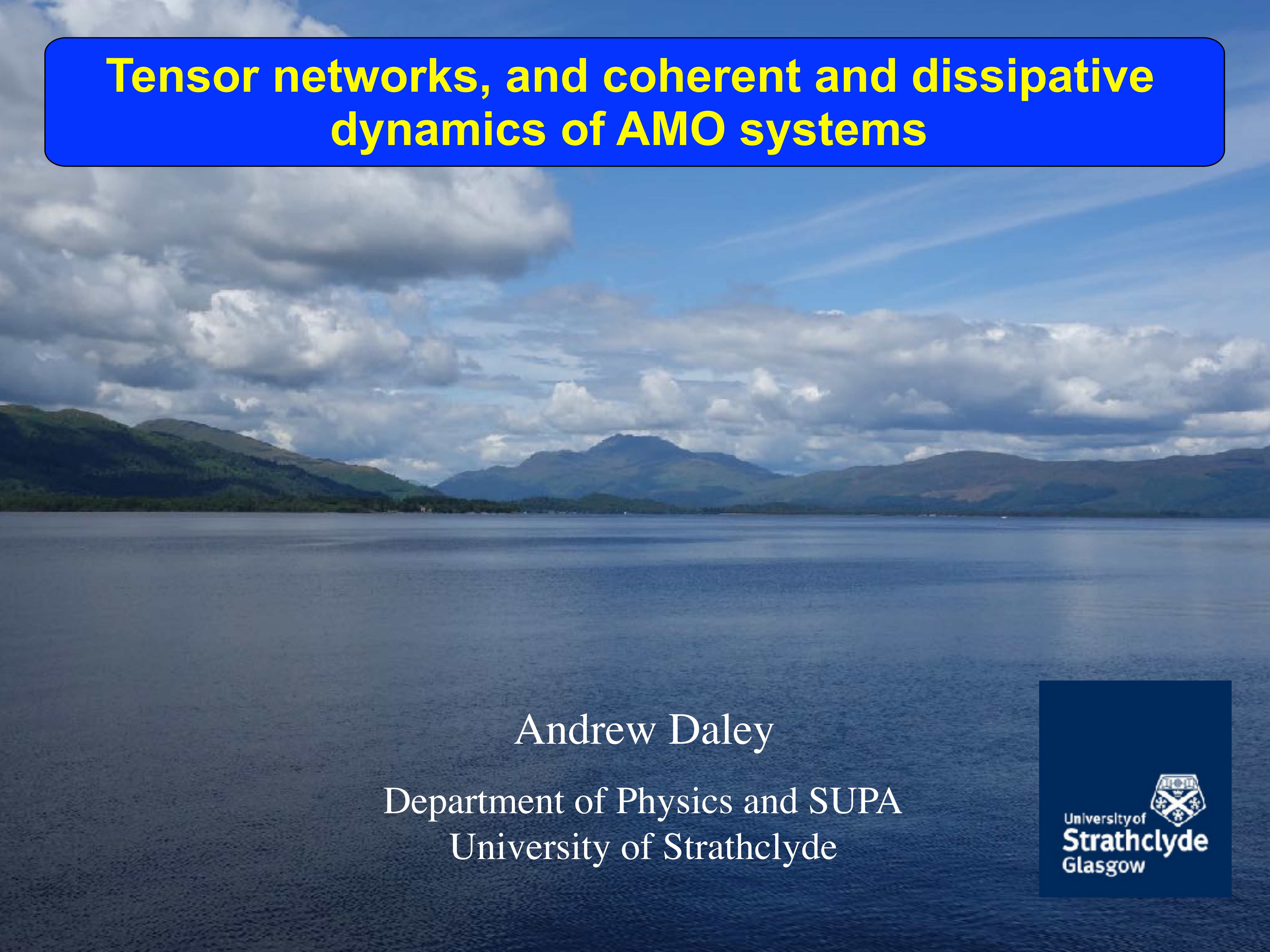


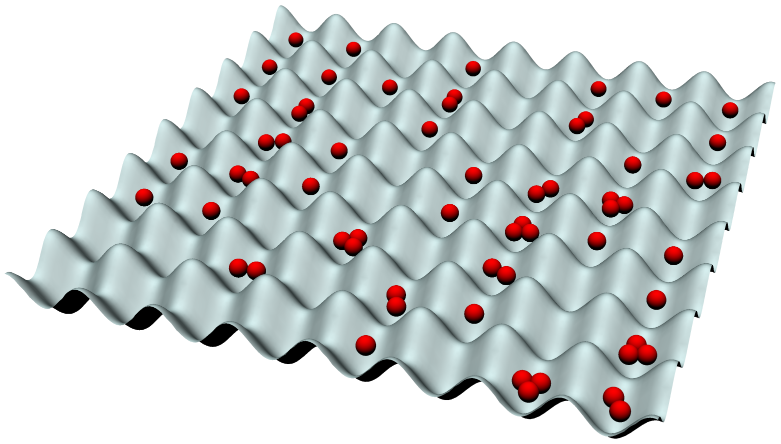
Tensor networks, and coherent and dissipative dynamics of AMO systems

Andrew Daley

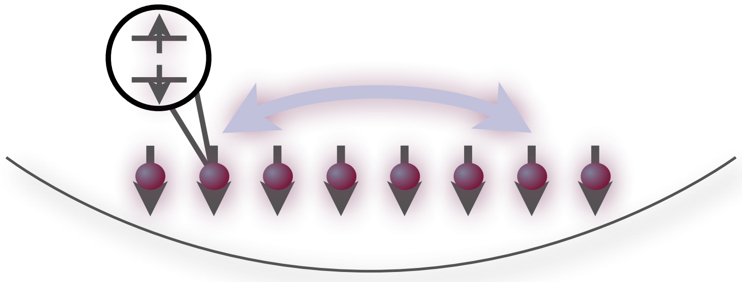
Department of Physics and SUPA
University of Strathclyde

AMO systems for studying many-body physics

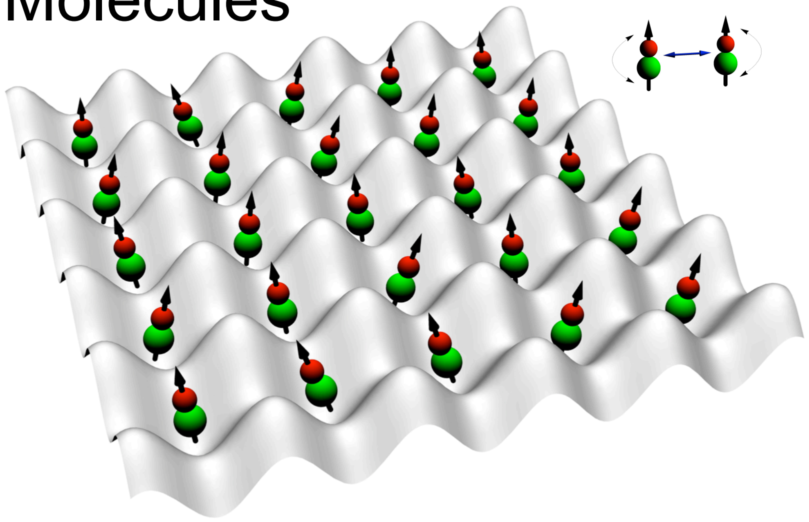
- Atoms



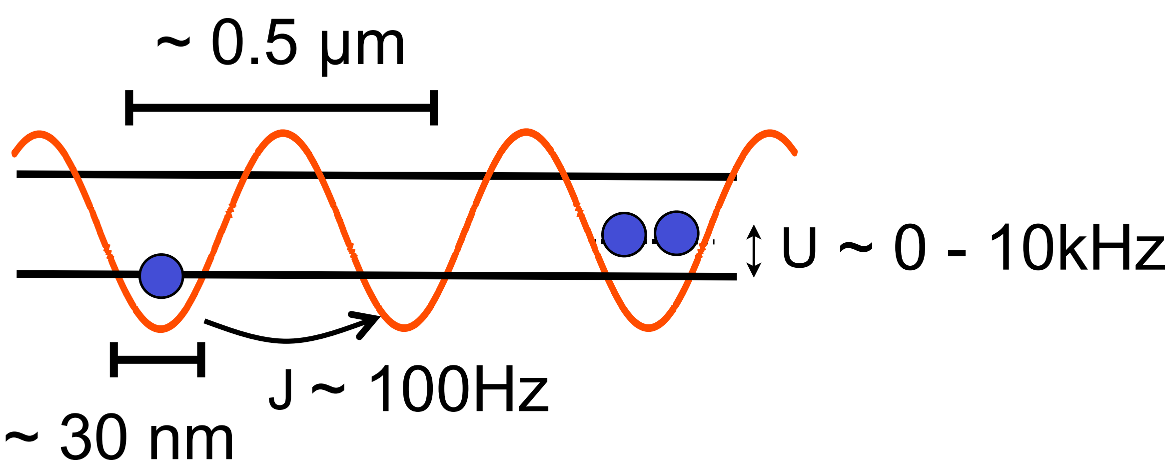
- Ions



- Molecules



e.g., Bose-Hubbard: D. Jaksch et al. PRL ’98



$$H = -J \sum_{\langle i,j \rangle} \hat{b}_i^\dagger \hat{b}_j + \frac{U}{2} \sum_i \hat{n}_i(\hat{n}_i - 1)$$

- Microscopic understanding / control
- Extendable to many well-controlled models
- Study thermodynamics / quantum phases
- Study out of equilibrium dynamics

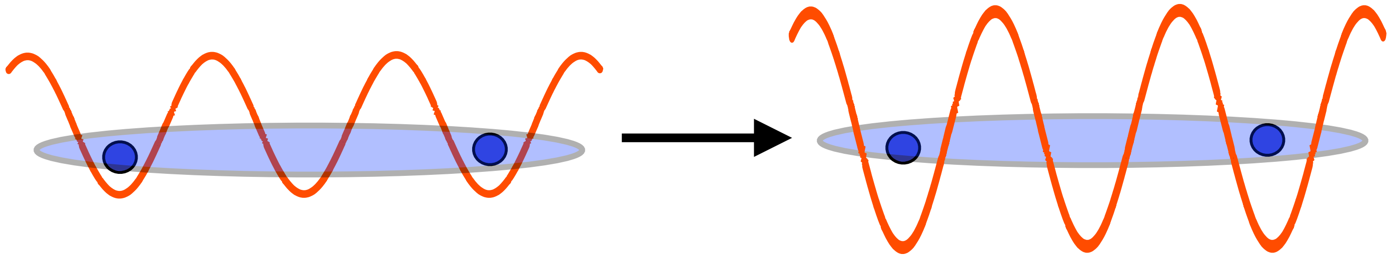
e.g., variable-range Ising model:
D. Porras, J. I. Cirac, PRL ‘04

$$H = \sum_{kl} \frac{\bar{J}}{|k-l|^\alpha} \sigma_k^x \sigma_l^x + B \sum_l \sigma_l^z$$

Experiments – cold gases:
Munich, Zurich, NIST / JQI, MIT, Harvard, Innsbruck, Hamburg, Pisa, Florence, Oxford, Cambridge, Austin, Chicago, Penn State, Kyoto, Toronto, Stony Brook, Paris, Strathclyde, Illinois, Cornell, Stanford, Berkeley, Heidelberg ......

