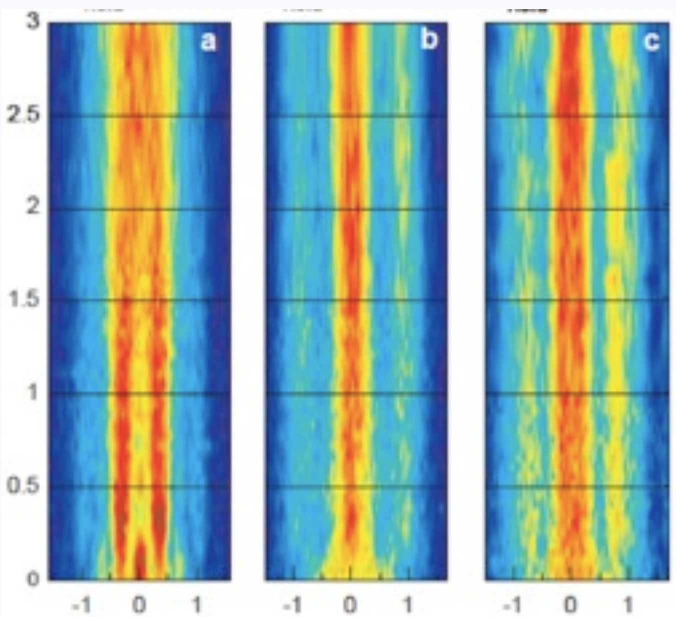
A quantum dynamical simulator

Classical digital meets quantum analog



Ulrich Schollwöck

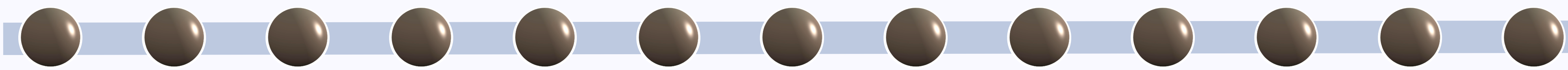
LMU Munich

Jens Eisert

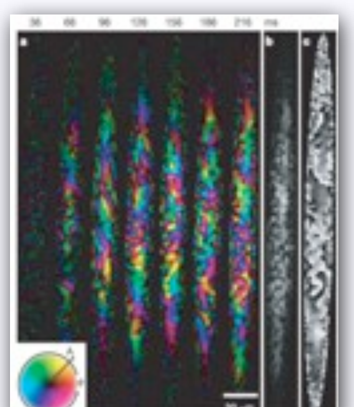
Freie Universität Berlin

Mentions joint work with I. Bloch, S. Trotzky, I. McCulloch, A. Flesch, Y.-U. Chen, C. Gogolin, M. Mueller, A. Riera

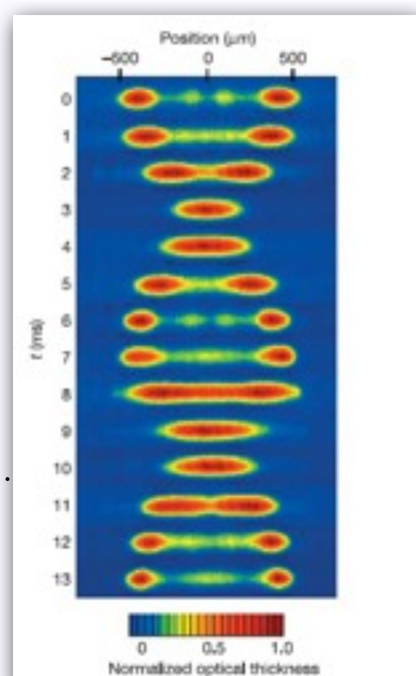
Equilibration



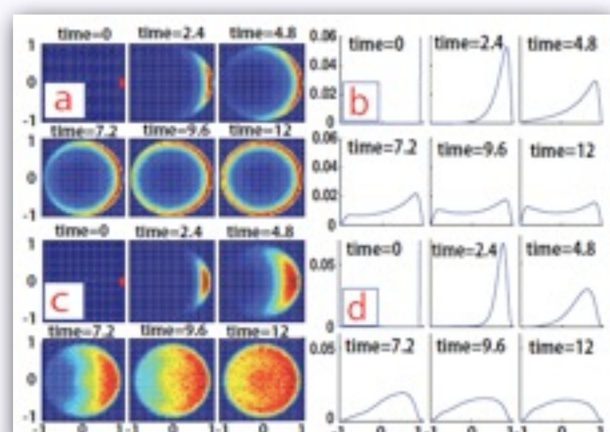
- How do quantum many-body systems come to equilibrium?
- How does temperature dynamically appear?



Sadler, Stamper-Kurn et al.



Kinoshita et al.



Schmiedmayer et al.

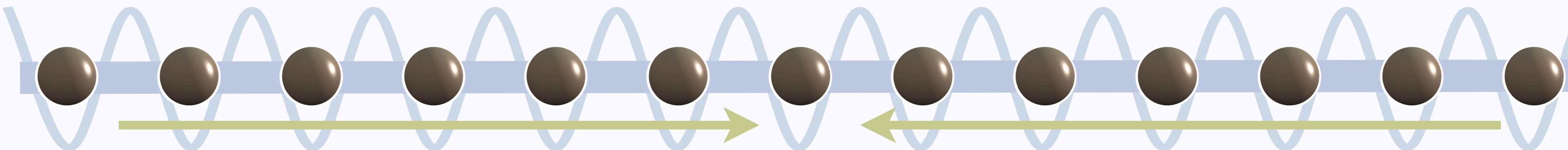
Quenched dynamics

- Start in some **initial state** $\rho(0)$ with clustering correlations (e.g. product)
- Many-body free **unitary time evolution**

$$\rho(t) = e^{-iHt}\rho(0)e^{iHt}$$

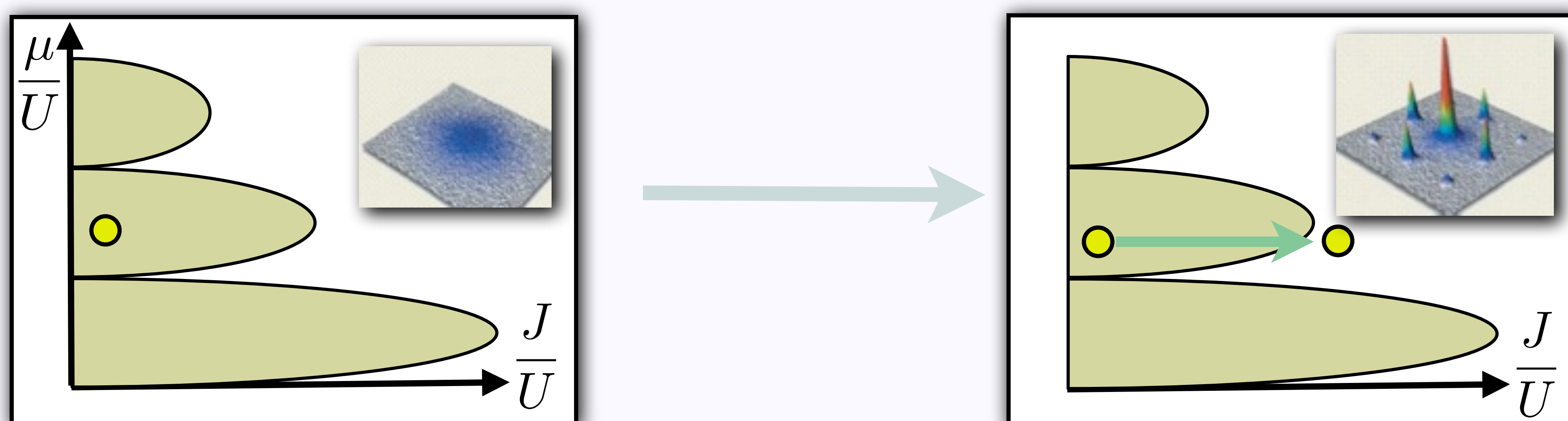
(Compare also Corinna Kollath's, John Cardy's, Ferenc Igloi's, Alexei Tsvelik's, Eugene Demler's, Allessandro Silva's, Maurizio Fagotti's, Jean-Sebastien Caux's talks)

Cold atoms in optical lattices



- **Paradigmatic situation:** Quench from deep Mott to superfluid phase in Bose-Hubbard model

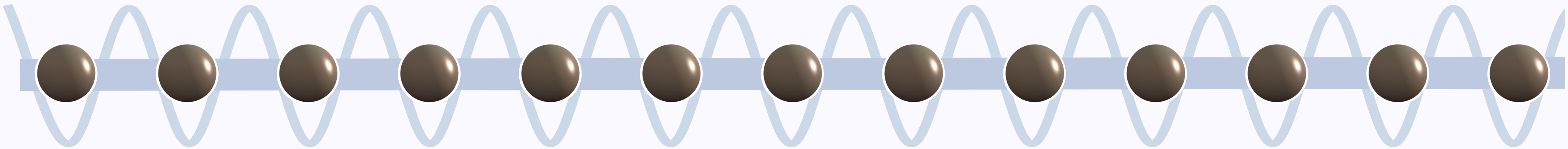
$$H = -J \sum_{\langle j,k \rangle} b_j^\dagger b_k + \frac{U}{2} \sum_k b_k^\dagger b_k (b_k^\dagger b_k - 1) - \mu \sum_k b_k^\dagger b_k$$



Mott phase

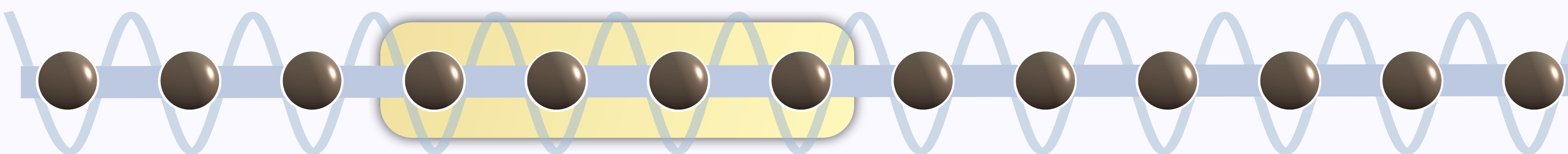
Superfluid

Where does it relax to?



- **What happens?**
- What can be said analytically?

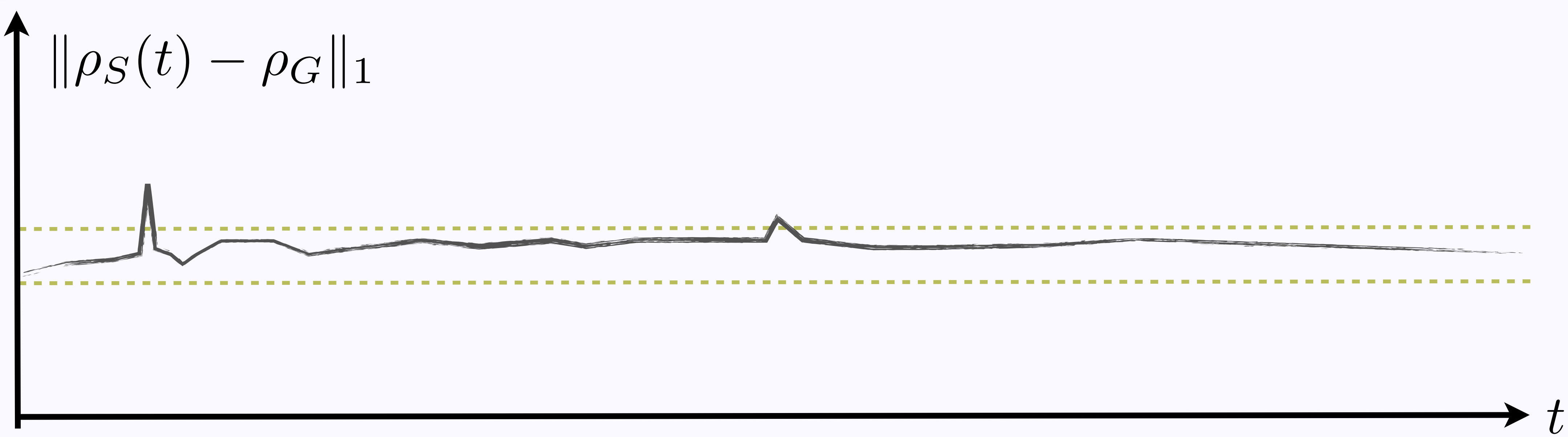
Relaxation theorems



- **Equilibration** (true for all Hamiltonians with non-degenerate energy gaps)

$$\mathbb{E}(\|\rho_S(t) - \rho_G\|_1) \leq \frac{1}{2}\sqrt{\frac{d_2^2}{d^{\mathrm{eff}}}}, \qquad d^{\mathrm{eff}} = \frac{1}{\sum_k |\langle E_k|\psi_0\rangle|^4}$$

