\beta = Z(\beta)^{-1}\langle\psi(0)|\mathrm{e}^{-\beta\hat{H}_P/2}\mathrm{e}^{\mathrm{i}\hat{H}_Pt}\hat{B}_P\mathrm{e}^{-\mathrm{i}\hat{H}_Pt}\hat{A}_P\mathrm{e}^{-\beta\hat{H}_P/2}|\psi(0)\rangle$$

$$\langle \hat{B}_P(t)\hat{A}_P\rangle_\beta = Z(\beta)^{-1}\langle\psi(0)|\boxed{\hat{T}_Q^{-1}}\mathrm{e}^{-\beta\hat{H}_P/2}\mathrm{e}^{\mathrm{i}\hat{H}_Pt}\hat{B}_P\mathrm{e}^{-\mathrm{i}\hat{H}_Pt}\hat{A}_P\mathrm{e}^{-\beta\hat{H}_P/2}\boxed{\hat{T}_Q}|\psi(0)\rangle$$

- proposal by Karrasch *et al.* (PRL 2012): $\hat{T}_Q(t) = \mathrm{e}^{\mathrm{i}\hat{H}_Qt}$
  time-evolve Q using physical Hamiltonian *backwards in time*
- substantial improvement over original approach
- questions:
  - why does time range improve?
  - can we do even better?

a new notation

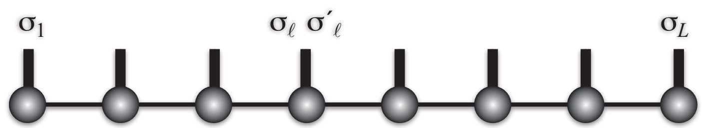
- isomorphism between „doubled“ Hilbert space and linear bounded operators on Hilbert space $\mathcal{H}_P = \mathcal{H}_Q \equiv \mathcal{H}$

$$|\psi\rangle \in \mathcal{H} \otimes \mathcal{H} \qquad \hat{\Psi} \in \mathcal{B}(\mathcal{H}) : \mathcal{H} \mapsto \mathcal{H}$$

$$\langle \{\sigma\}, \{\sigma'\} | \psi \rangle \equiv \langle \{\sigma\} | \hat{\Psi} | \{\sigma'\} \rangle$$

- in MPS language: *matrix product operator*

$$|\psi\rangle = \sum_{\{\sigma\},\{\sigma'\}} A^{\sigma_1,\sigma'_1} \dots A^{\sigma_L,\sigma'_L} |\{\sigma\}, \{\sigma'\}\rangle \qquad \hat{\Psi} = \sum_{\{\sigma\},\{\sigma'\}} A^{\sigma_1,\sigma'_1} \dots A^{\sigma_L,\sigma'_L} |\{\sigma\}\rangle\langle\{\sigma'\}|$$

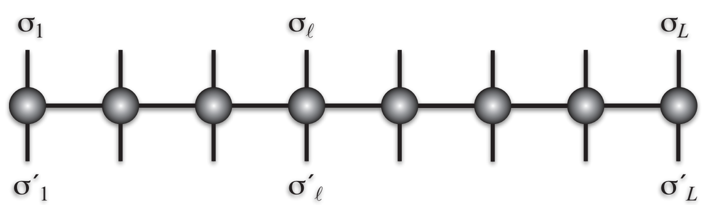


- translation rules:

$$|\psi(0)\rangle \propto \sum_{\{\sigma\},\{\sigma'\}} |\{\sigma\}, \{\sigma'\}\rangle \equiv |I\rangle \qquad \hat{I}$$

$$|\psi(\beta)\rangle \propto \mathrm{e}^{-\beta \hat{H}} |I\rangle \qquad \mathrm{e}^{-\beta \hat{H}}$$

$$(\hat{P} \otimes \hat{Q}) |\psi\rangle \leftrightarrow \hat{P} \hat{\Psi} \hat{Q}^T$$



reexpress approaches ...

$$\langle \hat{B}(t)\hat{A}\rangle_\beta = Z(\beta)^{-1}\langle I|\mathrm{e}^{-\beta\hat{H}/2}\mathrm{e}^{\mathrm{i}\hat{H}t}\hat{B}\mathrm{e}^{-\mathrm{i}\hat{H}t}\hat{A}\mathrm{e}^{-\beta\hat{H}/2}|I\rangle$$

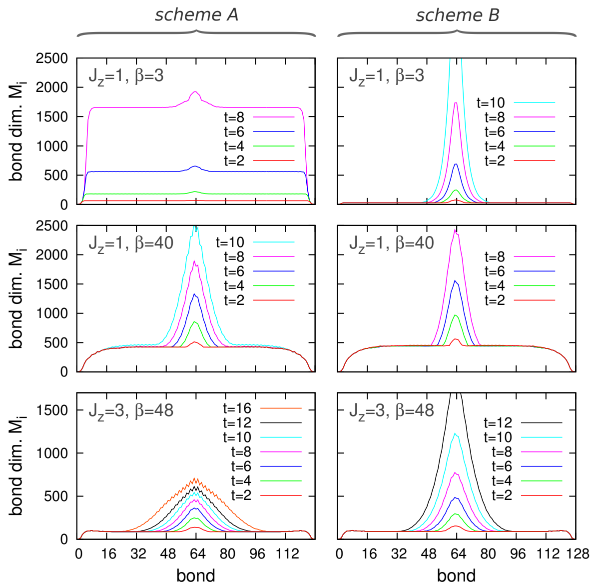
- original approach:

matrix product operator

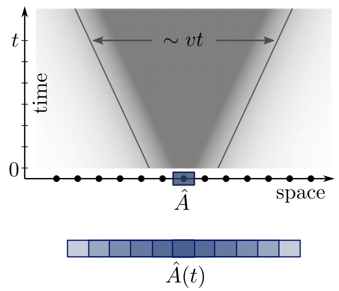
$$\langle \hat{B}(t)\hat{A}\rangle_\beta = Z(\beta)^{-1}\mathrm{Tr}\left(\boxed{[\mathrm{e}^{-\beta\hat{H}/2}\mathrm{e}^{+\mathrm{i}\hat{H}t}]}\hat{B}\boxed{[\mathrm{e}^{-\mathrm{i}\hat{H}t}\hat{A}\mathrm{e}^{-\beta\hat{H}/2}]}\right)$$

- approach by Karrasch *et al.*:

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



can be simplified



works well because of lightcone argument

Barthel, NJP (2013)

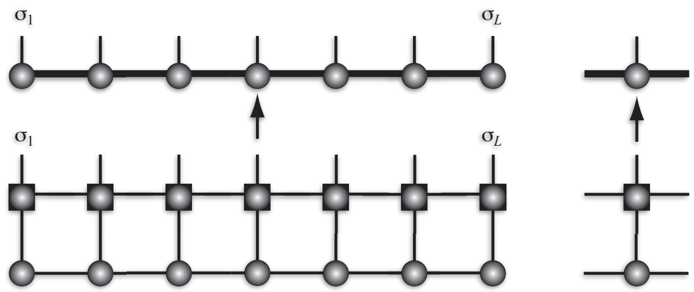
long-ranged interactions

what can we do if interactions are not just nearest-neighbour?

- larger unit cells for Trotter scheme
    - becomes very costly
- swap gates + Trotter scheme
    - treat all interactions as nearest-neighbour
    - to make this possible you have to swap sites into different positions
    - sequence of nearest-neighbour swaps
    - build one large *M*-matrix from *two* sites, exchange local sites, deconstruct into two *M*-matrices by SVD

long-ranged interaction: Krylov

- 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

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