Experiments – ions and molecules:
Maryland, Innsbruck, NIST, JILA, ……

Non-equilibrium dynamics with quantum simulators:



M. Greiner *et al.*, Nature **419**, 51 (2002).
S. Will *et al.*, Nature **465**, 197 (2010).

M. Cheneau *et al.*, Nature **481**, 484 (2012)
J.-S. Bernier *et al.*, PRL **106**, 200601 (2011)

Calabrese, Cardy, Essler, Olshanii, Rigol,……

Läuchli, Kollath, Heidrich-Meissner, Fazio, Montangero, Schollwöck, White, ……

- Millisecond timescales - track+control in real time
- Long coherence times; isolated system

- Intrinsic / fundamental questions

  - Quench Dynamics / correlation spreading / growth of entanglement
  - Thermalisation in quantum systems
  - Behaviour near critical points
  - Emergence of many-body states in driven/dissipative dynamics
  - …

Tensor network methods

Matrix product states

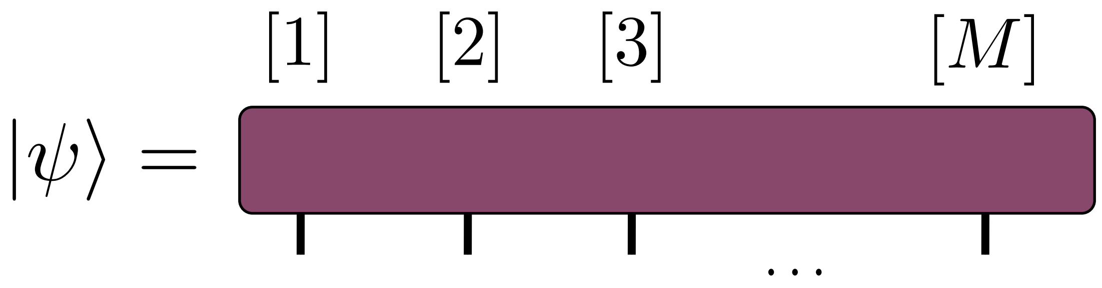
6 particles, 6 sites: 462 states

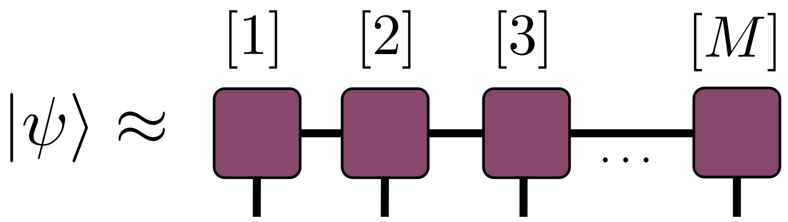
50 particles, 50 sites: 5 x 10^{28} states

$$|\psi\rangle = \sum_{i_1,i_2,\ldots,i_L=1}^{d} c_{i_1 i_2 \ldots i_L} |i_1\rangle_{[1]} \otimes |i_2\rangle_{[2]} \otimes \cdots \otimes |i_L\rangle_{[L]}$$

Full lattice quantum state (M sites)

Matrix product state





d^M-dimensional tensor

D-dimensional matrices

- State coefficients expressed as a product of dMD^2 coefficients

G. Vidal, Phys. Rev. Lett. **91**, 147902 (2003)
G. Vidal, Phys. Rev. Lett. **93**, 040502 (2004)
A. J. Daley et al., J. Stat. Mech. P04005 (2004)
S. R. White and A. E. Feiguin, PRL **93**, 076401 (2004)
F. Verstraete et al., Adv. in Phys. 57, 143 (2008).

Ground state calculations

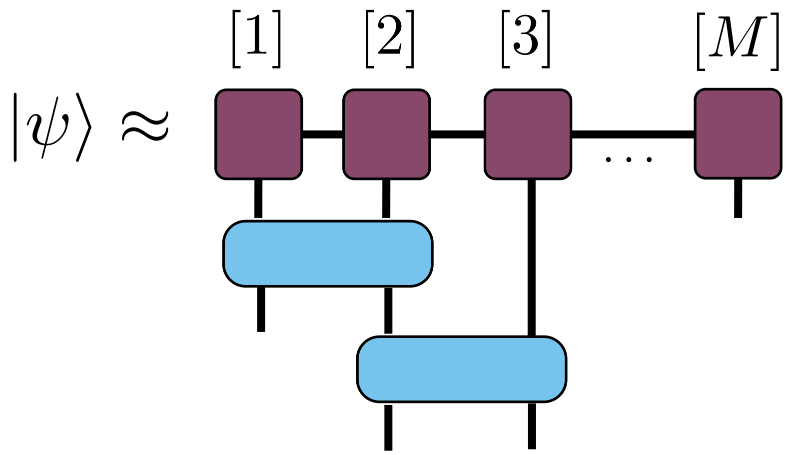
- Density Matrix Renormalisation Group
- Direct tensor optimisation
- Imaginary time evolution

S. R. White, PRL 69, 2863 (1992)

Time evolution

- Time evolution via operations on states, e.g., via Trotter decomposition (Time Evolving Block Decimation algorithm / adaptive time-dependent DMRG)

G. Vidal, Phys. Rev. Lett. **93**, 040502 (2004)
A. J. Daley et al., J. Stat. Mech. P04005 (2004)
S. R. White and A. E. Feiguin, PRL 93, 076401 (2004)



$$H = \sum_i H_{i,i+1}$$

$$\mathrm{e}^{-iH\delta t} = \prod_i \mathrm{e}^{-iH_{i,i+1}\delta t} + O(\delta t^2)$$

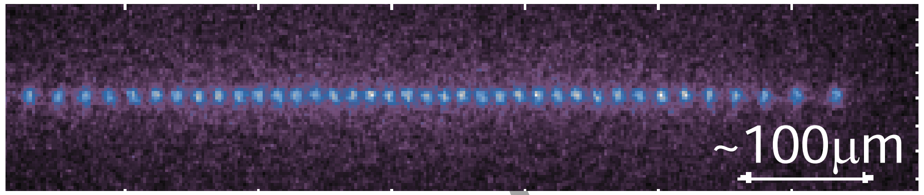
- Also time-dependent variational principle

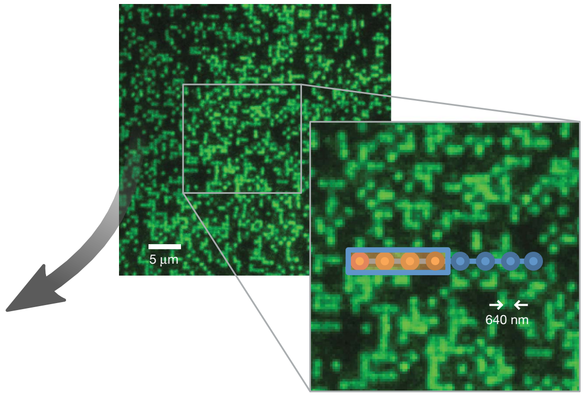
J. Haegeman et al., PRL 107, 070601 (2011)

- Quench dynamics lead to entanglement growth, and limit computations
- Short-time dynamics after a quench, and long time near-adiabatic dynamics computable

Review: U. Schollwöck, Annals of Physics **326**, 96 (2011)

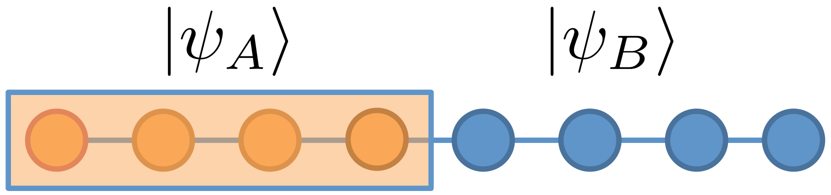
Spatial Entanglement in Many-body states



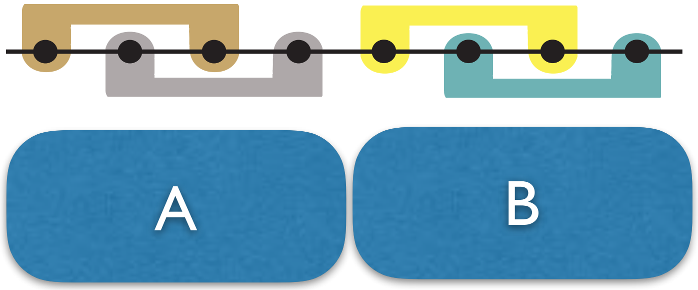


$$|\psi\rangle \neq |\psi_A\rangle \otimes |\psi_B\rangle$$

State with spatial entanglement:



$= |\psi\rangle$



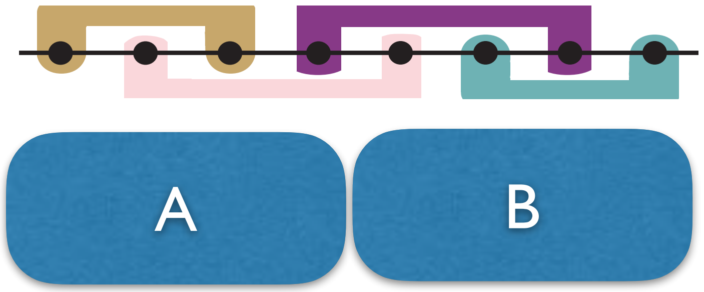
$$|\psi\rangle = |\psi_A\rangle \otimes |\psi_B\rangle$$

$$\rho_A = \mathrm{tr}_B\left(|\psi\rangle\langle\psi|\right)$$

PURE TRACE

Von Neumann entropy

$$S_{\mathrm{vN}}(\rho_A) = -\mathrm{tr}_{\mathrm{A}}\left[\rho_A(\log_2 \rho_A)\right]$$



$$|\psi\rangle \neq |\psi_A\rangle \otimes |\psi_B\rangle$$

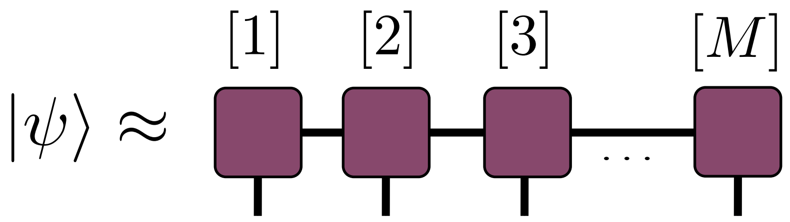
MIXED TRACE

Rényi entropy

$$S_n(\rho_A) = \frac{1}{1-n}\log \mathrm{tr}\{\rho_A^n\}$$

L. Amico, R. Fazio, A. Osterloh and V. Vedral, Rev. Mod. Phys. 80, 517 (2008).
J. Eisert, M. Cramer and M. B. Plenio, Rev. Mod. Phys. 82, 277 (2010).