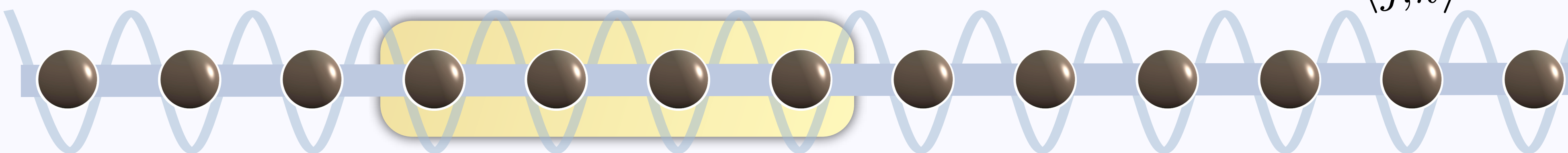
ρ_G is a *maximum entropy state* given all constants of motion



Linden, Popescu, Short, Winter, *Phys Rev E* **79** (2009)
Gogolin, Mueller, Eisert, *Phys Rev Lett* **106** (2011)

Relaxation theorems

$$H = -J \sum_{\langle j,k \rangle} b_j^\dagger b_k - \mu \sum_k b_k^\dagger b_k$$



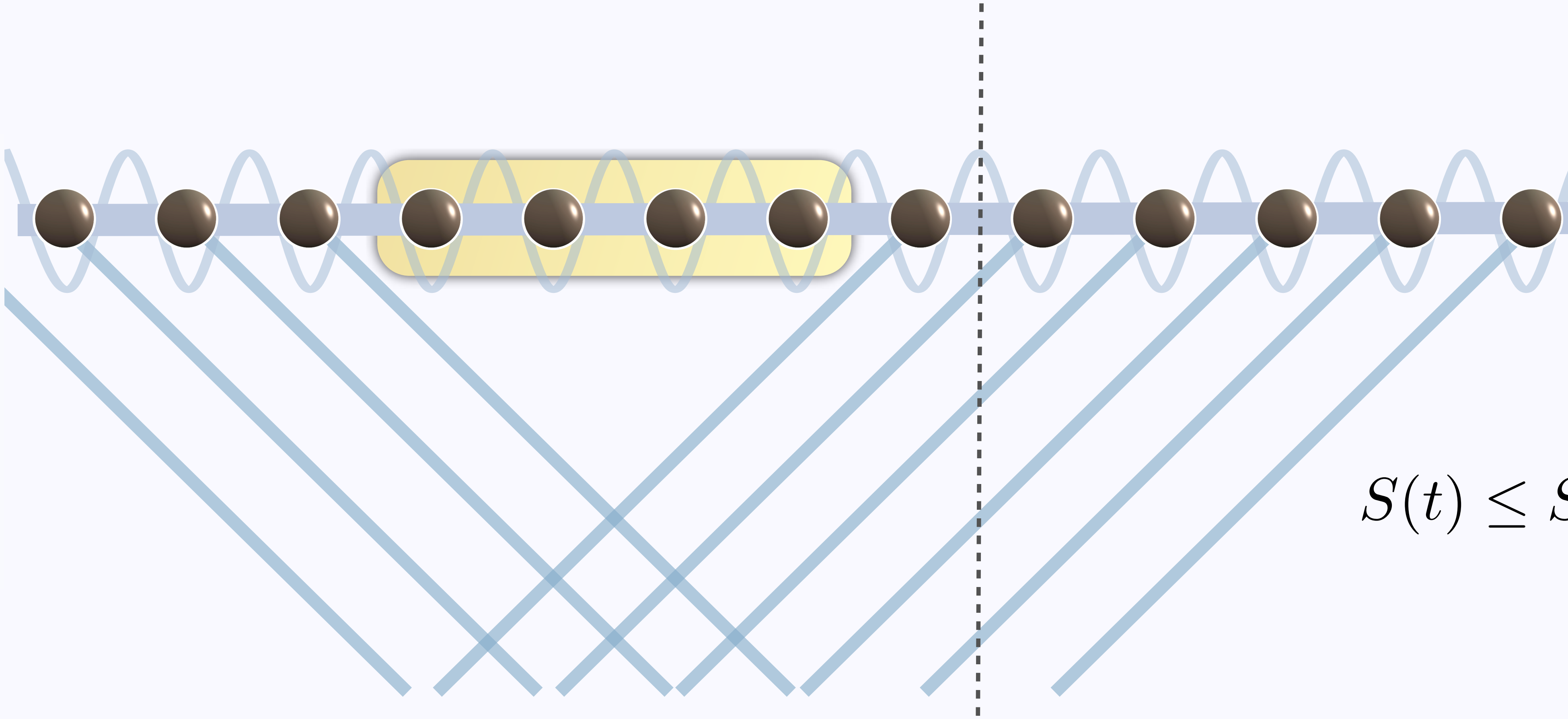
- **Strong equilibration** (infinite free bosonic, integrable models): For clustering initial states (not Gaussian), $\forall \varepsilon > 0 \ \exists t_{\text{relax}}$

$$\|\rho_S(t) - \rho_G\|_1 < \varepsilon, \ \forall t > t_{\text{relax}}$$

ρ_G is a *maximum entropy state* given all constants of motion

Cramer, Eisert, *New J Phys* **12** (2010)
Cramer, Dawson, Eisert, Osborne, *Phys Rev Lett* **100** (2008)
Dudnikova, Komech, Spohn, *J Math Phys* **44** (2003) (classical)

Light cone dynamics and entanglement growth



$$S(t) \leq S(0) + ct$$

- Non-commutative central limit theorems for equilibration

  Cramer, Eisert, *New J Phys* **12** (2010)
  Cramer, Dawson, Eisert, Osborne, *Phys Rev Lett* **100** (2008)

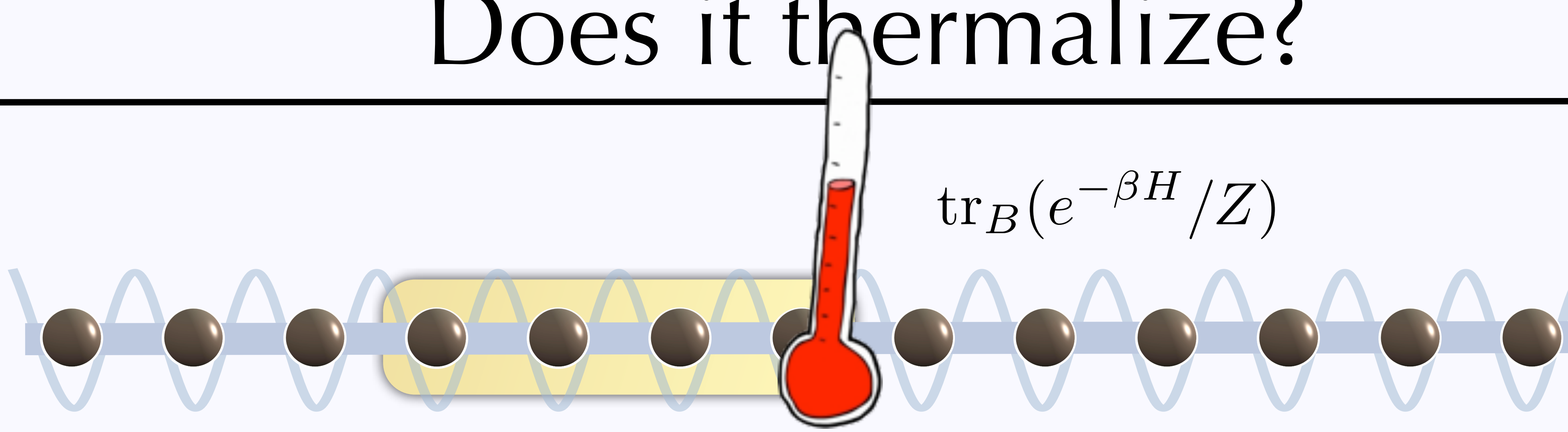
- Entanglement growth

  Eisert, Osborne, *Phys Rev Lett* **97** (2006)
  Bravyi, Hastings, Verstraete, *Phys Rev Lett* **97** (2006)
  Schuch, Wolf, Vollbrecht, Cirac, *New J Phys* **10** (2008)
  Barthel, Schollwoeck, *Phys Rev Lett* **100** (2008)
  Laeuchli, Kollath, *J Stat Mech* (2008) P05018

- Light cone dynamics in conformal field theory

  Calabrese, Cardy, *Phys Rev Lett* **96** (2006)

Does it thermalize?

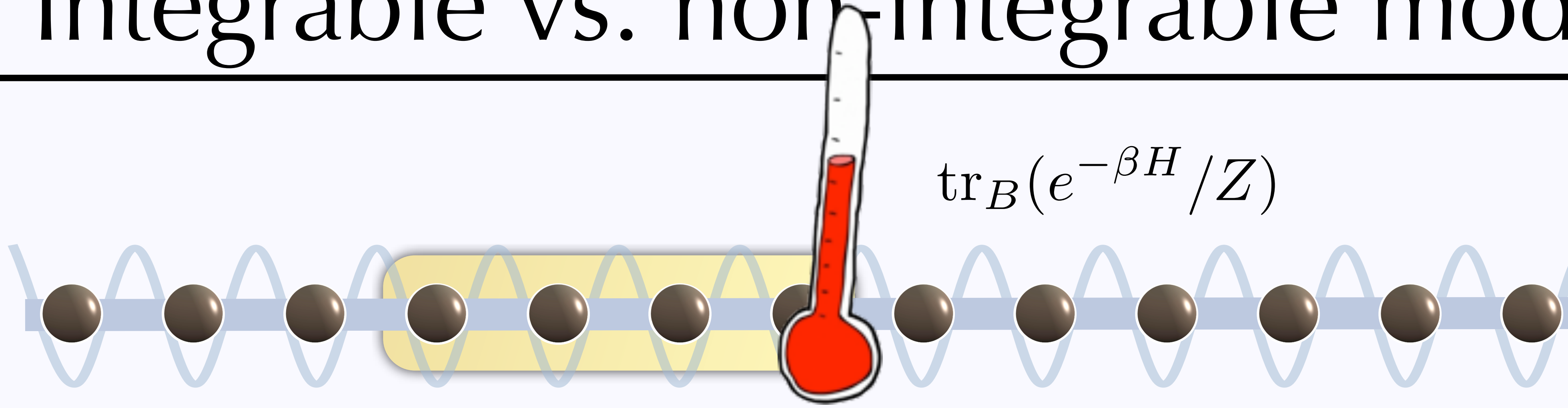


$$\mathrm{tr}_B(e^{-\beta H}/Z)$$

- **Complicated process:**
  - Equilibration
  - Subsystem initial state independence
  - Weak "bath" dependence
  - Gibbs state

Goldstein, Lebowitz, Tumulka, Zanghi, *Phys Rev Lett* **96** (2006)
Reimann, *New J Phys* **12** (2010)
Linden, Popescu, Short, Winter, *Phys Rev E* **79** (2009)
Gogolin, Mueller, Eisert, *Phys Rev Lett* **106** (2011)

Integrable vs. non-integrable models



- Steps towards proving thermalization in certain *weak-coupling limits*

Riera, Gogolin, Eisert, *Phys Rev Lett* **108** (2012)
In preparation (2012)

- **Common belief:** "Non-integrable models thermalize"

- **Notions of integrability:**

(A) Exist *n* (local) conserved commuting linearly independent operators

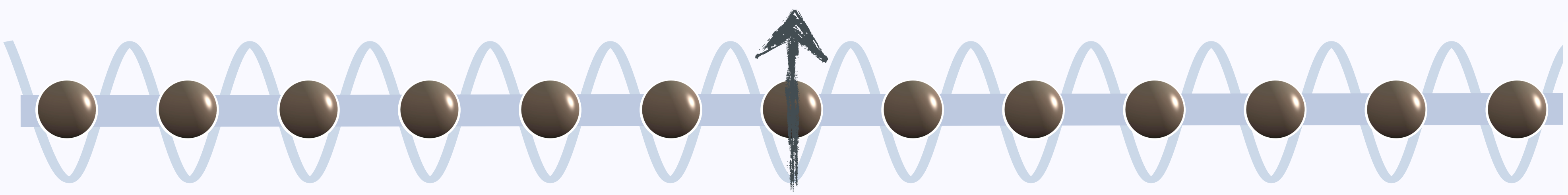
(B) Like (A) but with linear replaced by algebraic independence

(C) The system is integrable by the Bethe ansatz or is a free model

(D) The quantum many-body system is exactly solvable

Beautiful models, Sutherland (World Scientific, Singapore, 2004)
Faribault, Calabrese, Caux, *J Stat Mech* (2009)
Exactly solvable models, Korepin, Essler (World Scientific, Singapore, 1994)

Non-thermalizing non-integrable models



- Not even non-integrable systems necessarily thermalize:

- **Non-thermalization:** There are weakly non-integrable models,

  - translationally invariant
  - nearest-neighbor,

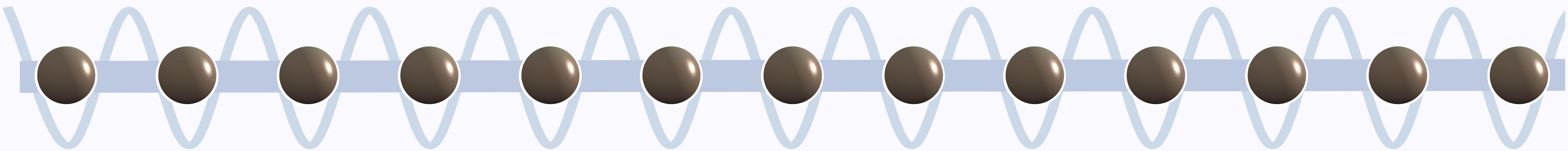
  for which for two initial conditions $\psi^{(i)}(0) = \psi_S^{(i)}(0) \otimes \psi_B^{(i)}(0)$, $i = 1, 2$,
  two time-averaged states $\omega^{(i)}$ remain distinguishable,

$$\|\omega^{(1)} - \omega^{(2)}\|_1 \geq c$$

- Infinite memory of initial condition

Gogolin, Mueller, Eisert, *Phys Rev Lett* **106** (2011)
Eisert, Friesdorf, in preparation (2012)

Lots of open questions



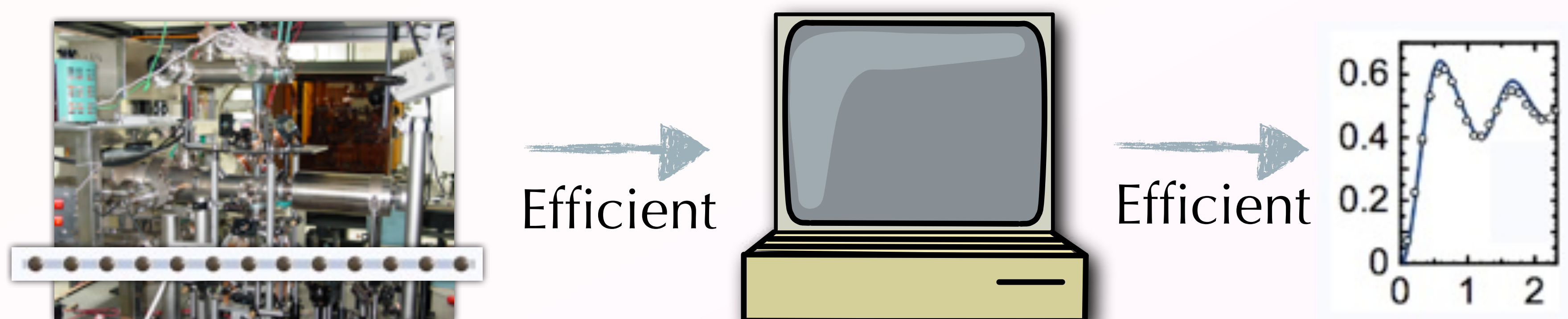
- **Situation is far from clear**
  - Time scales of equilibration?
  - Algebraic vs exponential decay?
  - When does it thermalize?
  - Role of conserved quantities/integrability?
- **Need for simulation**

Digital vs. "quantum simulation"

- **Classical simulation**

Classical simulation
(t-DMRG)

- **"Quantum simulation"**



Quantum simulation

Postprocessing

Key issues with quantum simulation

1. Hardness problem:

One has to solve a quantum problem that presumably is *"hard" classically*

2. Certification problem:

How does one *certify correctness* of quantum simulation?

- **Realize some feasible device** (not universal) outperforming classical ones?

compression of information

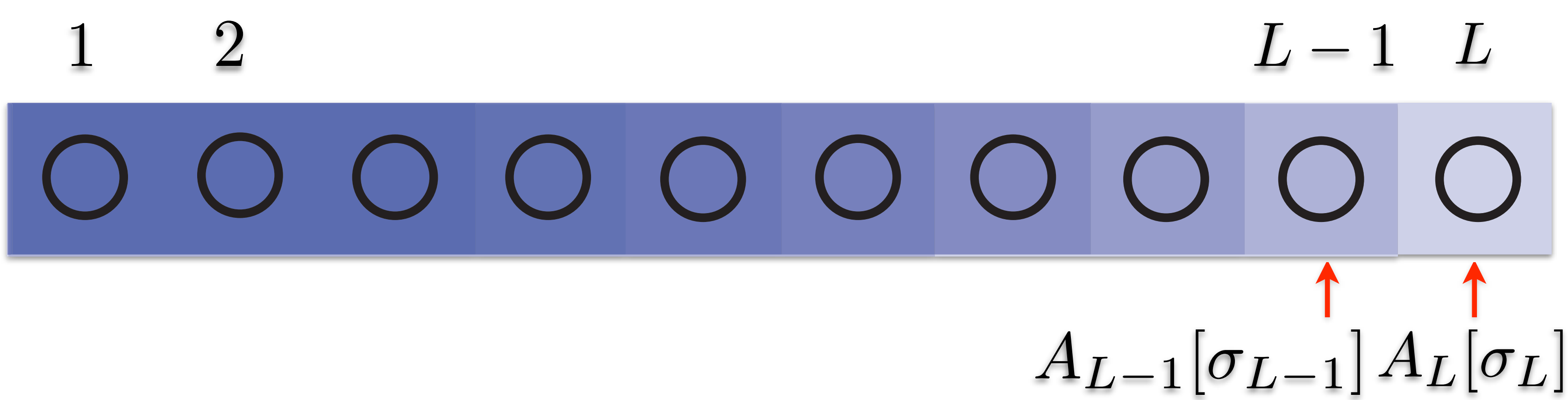
- compression of information necessary and desirable
  - diverging number of degrees of freedom
  - emergent macroscopic quantities: temperature, pressure, ...
- classical spins
  - thermodynamic limit: $N \to \infty$ $2N$ degrees of freedom (linear)
- quantum spins
  - superposition of states
  - thermodynamic limit: $N \to \infty$ 2^N degrees of freedom (exponential)

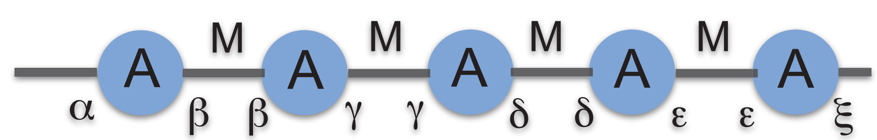
classical simulation of quantum systems

- 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?**

matrix product states

- identify each site with a set of matrices depending on local state





- total system wave functions

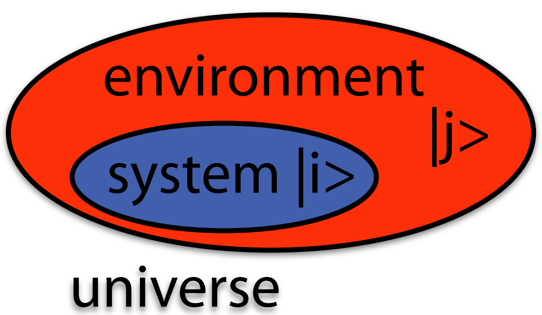
$$|\psi\rangle = \sum_{\sigma_1 \ldots \sigma_L} \boxed{(A_1[\sigma_1] \ldots A_L[\sigma_L])} |\sigma_1 \ldots \sigma_L\rangle$$

scalar coefficient:
~ matrix product

- matrix product state (MPS):
  - control parameter: matrix dimension *M*
  - *A*-matrices determined by decimation prescription