Entanglement and the matrix product state ansatz

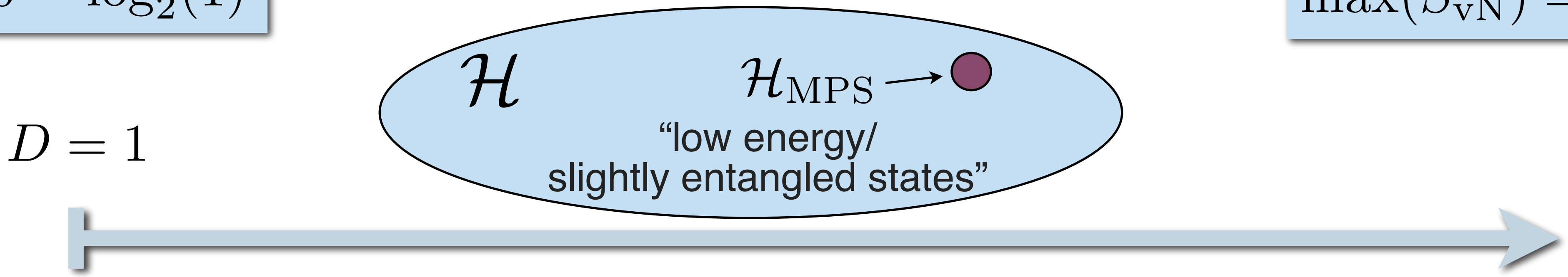


Matrices
$D \times D$

D= matrix/bond dimension

$\max(S_{\rm vN}) = 0 = \log_2(1)$

$\max(S_{\rm vN}) = \log_2(D)$



product state

$\max(S_{\rm vN}) = M/2$

(for spins)

- Matrix product states can represent a state exactly if entanglement is small (necessary condition: von Neumann; sufficient condition: Rényi, order < 1)

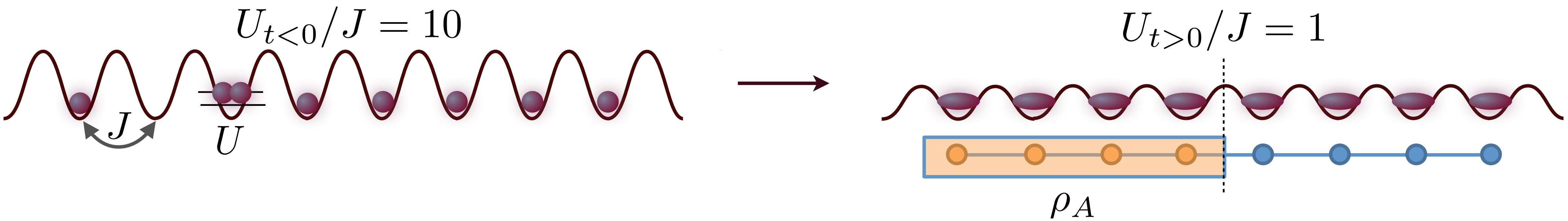
F. Verstraete and J.I. Cirac Phys. Rev. B **73**, 094423 (2006)

N. Schuch, M. M. Wolf, K. G. H. Vollbrecht, and J. I. Cirac, New J. Phys. **10**, 033032 (2008)
N. Schuch, M. M. Wolf, F. Verstraete, and J. I. Cirac, Phys. Rev. Lett. **100**, 030504 (2008)

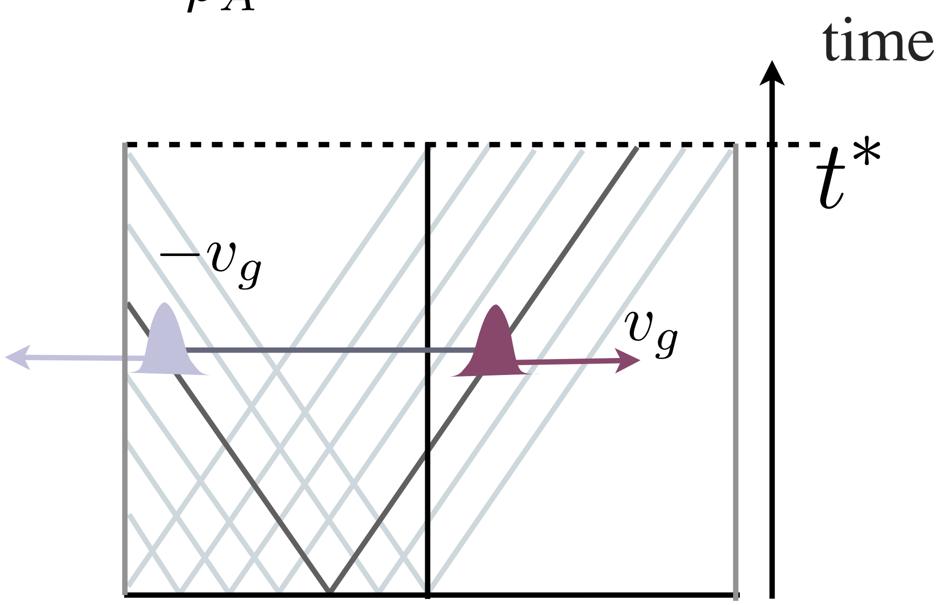
- 1D systems with local Hamiltonians have low ground state entanglement (S bounded in *M* for gapped systems; grows as log(*M*) for critical systems)

Entanglement and quench dynamics (local 1D system)

- Quench experiment for bosons



- Propagation of quasi-particle pairs, velocity limited by Lieb-Robinson bound



E. H. Lieb and D. W. Robinson, Comm. Math. Phys. 28, 251 (1972).

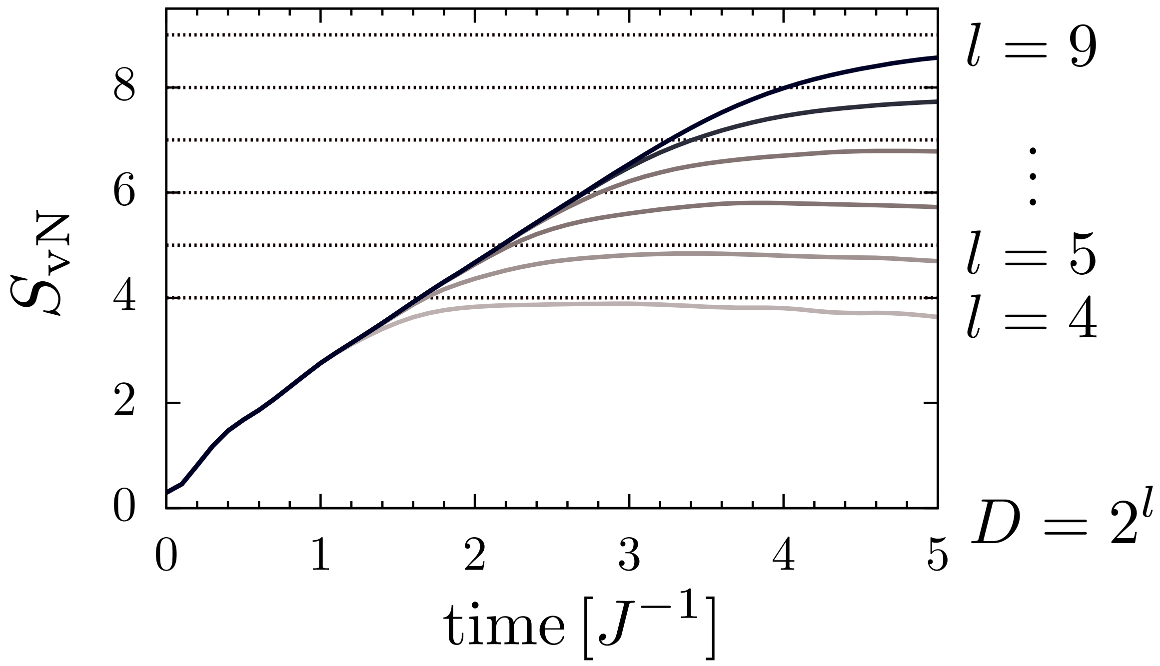
P. Calabrese and J. Cardy, *J. Stat. Mech*, P04010 (2005)

- Linear von Neumann entropy increase

$$\boxed{\max(S_{\rm vN}) = \log_2(D)}$$

  - For exact simulation: $D \propto \exp[ct]$
  - In practice:

D	Runtime:
512	1 day
1024	8 days
2048	2 months

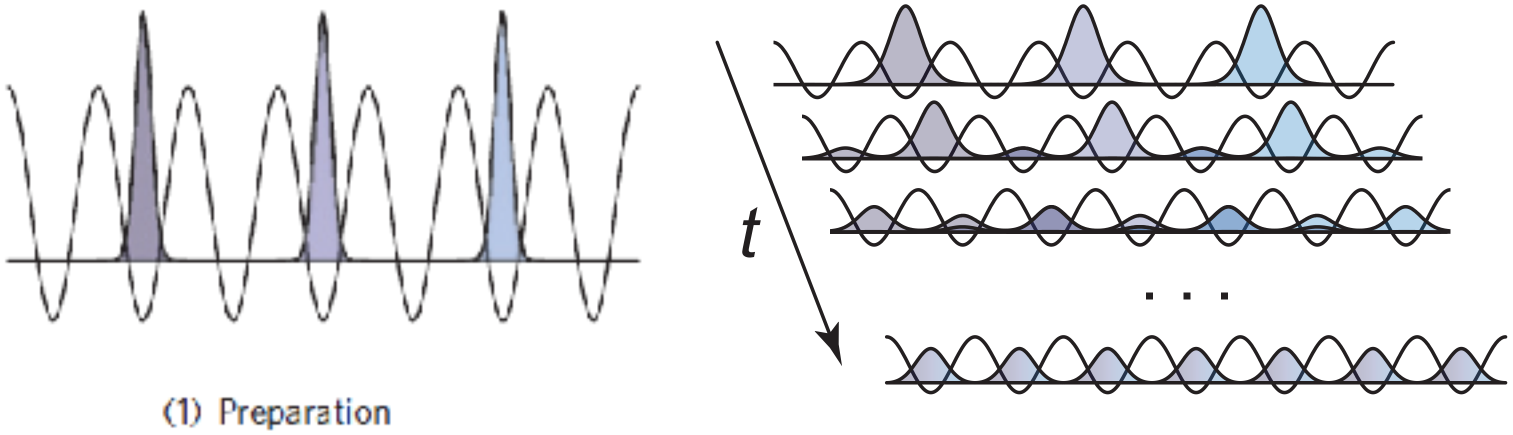


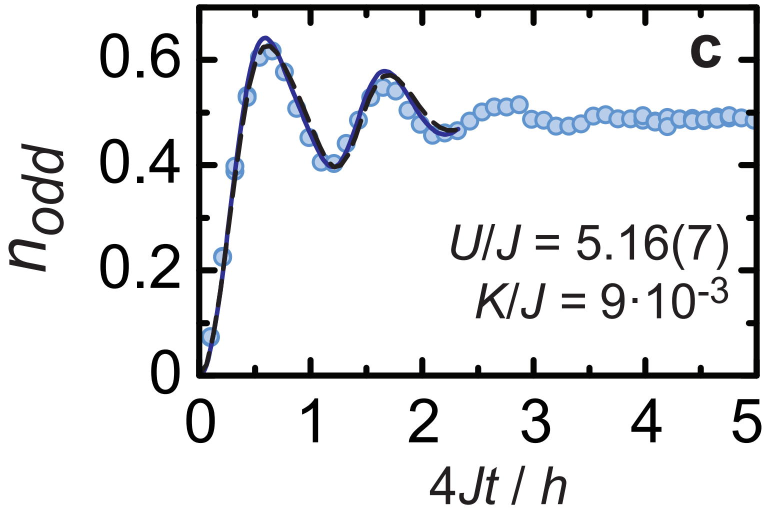
Control over accuracy

- Convergence in the maximum allowed truncation error is used to control validity of the calculation