bipartite entanglement in MPS

- measuring bipartite entanglement *S*: reduced density matrix



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

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

- arbitrary bipartition

AAAAAAAA AAAAAAAAAAAAAAA

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

Schmidt decomposition

- reduced density matrix and bipartite entanglement

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

$$\boxed{S = -\sum_\alpha w_\alpha \log_2 w_\alpha \quad \leq \log_2 M}$$

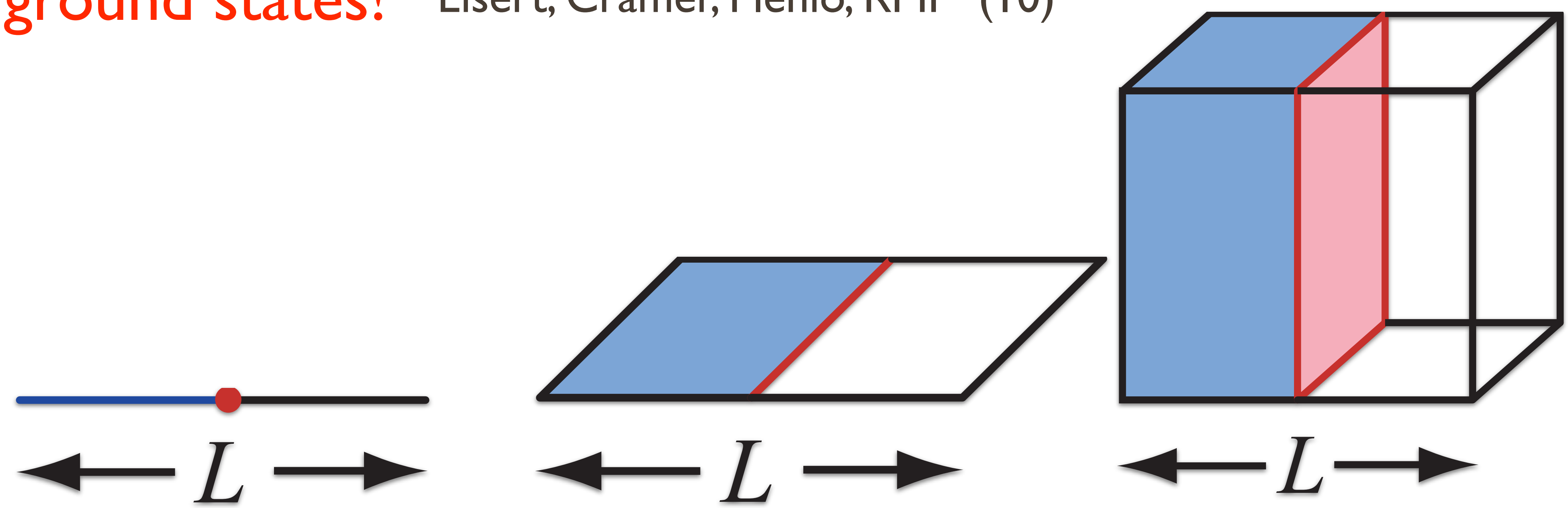
codable maximum

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

$$\boxed{S \leq \log_2 M \Rightarrow M \geq 2^S}$$

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

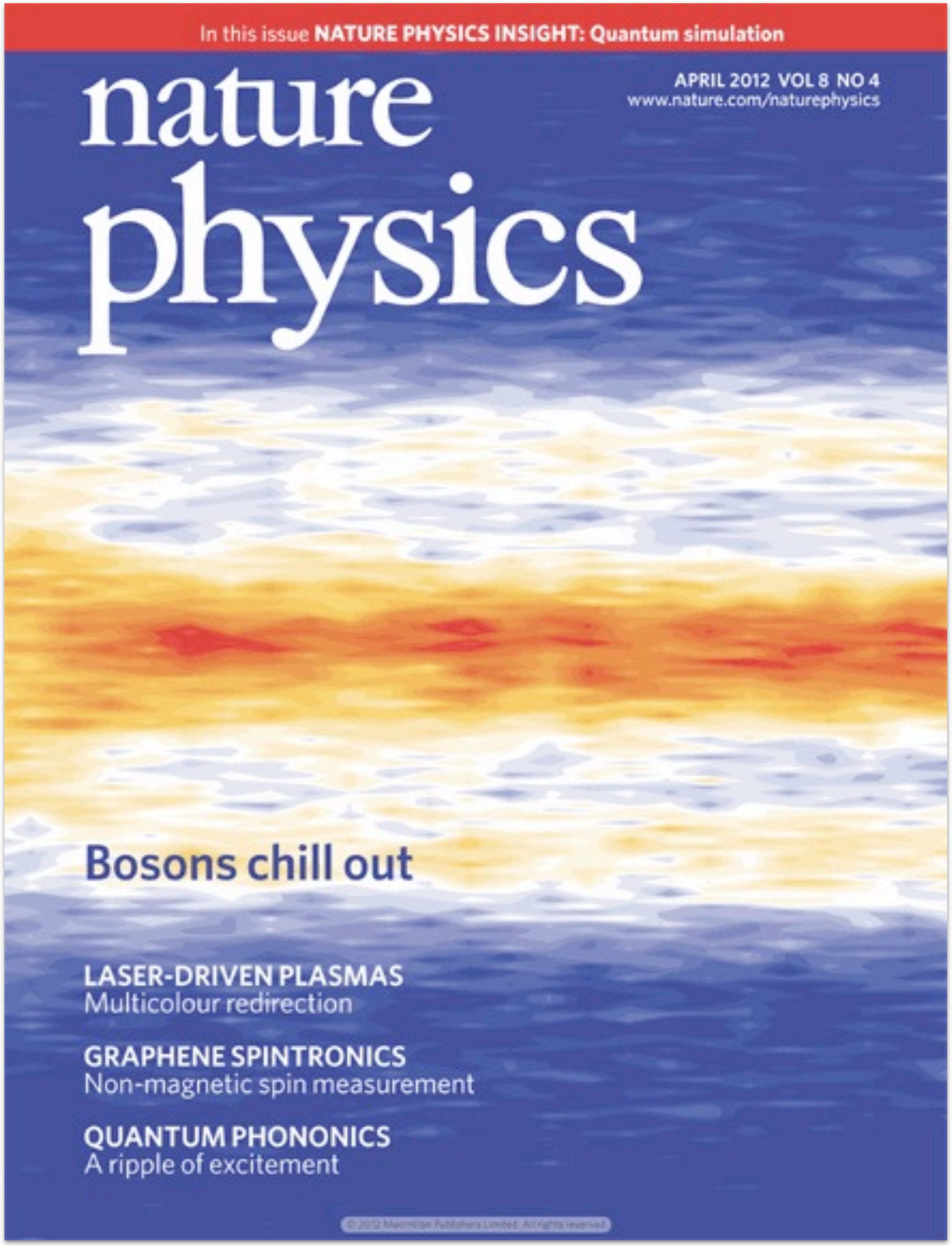
entanglement & matrix scaling

- TEBD/t-DMRG/t-MPS: time evolution of MPS (Trotter-based)

  Vidal PRL `04; Daley, Kollath, US, Vidal, J. Stat. Mech (2004) P04005;
  White, Feiguin PRL '04; Verstraete, Garcia-Ripoll, Cirac PRL `04;
  US, RMP 77, 259 (2005); US, Ann. Phys. 326, 96 (2011)

- linear entanglement growth after global quenches

- consequences for simulation:
  - up to exponential growth in M ! $\boxed{M \propto c^{vt}}$
  - steady states / thermal states dynamically inaccessible



a dynamical quantum simulator: certification vs. prediction

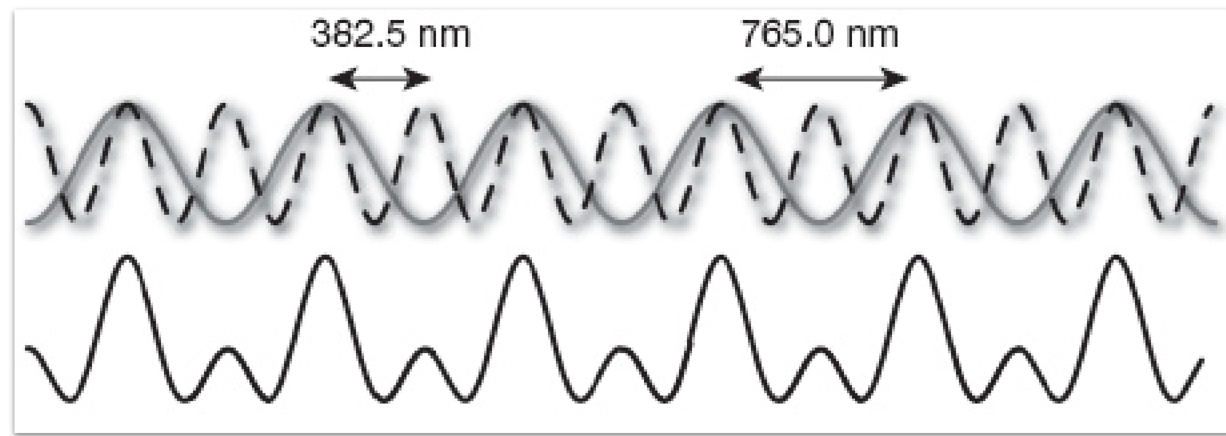
Cramer, Flesch, McCulloch, US, Eisert, PRL 101, 063001 (2008)
Flesch, Cramer, McCulloch, US, Eisert, PRA 78, 033608 (2008)
Trotzky, Chen, Flesch, McCulloch, US, Eisert, Bloch, Nat. Phys. 8, 325(2012)

preparation and local observation

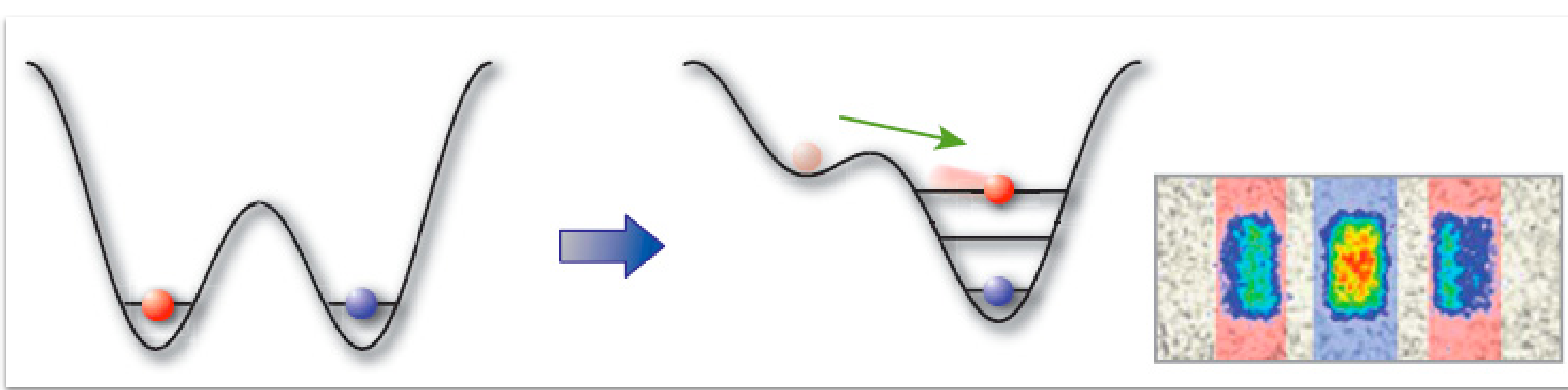
ultracold atoms provide coherent out of equilibrium dynamics

controlled preparation of initial state?   local measurements?

period-2 superlattice
- double-well formation
- staggered potential bias



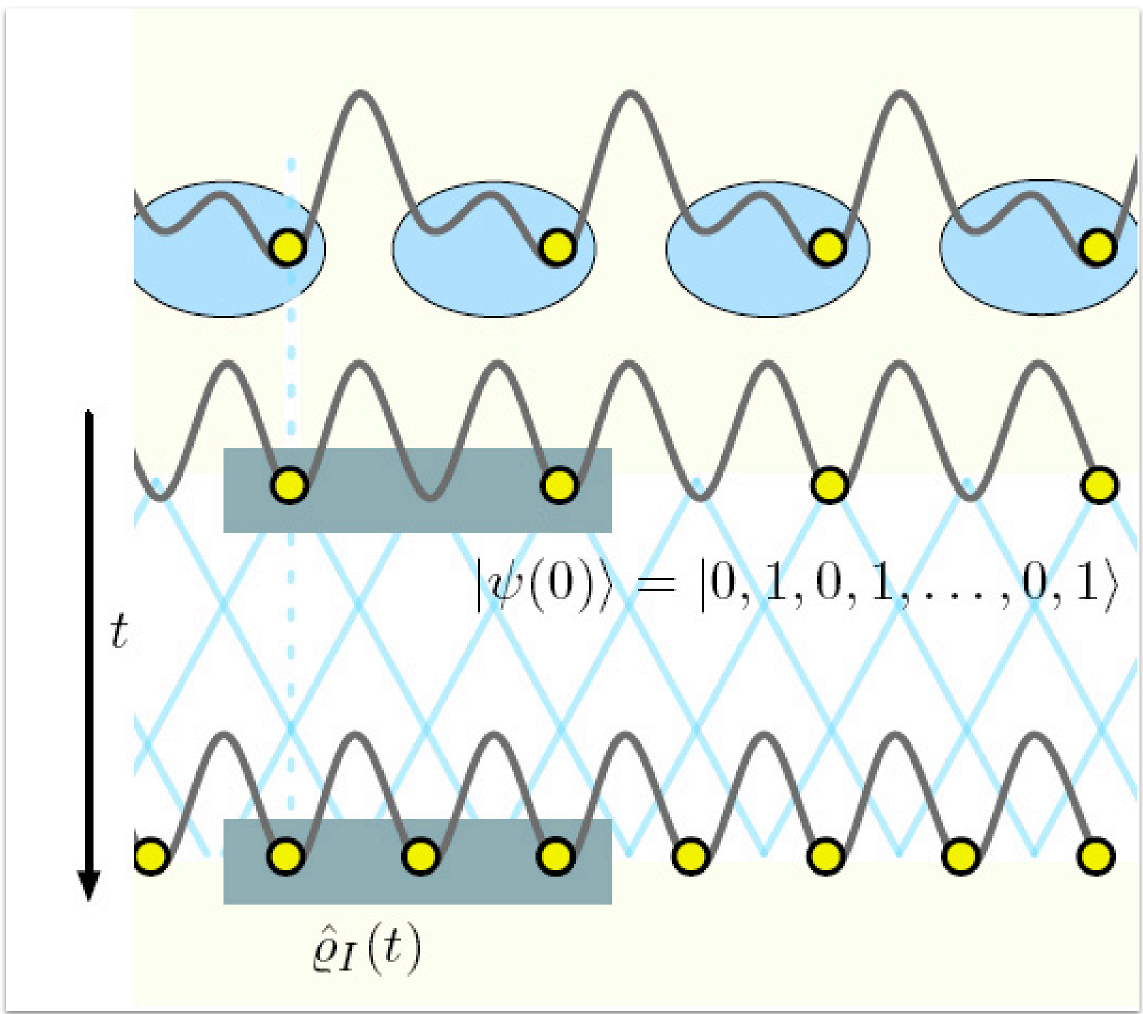
pattern-loading and odd-even resolved local measurement



- bias superlattice
- unload to higher band
- time-of-flight measurement: mapping to different Brillouin zones

(Fölling *et al.*, Nature 448, 1029 (2007))

experimental proposal



prepare $|\psi\rangle = |1,0,1,0,1,0,\ldots\rangle$

switch off superlattice

observe Bose-Hubbard dynamics

$$\hat{H} = -J\sum_i(\hat{b}_i^\dagger\hat{b}_{i+1} + \text{h.c.}) + \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) - \sum_i \mu_i\hat{n}_i$$

limiting cases

- *U*=0: non-interacting bosons: relax due to incommensurate mixing

$$\hat{H} = -J \sum_i (\hat{b}_i^\dagger \hat{b}_{i+1} + \mathrm{h.c.})$$

exactly solvable by Fourier transformation for PBC

$$\langle \hat{b}_i^\dagger(t)\hat{b}_j(t)\rangle = \frac{1}{2}\left(\delta_{ij} + (-\mathrm{i})^{i-j}(-1)^{j+1} J_{j-i}(4Jt)\right)$$

asymptotics $t^{-1/2}$

- *U*=∞: hardcore bosons: relax due to hardcore collisions
map to non-interacting spinless fermions

$$\hat{H} = -J \sum_i (\hat{c}_i^\dagger \hat{c}_{i+1} + \mathrm{h.c.})$$

exactly solvable by FT and Jordan-Wigner trafo for PBC

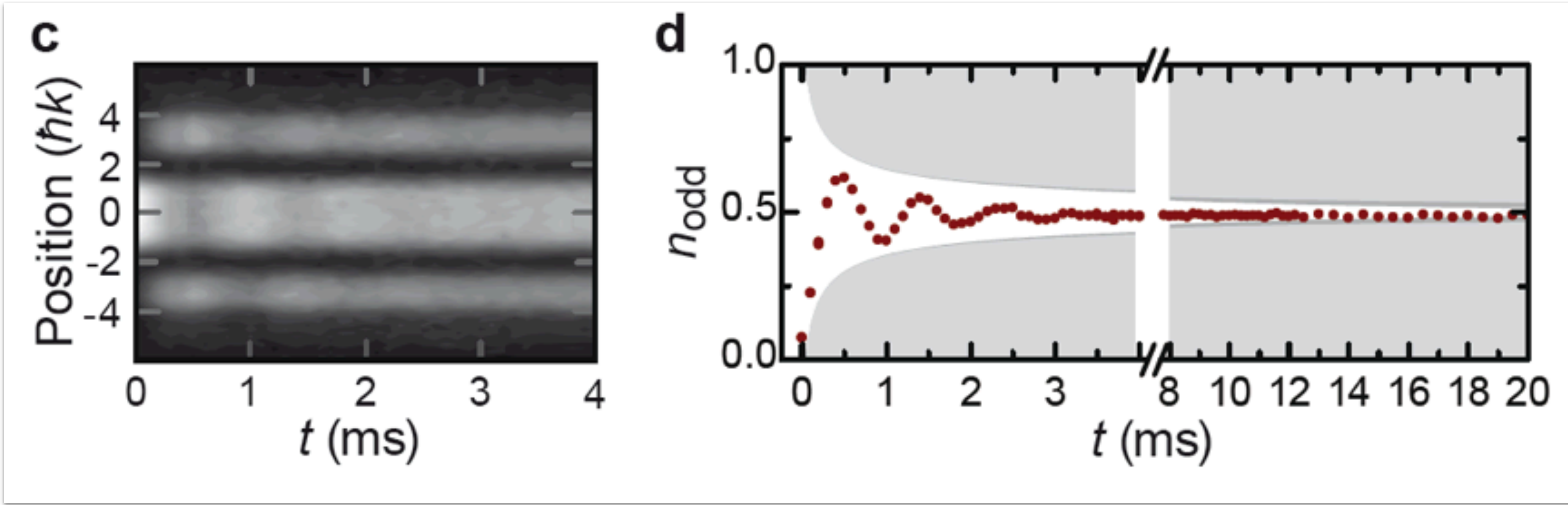
$$\langle \hat{n}_i(t)\rangle = \frac{1}{2}\left(1 - (-1)^i J_0(4Jt)\right)$$

some expressions agree with *U*=0,
e.g. local density, NN correlators

- 0<*U*<∞: interacting bosons: time-dependent DMRG

Daley, Kollath, US, Vidal, J. Stat. Mech (2004) P04005; White, Feiguin PRL ’04
US, Ann. Phys. 326, 96 (2011)

densities I

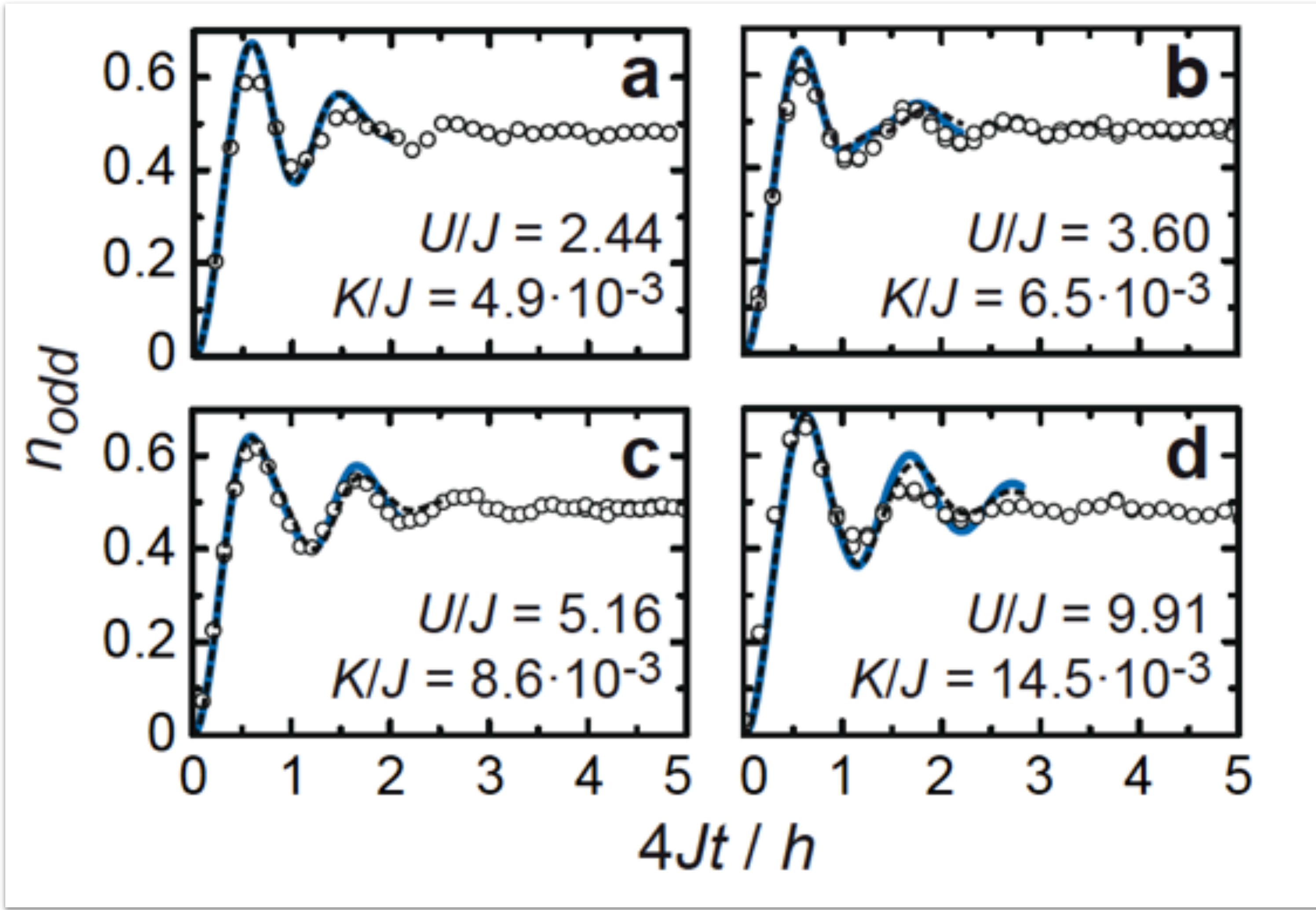


45,000 atoms, U=5.2
momentum distribution

relaxation of local occupation numbers:
fit to theory needs averaging over weighted set of chain lengths (multitube in trap)

classical tube dephasing minimal

densities II



no free fit parameters!

fully controlled relaxation in closed quantum system!

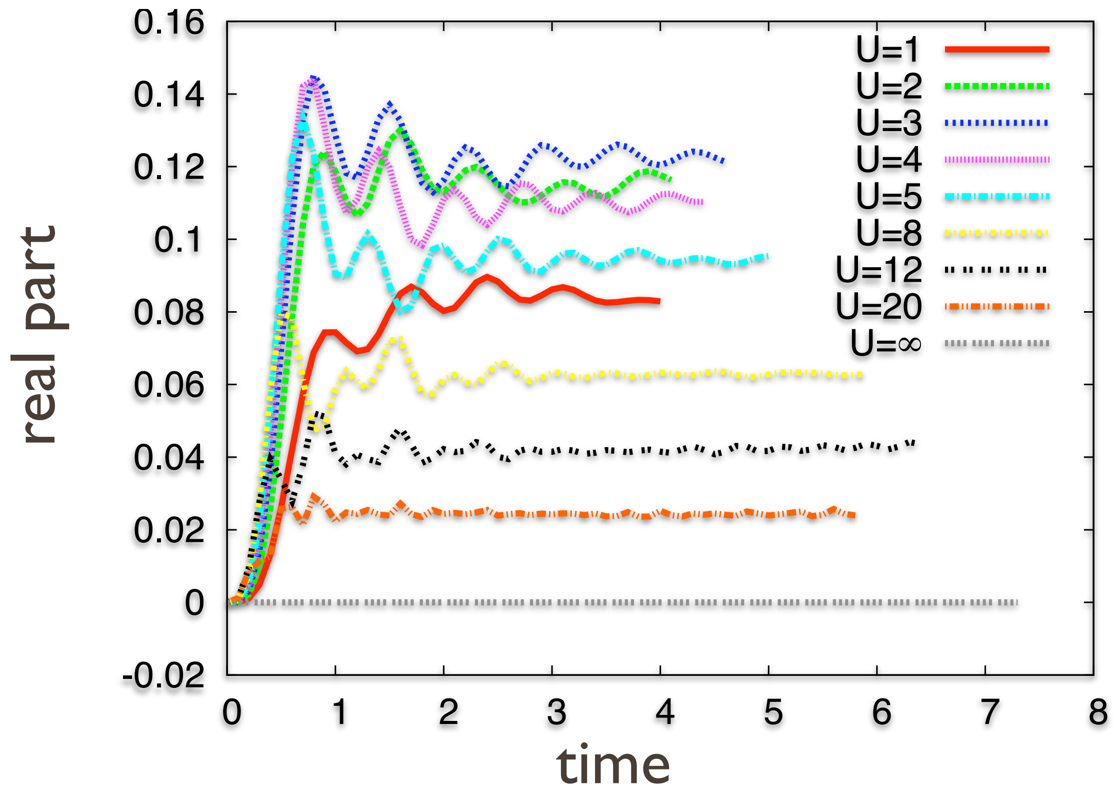
*validation of **dynamical** quantum simulator*

time range of experiment > 10 x time range of theory
real „analog computer“ that goes beyond theory

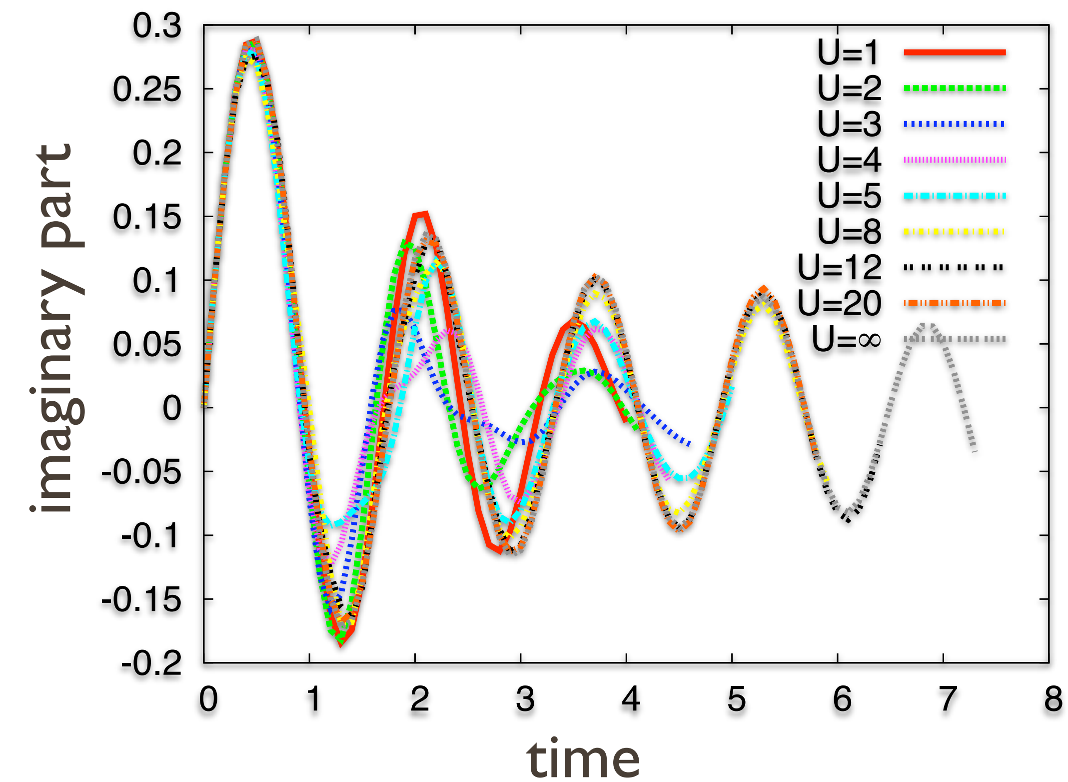
nearest-neighbour correlators

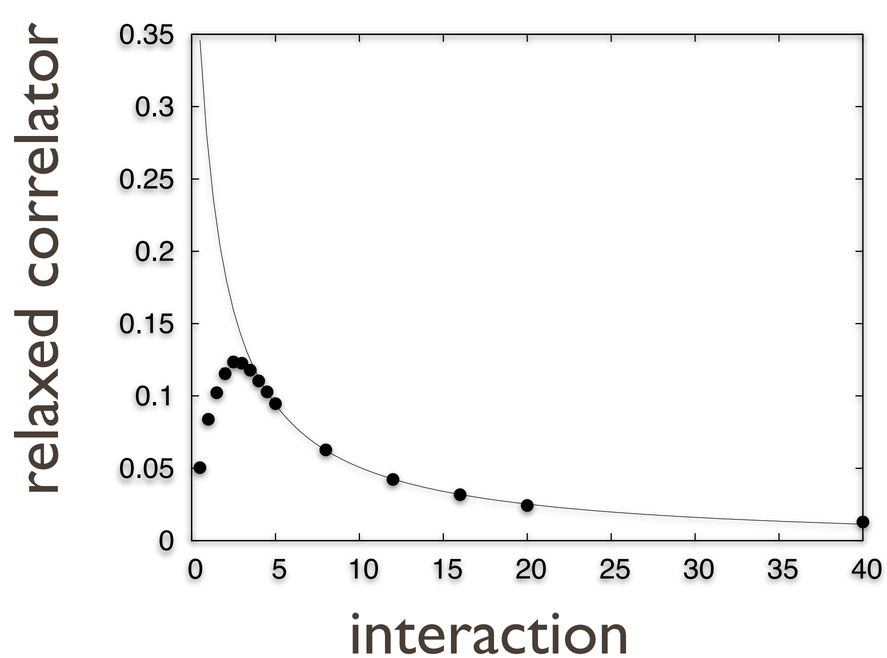
$$\langle \hat{b}_n^\dagger(t)\hat{b}_{n+1}(t)\rangle$$