e.g., experiment vs. t-DMRG
in a quantum quench

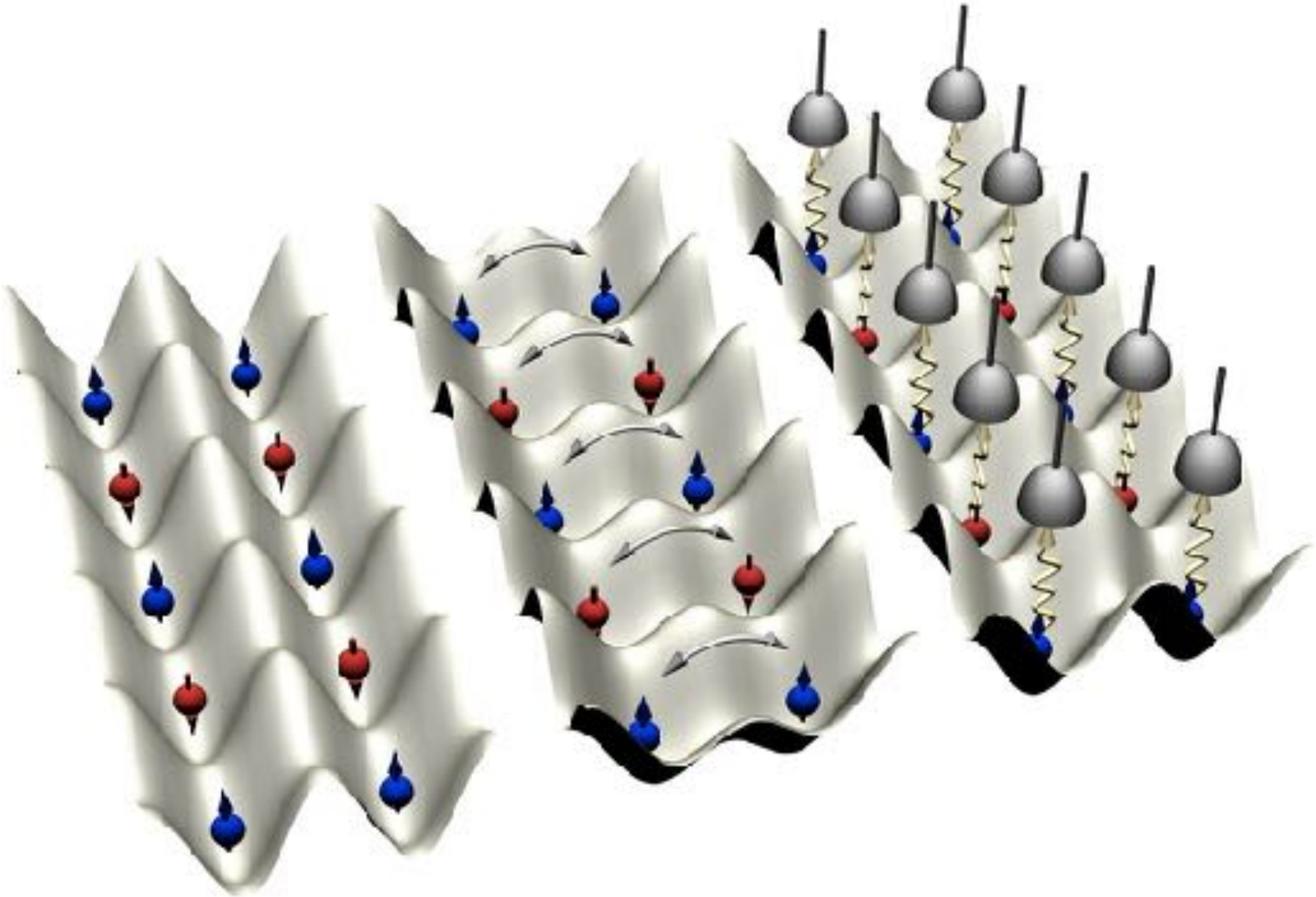
S. Trotzky et al.,
Nature Physics **8**, 325 (2012)

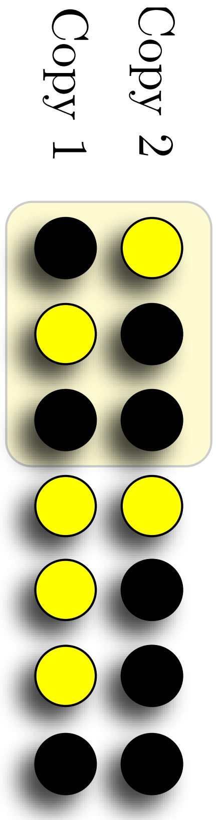




Entanglement growth leads to breakdown of simulation via tensor networks

How can we measure entanglement in an experiment?





- Parallel measurements:
  - Purity of the whole state
  - Entanglement for subsystems

Ingredients:

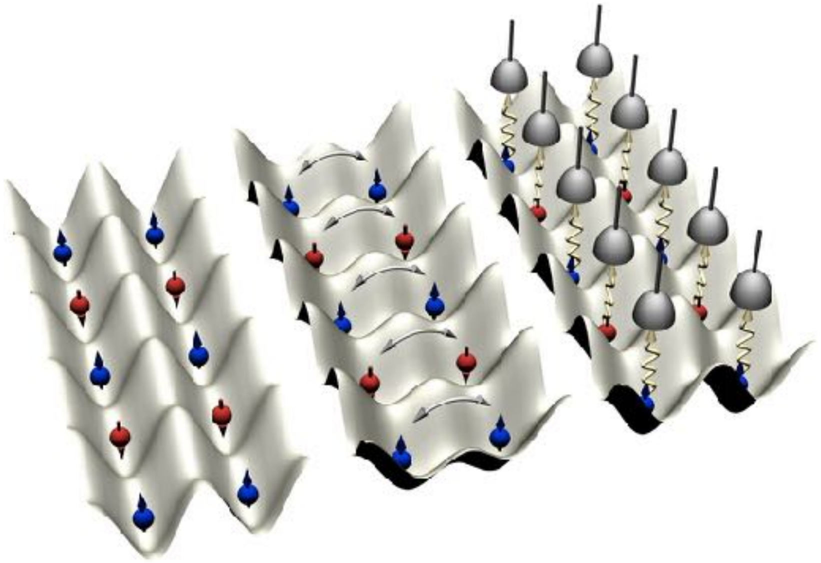
- Multiple copies prepared in low-entropy initial states in 1D tubes or 2D layers
- Coupling between copies
- Local occupation number measurements (quantum gas microscope)

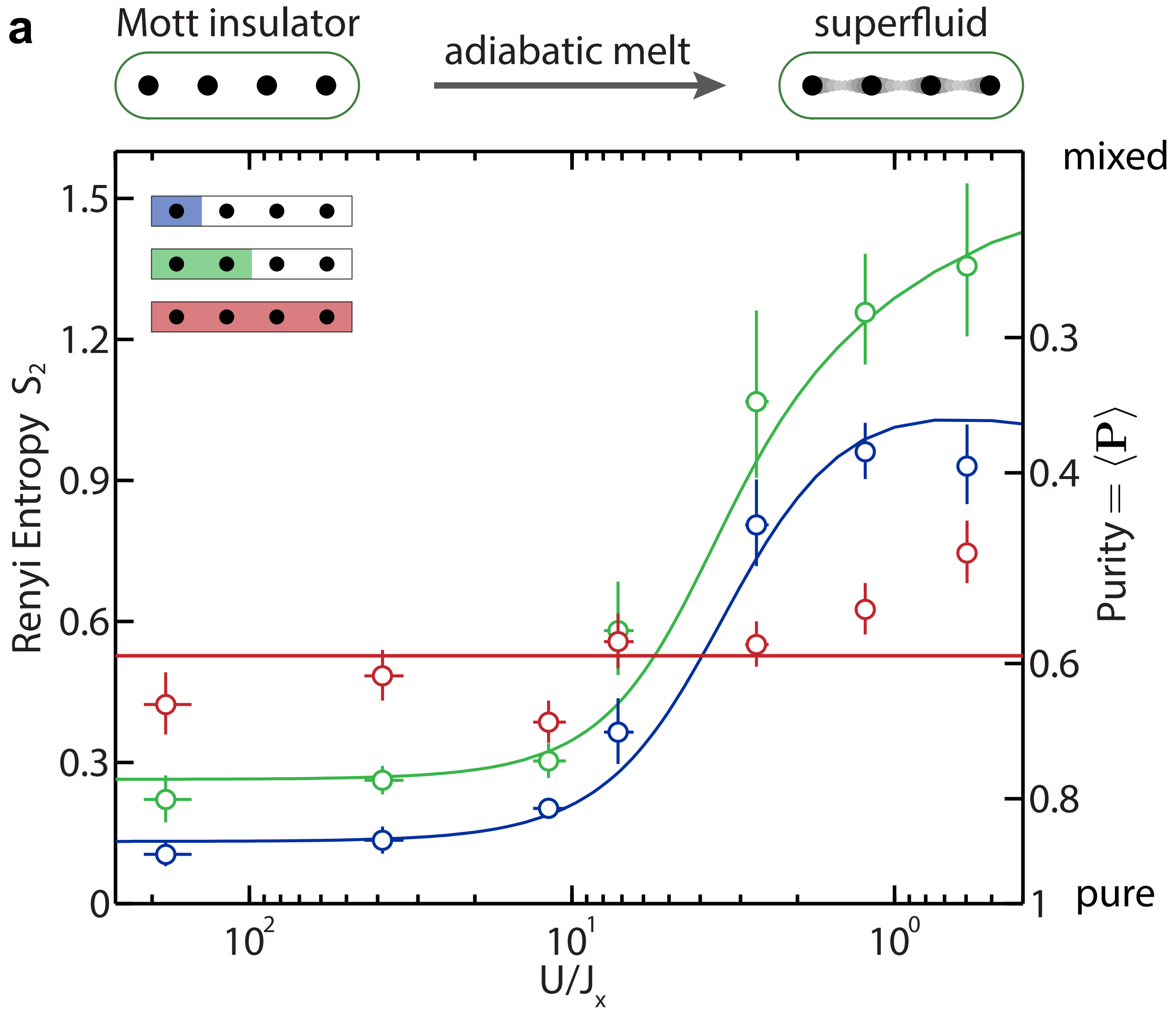
Measure: Purity/consistency of whole state; Renyi entropy of order n using n copies.