correlator



current



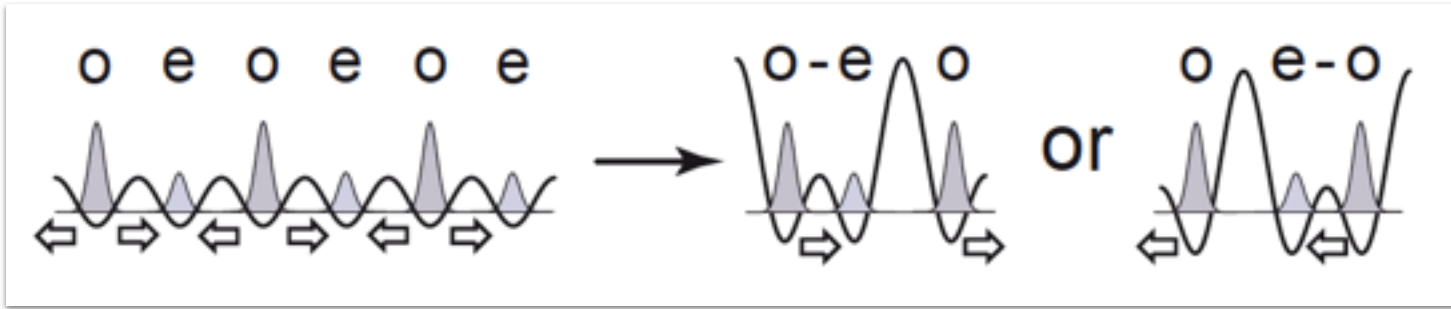


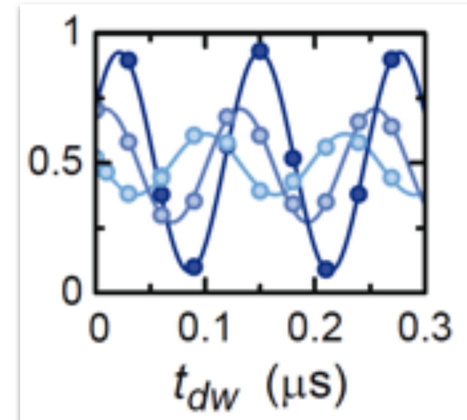
- again three regimes
- $U \approx 3$: crossover regime

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

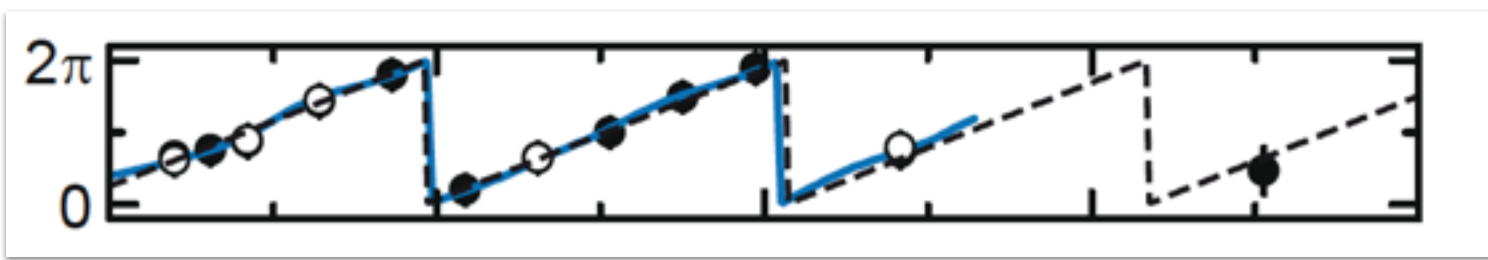
currents

measurement: split in double wells, measure well oscillations

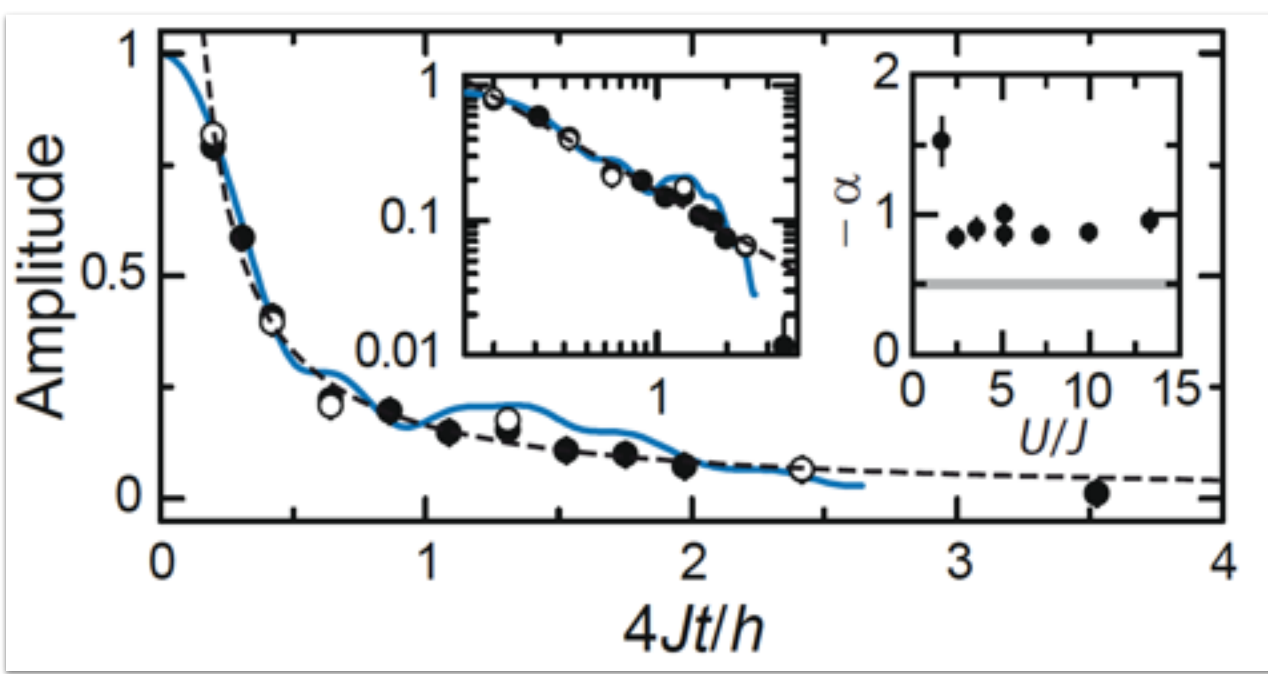




phase and amplitude

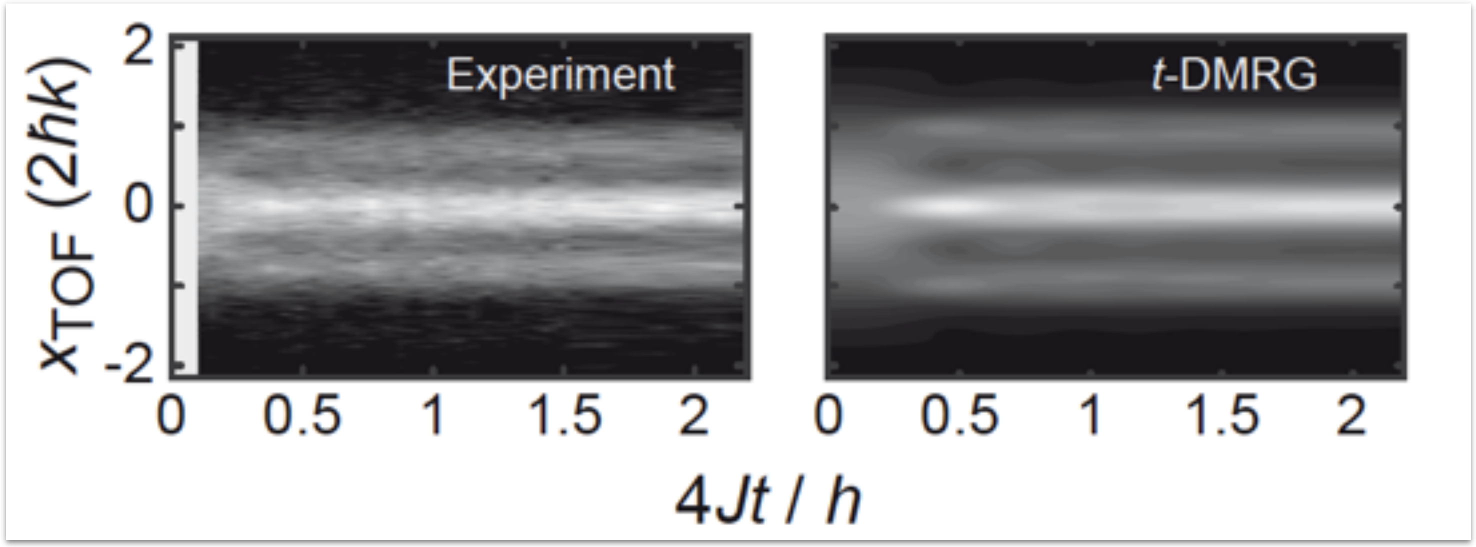


sloshing;
no c.m. motion



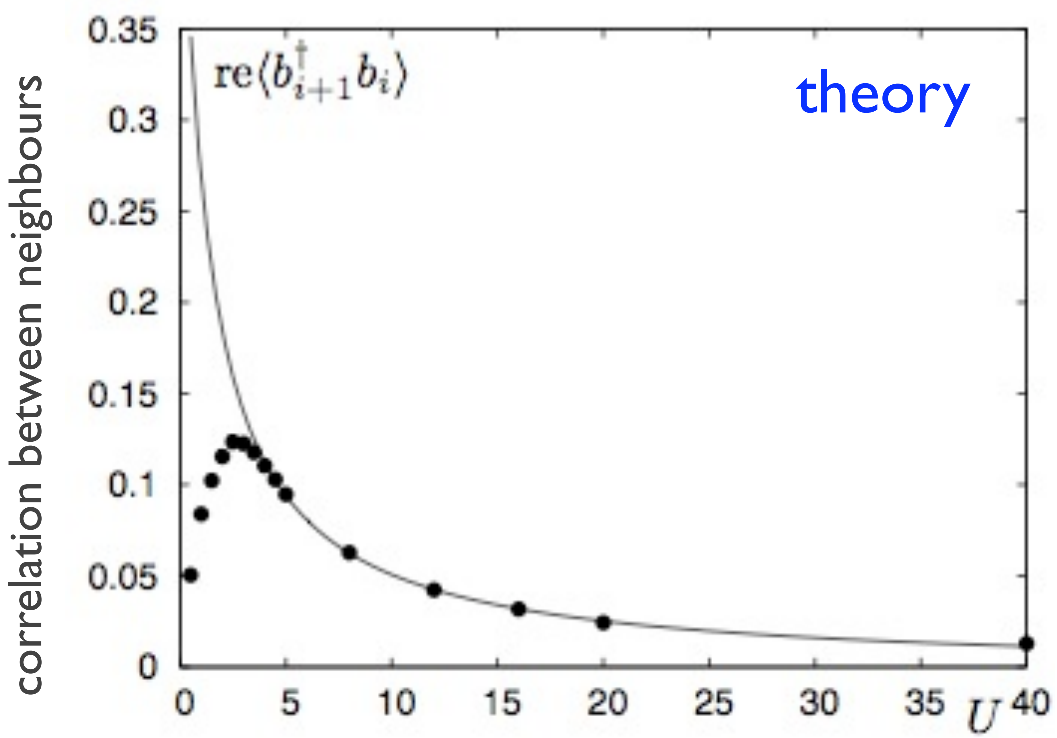
current decay as power law?

nearest neighbour correlations

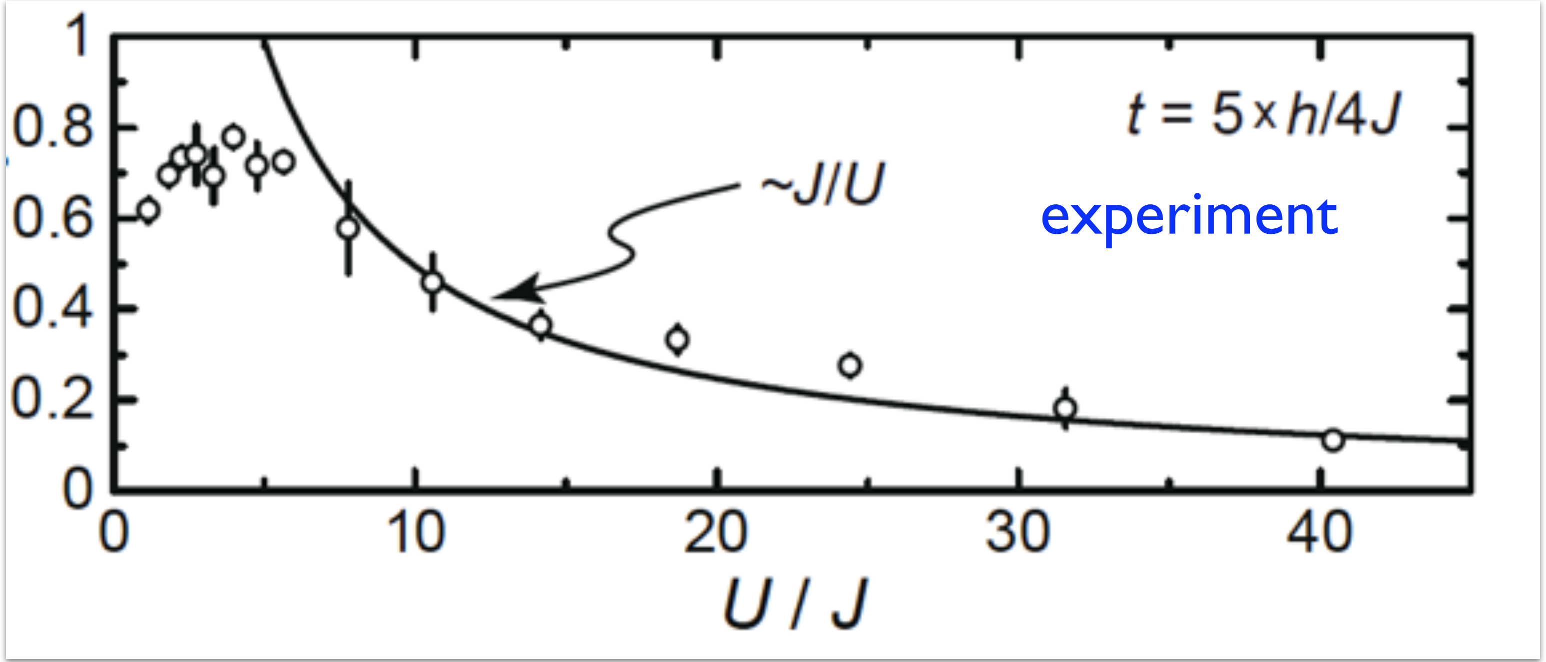


momentum distribution

visibility proportional to nearest neighbour correlations



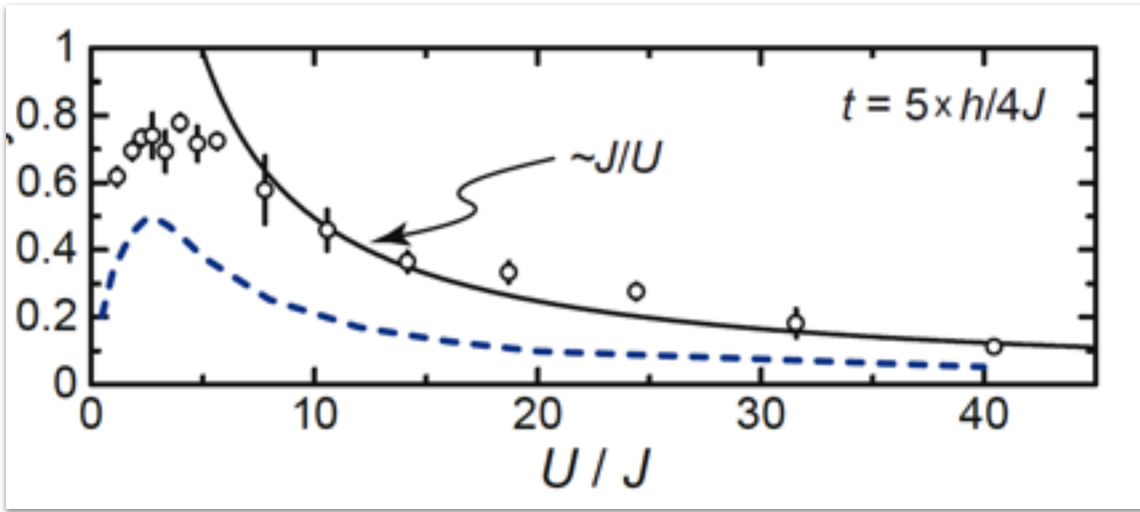
interaction strength



build-up of quantum coherence

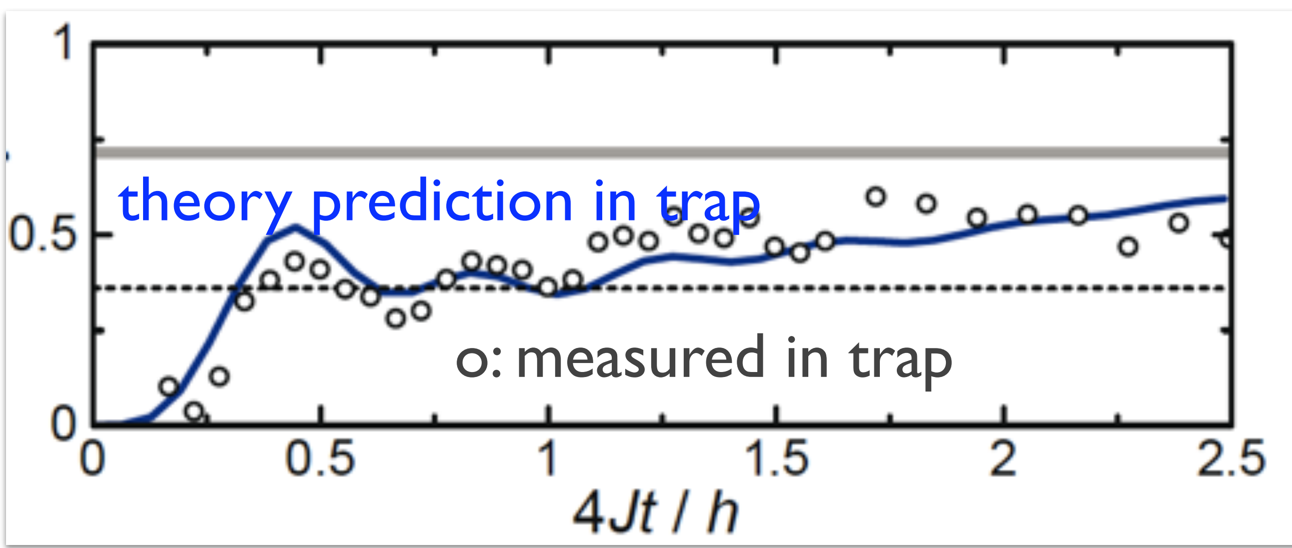
general trend, 1/U correct!

nearest neighbour correlations



a closer look:
effect stronger in experiment?

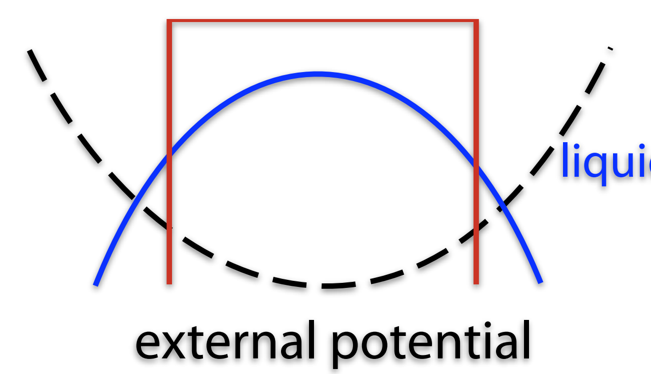
correlations grow over time; very good fit



measurement at „long time“

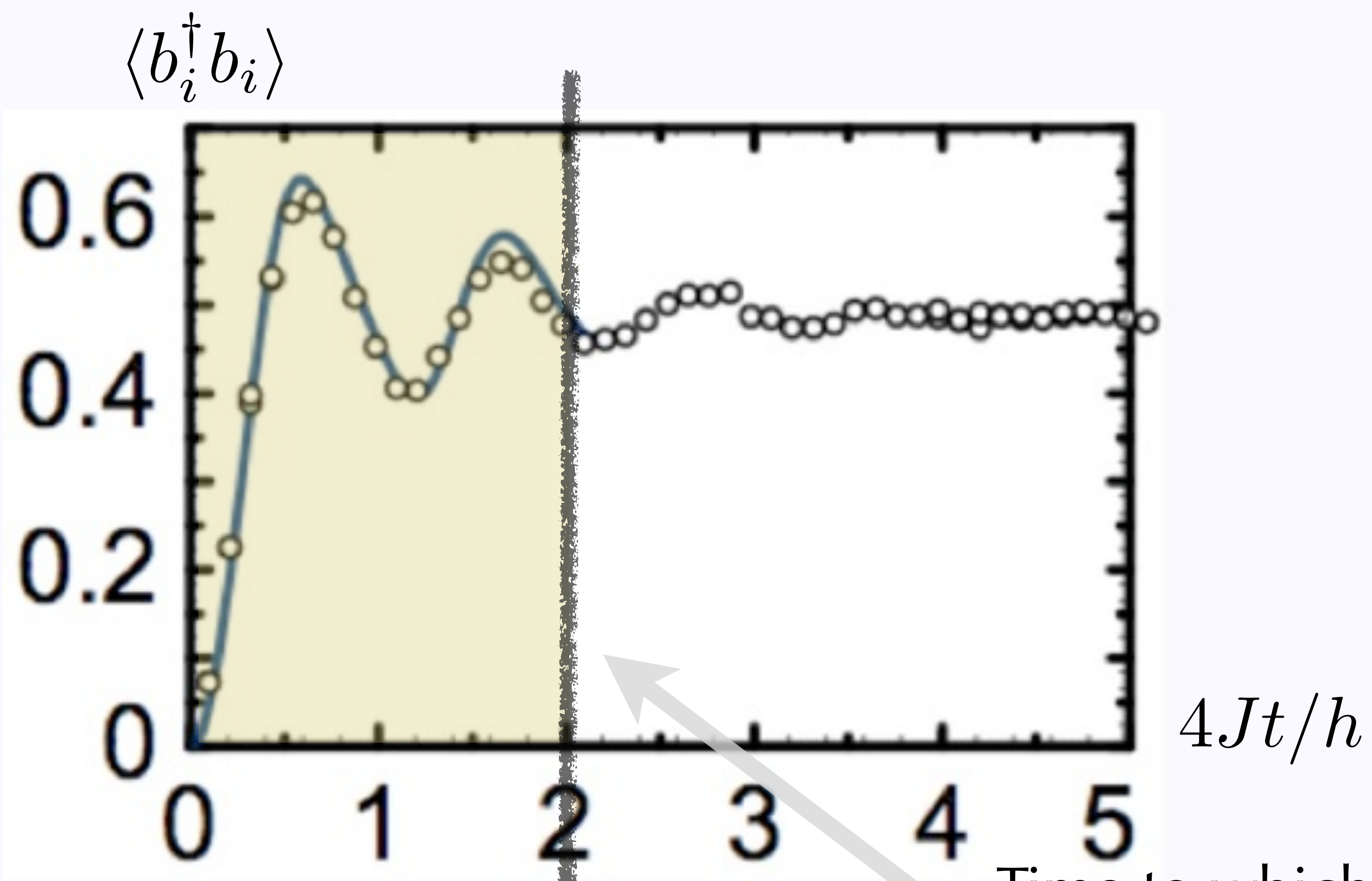
theory prediction

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



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

"Certify simulator for short times"