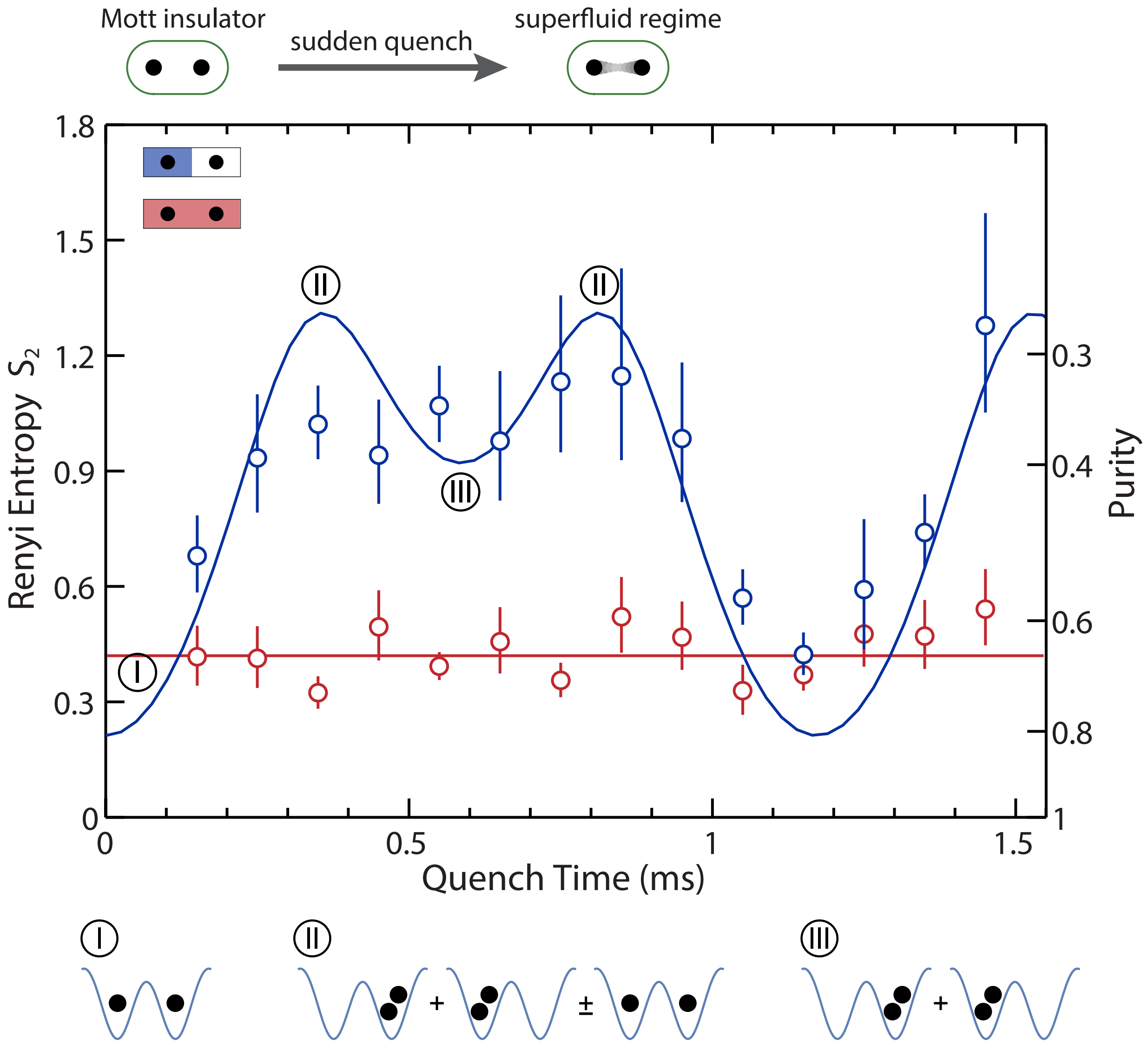
$$S_n(\rho_A) = \frac{1}{1-n}\log \mathrm{tr}\{\rho_A^n\} \leq S_{VN}(\rho_A)$$

Bosons: A. J. Daley, H. Pichler, J. Schachenmayer, P. Zoller, Phys. Rev. Lett. 109, 020505 (2012)
Fermions: H. Pichler, L. Bonnes, A. J. Daley, A. M. Läuchli, and P. Zoller, New J. Phys. 15 063003 (2013)

Experiment: Measurement of entanglement for itinerant bosons in optical lattices

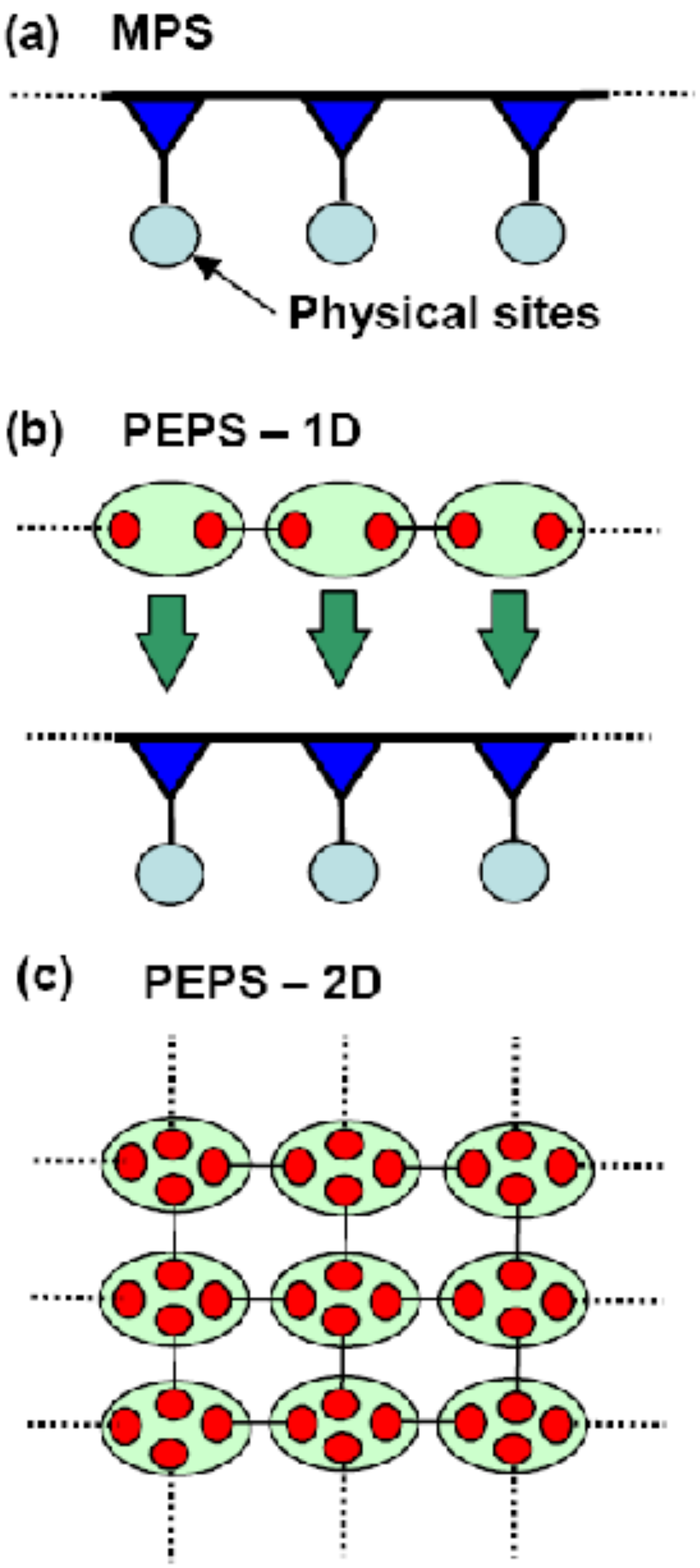


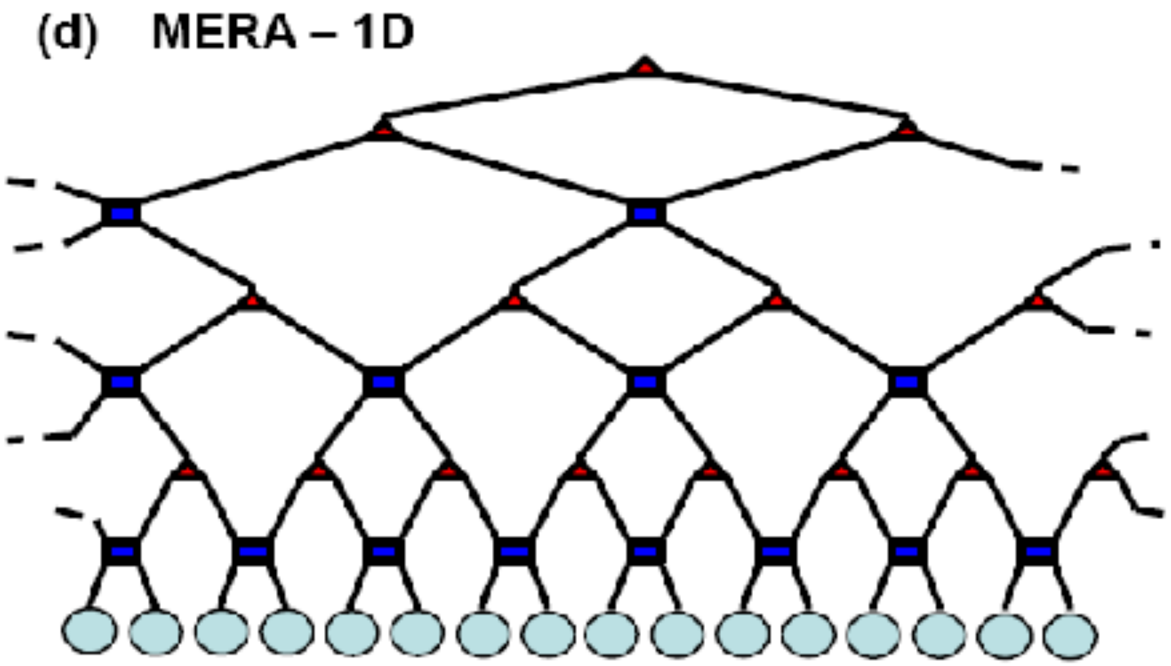




R. Islam et al., arXiv: 1509.01160

More general tensor networks:





G. Vidal Phys. Rev. Lett. 99, 220405 (2007)

- Different state representations, e.g.,
  MERA (G. Vidal) - critical 1D systems / 2D / 3D
  PEPS (F. Verstraete & I. Cirac) - 2D / 3D systems

- Optimisation of states / time-evolution are still numerically very time-consuming

- Example: lowest ground state energy of the tJ model (competing stripe vs. uniform d-wave)

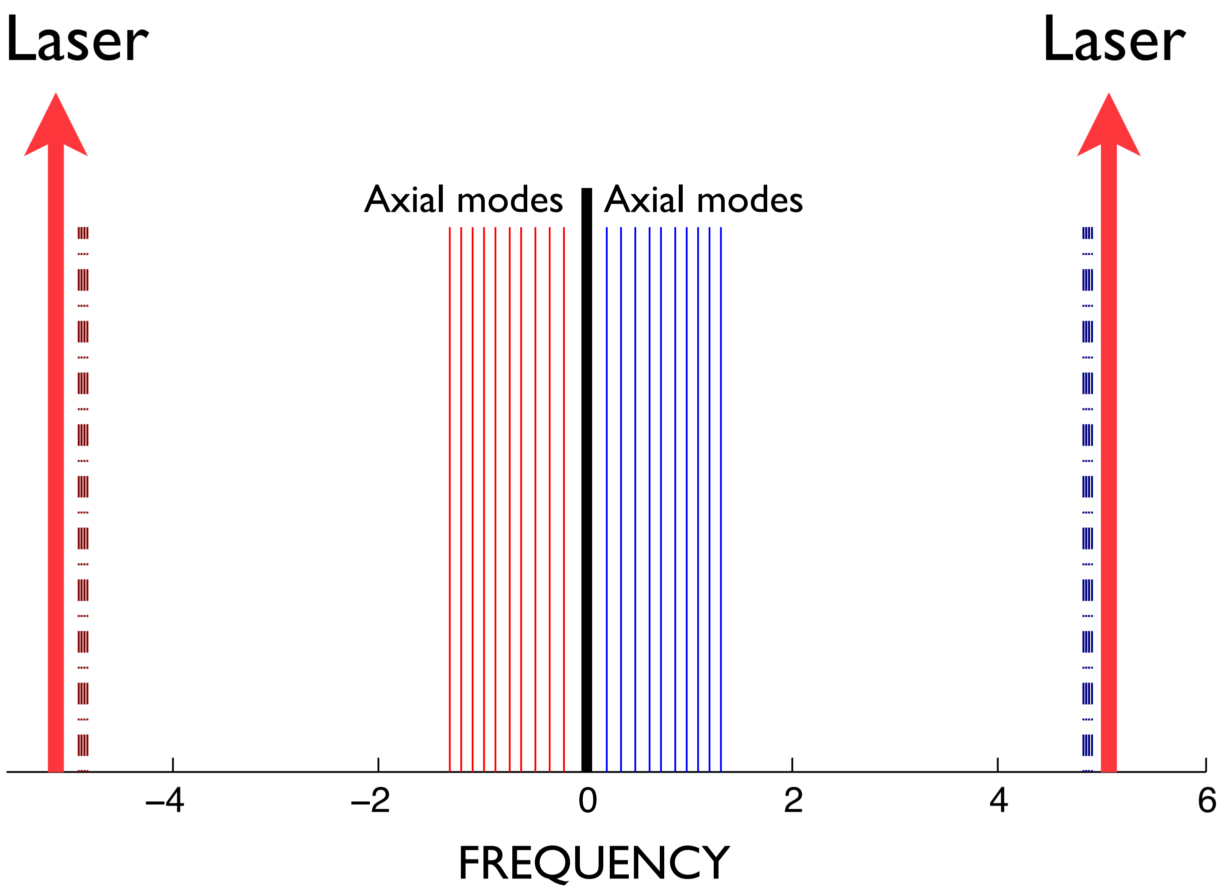
P. Corboz et al., PRL **113**, 046402 (2014)

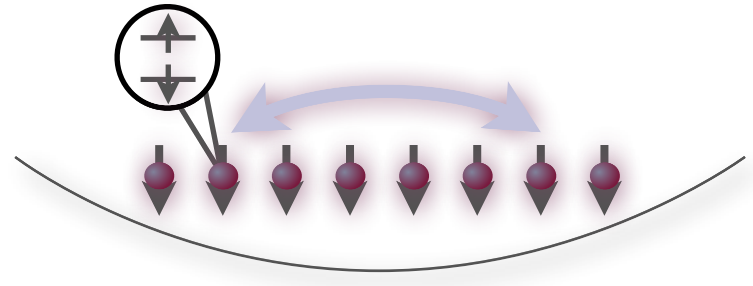
Review: F. Verstraete, V. Murg, and J. I. Cirac, Adv. Phys. **57**, 143 (2008).

Application to long-range interactions

Tuneable-range interactions in ion traps:

State-dependent-force, spin-flip process mediated by coupling many motional modes



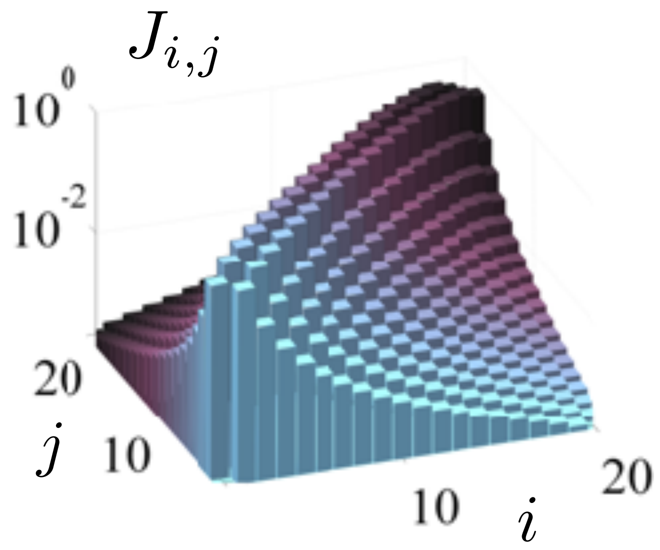


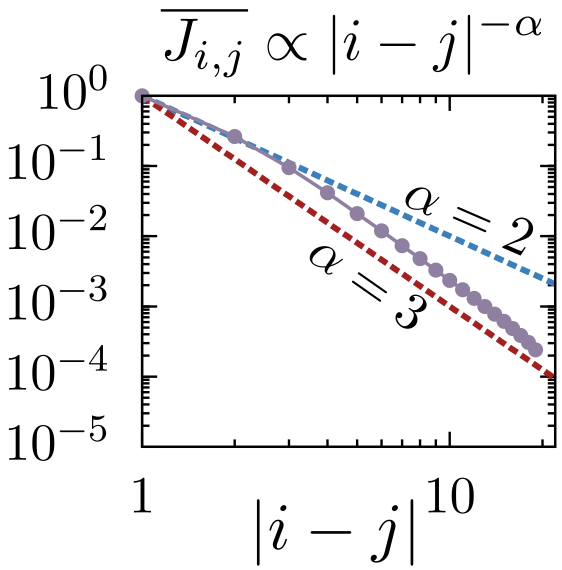
$$H = \sum_{k>l} \frac{\bar{J}}{|k-l|^{\alpha}} \sigma_k^x \sigma_l^x \qquad 0 \leq \alpha < 3$$

- Range determined by detuning (off-resonant contributions from different modes)

- Additional control varying axial confinement
- Long strings, hot axial modes

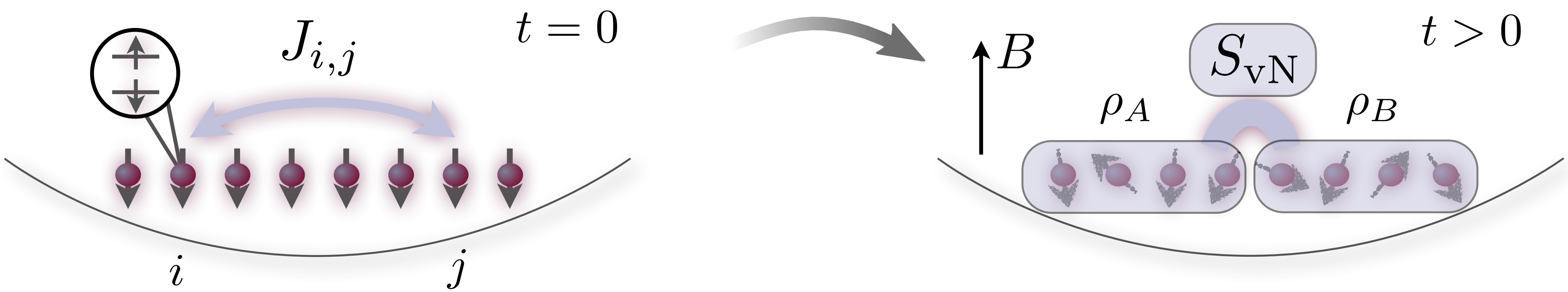
A. Sørensen and K. Mølmer, PRA 62, 022311 (2000)
D. Porras, J. I. Cirac, Phys. Rev. Lett. 92, 207901 (2004)
R. Islam et al, Science, 340, 583 (2013)
JW Britton et al. Nature 484, 489 (2012)
P. Jurcevic et al., Nature 511, 202 (2014)





Quench in an ion trap experiment

- Initial polarised state, then interactions switched on

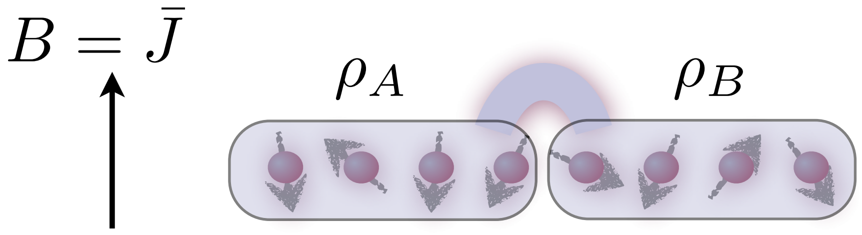


$$H=\sum_{k>l}\frac{\bar{J}}{|k-l|^{\alpha}}\sigma_k^x\sigma_l^x+B\sum_l\sigma_l^z$$