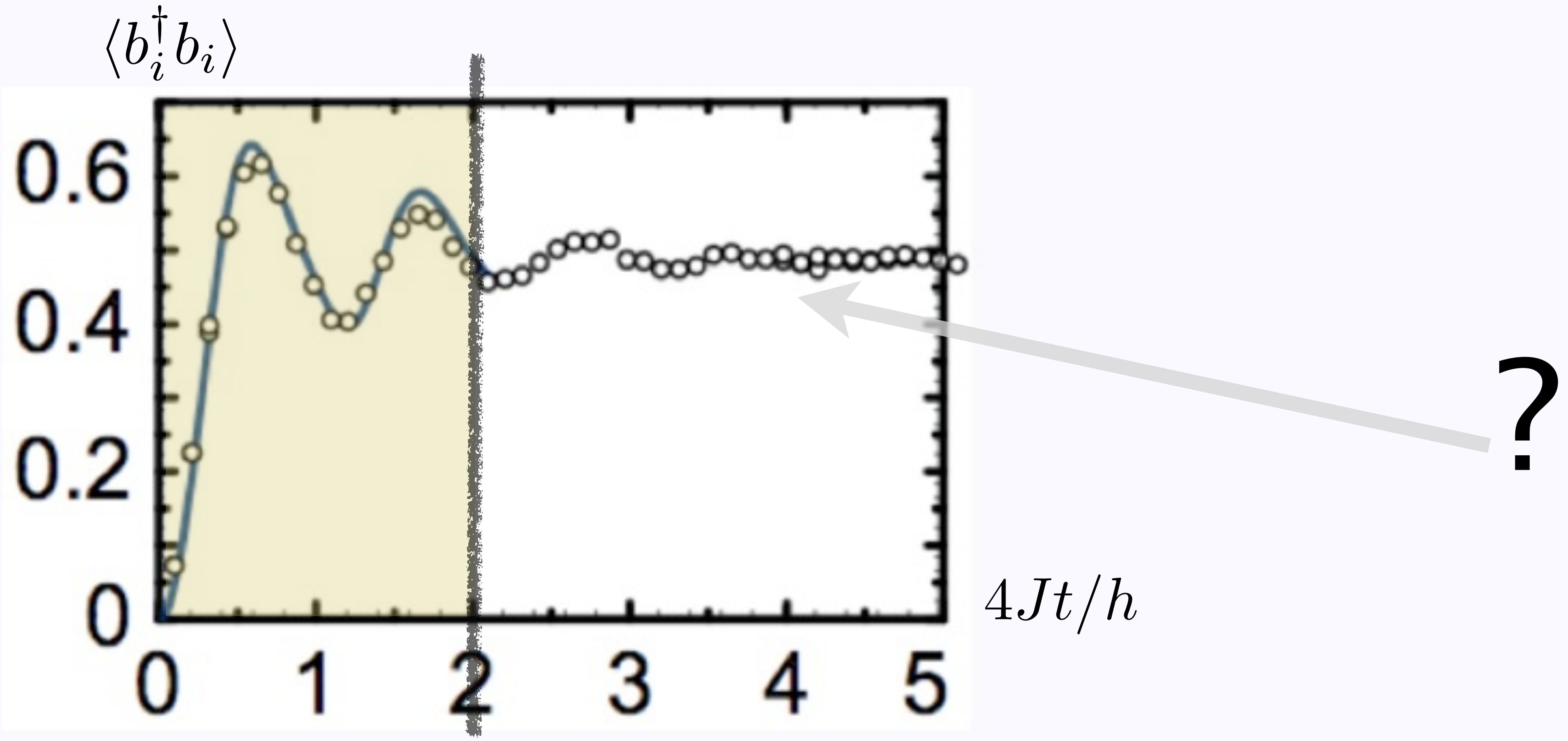


Time to which time-evolution can be simulated with MPS and $D = 5000$

Long times

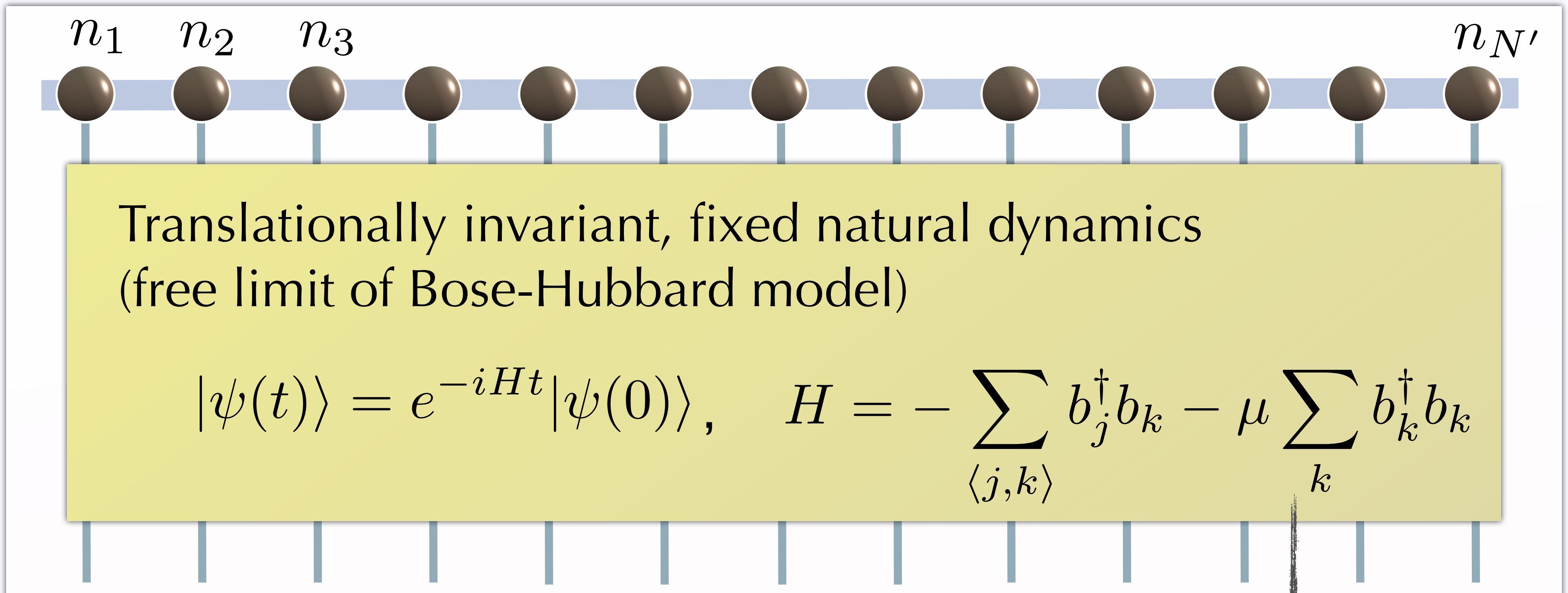
- **Quantum dynamics runs on...**

  ... ask physical questions about decay of correlations
  ... not explainable by mean field/Markovian evolution $\dot{\rho} = \mathcal{L}(\rho)$
  ... and is presumably a *hard problem*



Simulating cold atoms is classically hard

- Initially prepare product of atom numbers



Translationally invariant, fixed natural dynamics
(free limit of Bose-Hubbard model)

$$|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle\,, \quad H = -\sum_{\langle j,k\rangle} b_j^\dagger b_k - \mu \sum_k b_k^\dagger b_k$$

- Sample from output distribution

Polynomial reduction

"Boson sampling problem" for arbitrary linear optical circuits

Collapse of the polynomial hierarchy to the third level if classically efficiently sampled accurately

Kliesch, Eisert, in preparation (2012)
Aaronson, Arkhipov, arXiv:1011.3245

Simulating cold atoms is classically hard

- **Hardness of simulating cold atoms:** For arbitrary boson distributions, but translationally invariant natural Bose-Hubbard dynamics, the classical simulation is presumably hard for long times

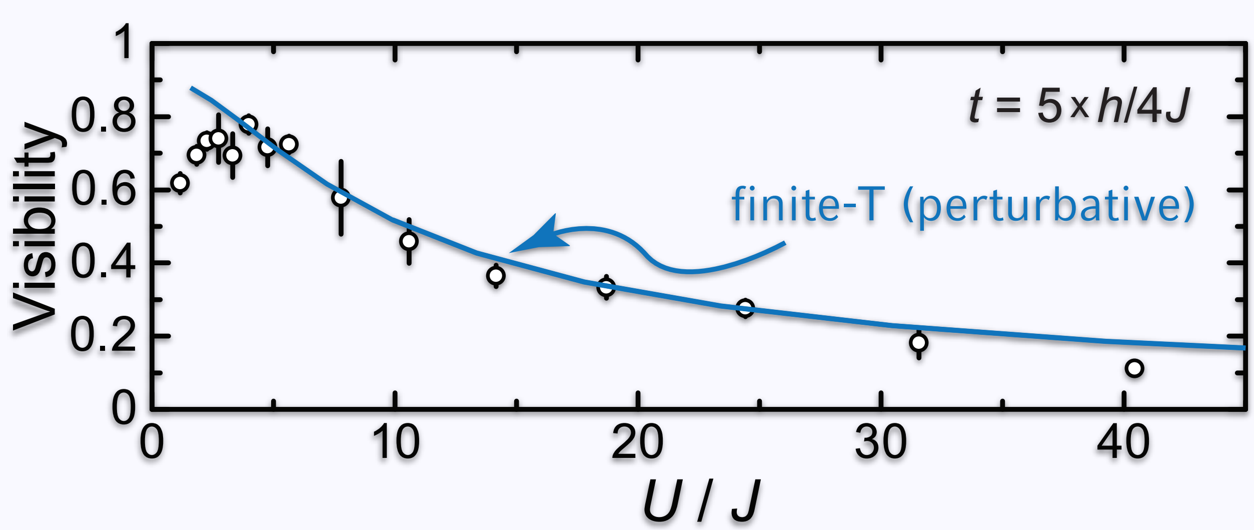
Kliesch, Eisert, in preparation (2012)
Aaronson, Arkhipov, arXiv:1011.3245

Summary

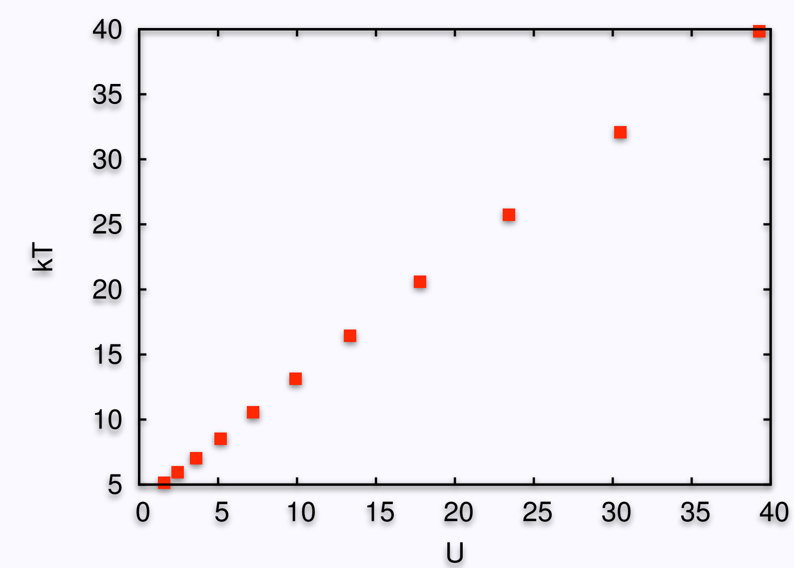
Quantum dynamical simulator for relaxation physics:

- Closed quantum system with coherent dynamics
- Non-trivial range of interactions
- Certified by parameter-free theory
- Prediction beyond theoretical time-range, classically hard problem
- Currents and correlators

- Non-trivial interaction dependencies, power laws?
- Much theory remains to be done ...



Correlators: thermal?



Chilling? No thank you!