$0 \leq \alpha \leq 3$

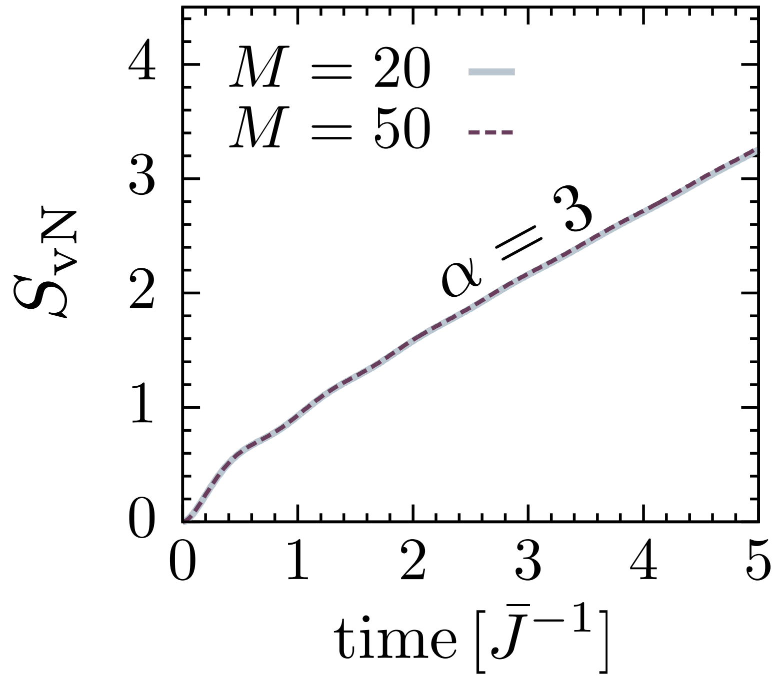
J. Schachenmayer et al., Phys. Rev. X **3**, 031015 (2013)
A. Buyskikh et al., Phys. Rev. A **93**, 053620 (2016)

Entanglement growth across bipartite splitting



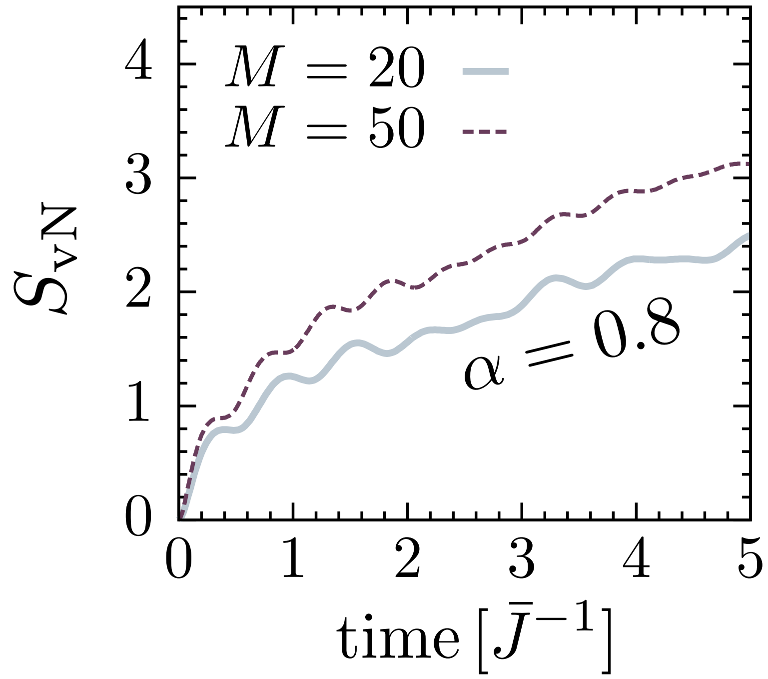
$\alpha \gtrsim 1$

linear increase

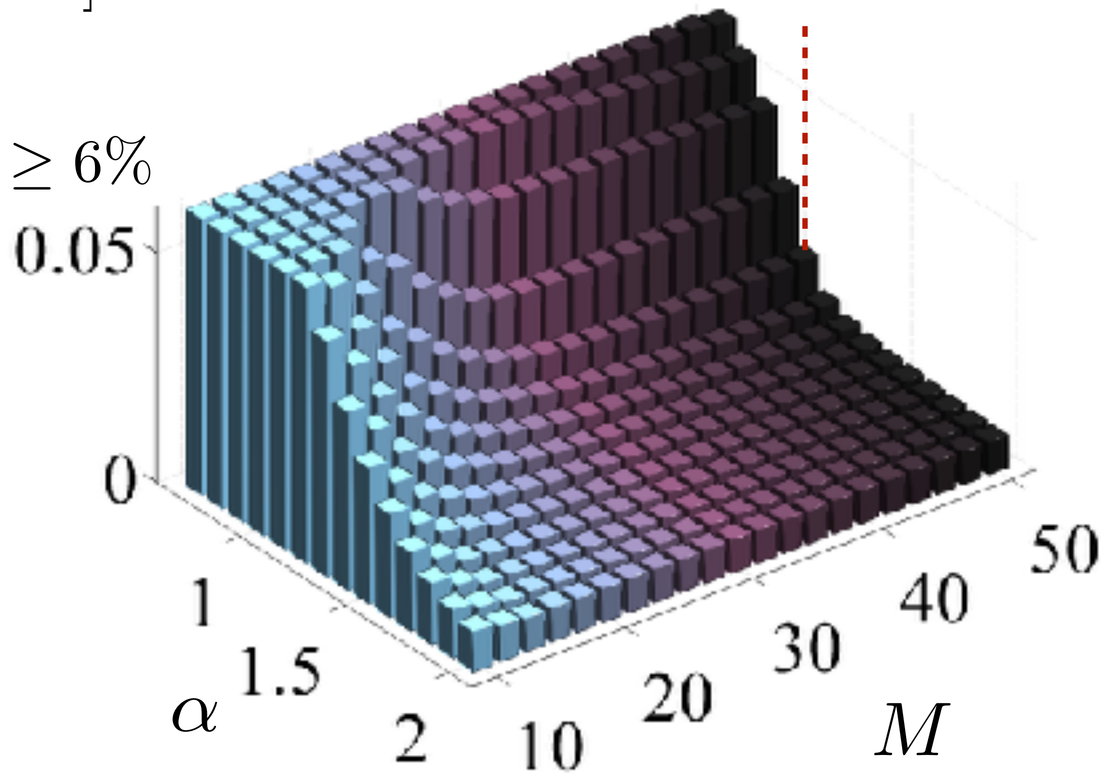


non-linear increase

$\alpha \lesssim 1$



Error of linear fit:



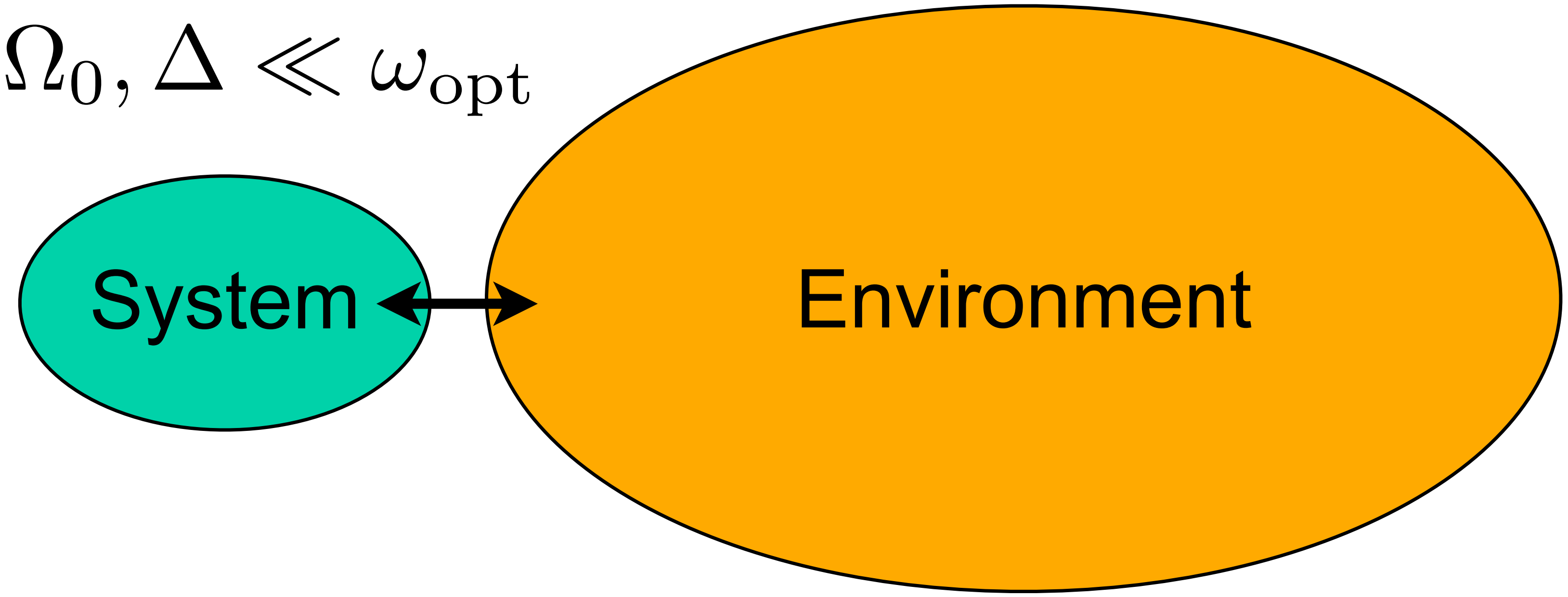
Logarithmic?
Algebraic?

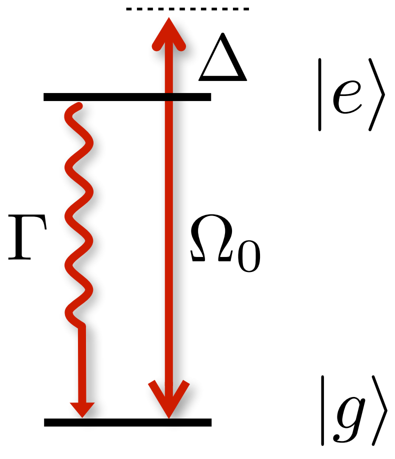
Open quantum systems

A. J. Daley, Advances in Physics 63, 77 (2014)

Dissipative dynamics / open many-body quantum systems:

$$\Gamma, \Omega_0, \Delta \ll \omega_{\mathrm{opt}}$$





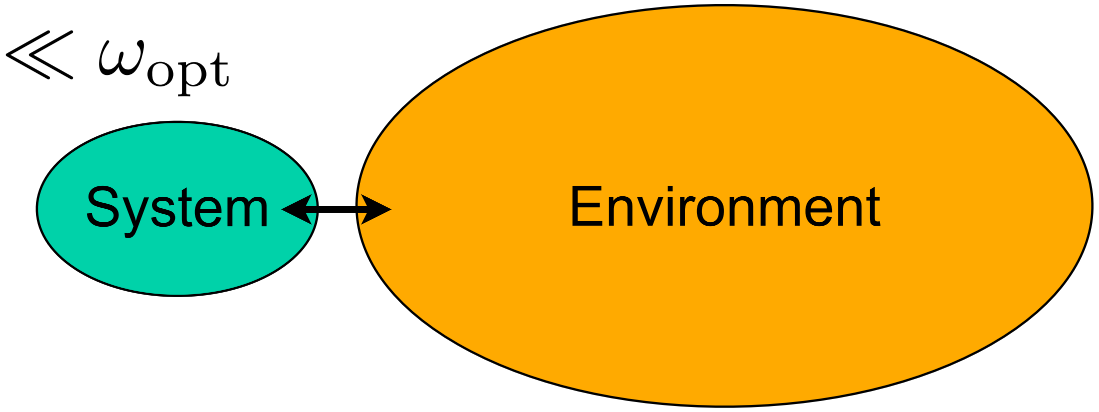
Analogies to quantum optics in many-body systems:

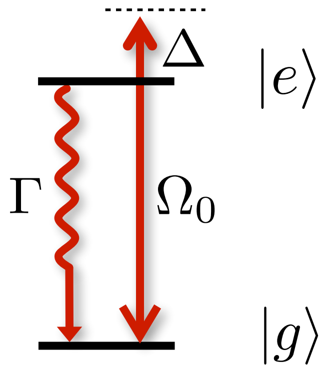
- Quantum Optics description - microscopic models, well-controlled approximations (master equation, quantum stochastic Schrödinger equations)
- Quantum Optics tools (laser cooling, optical pumping / dissipative preparation)

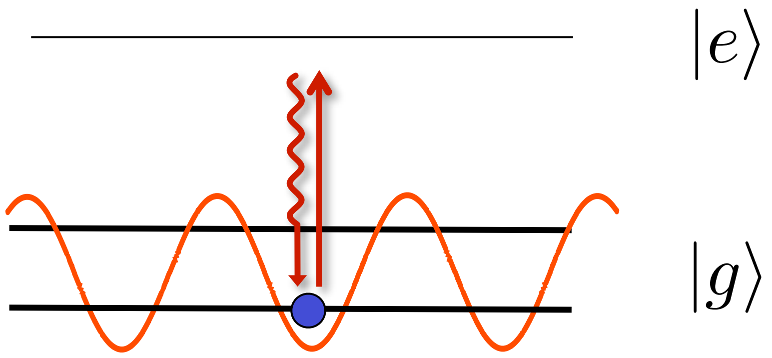
REVIEWS: A. J. Daley, Advances in Physics **63**, 77 (2014)
M. Müller, S. Diehl, G. Pupillo, and P. Zoller, Adv. At. Mol. Opt. Phys **61**, 1 (2012)

Dissipative dynamics / open many-body quantum systems:

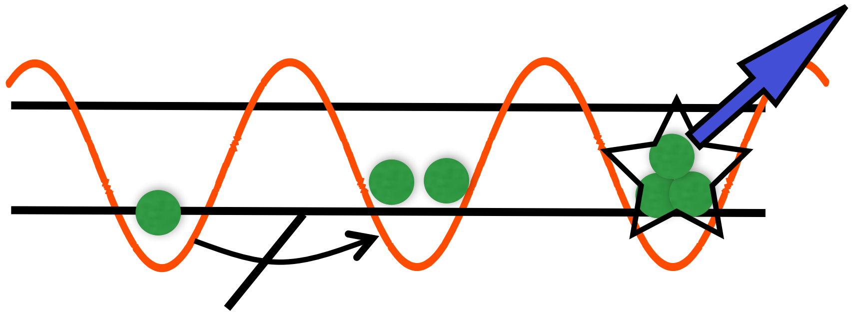
$$\Gamma, \Omega_0, \Delta \ll \omega_{\mathrm{opt}}$$

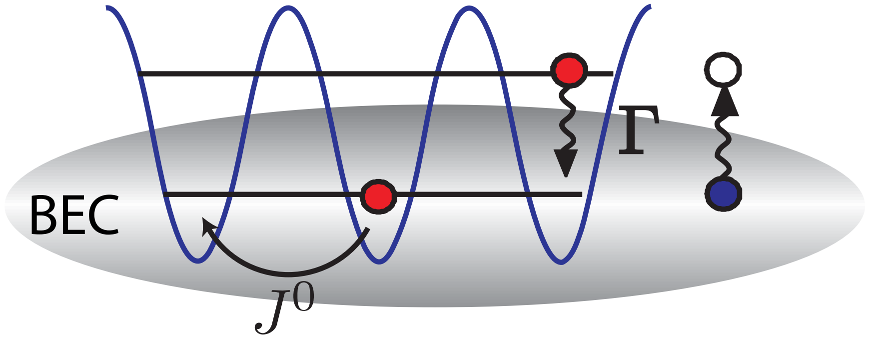






H. Pichler, A. J. Daley, and P. Zoller, PRA **82**, 063605 (2010)
S. Sarkar, S. Langer, J. Schachenmayer, and A. J. Daley, PRA. 90, 023618 (2014)
J. Schachenmayer, L. Pollet, M. Troyer, and A. J. Daley, PRA 89, 011601(R) (2014)





Two-body loss experiments: Rempe group (2008); Jin/Ye (2013) De Marco group (2014); Oberthaler group (2013); Porto/Rolston

Three-body loss:
A. J. Daley et al., PRL **102**, 040402 (2009)
A. Kantian et al., A. J. Daley, PRL **103**, 240401 (2009)

Single atom or Dark state cooling:
A. J. Daley et al., PRA **69**, 022306 (2004)
A. Griessner et al., PRL **97**, 220403 (2006)

REVIEWS: A. J. Daley, Advances in Physics **63**, 77 (2014)
M. Müller, S. Diehl, G. Pupillo, and P. Zoller, Adv. At. Mol. Opt. Phys **61**, 1 (2012)

Spontaneous emissions in optical lattices

- Master equation (Born/Markov)
- Adiabatic elimination of excited state

For single particle version, see:
J. P. Gordon and A. Ashkin, PRA **21,** 1606 (1980)
F. Gerbier and Y. Castin, PRA **82,** 013615 (2010)

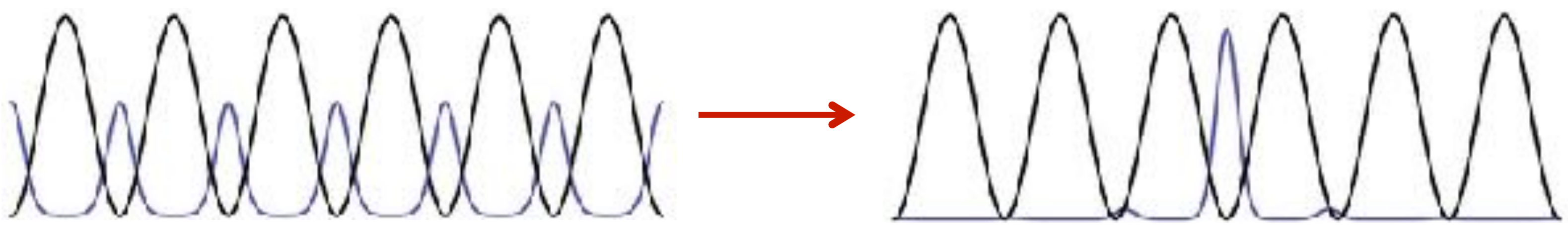
$$\dot{\rho} = -i\left[\hat{H},\rho\right] - \frac{1}{2}\frac{\Gamma}{4\Delta^2}\sum_{\mu}|\Omega_{0,\mu}|^2\int d^3x\int d^3y F_{\mathbf{e}_\mu}(k(\mathbf{x}-\mathbf{y}))\epsilon_\mu(\mathbf{x})\epsilon_\mu(\mathbf{y})\left[\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}(\mathbf{x}),\left[\hat{\psi}^\dagger(\mathbf{y})\hat{\psi}(\mathbf{y}),\rho\right]\right]$$

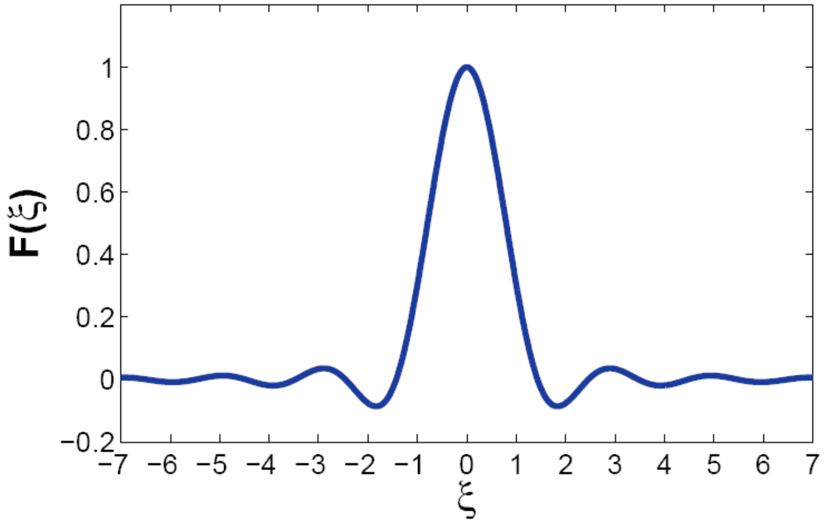
Many-body Hamiltonian
(including optical potential)

multiple beams

bosonic field operator

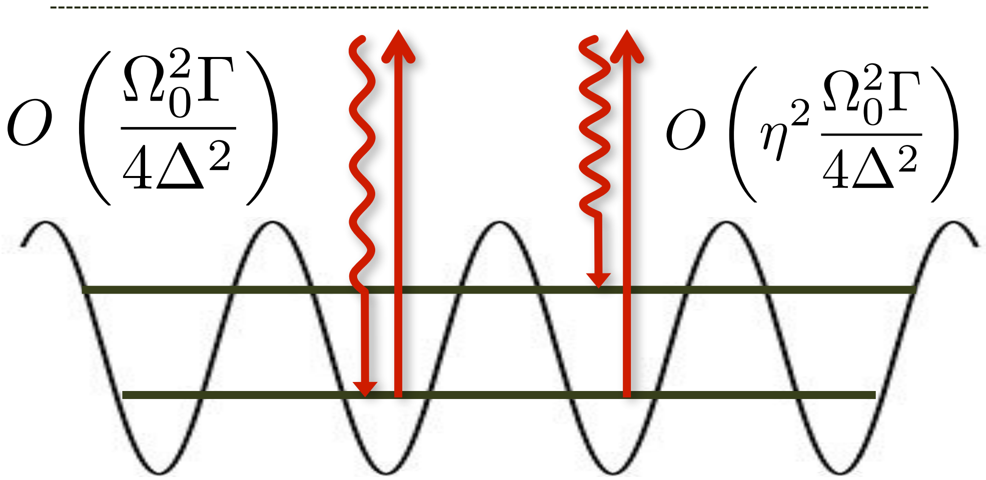
- Localization (position measurement) on scale of wavelength





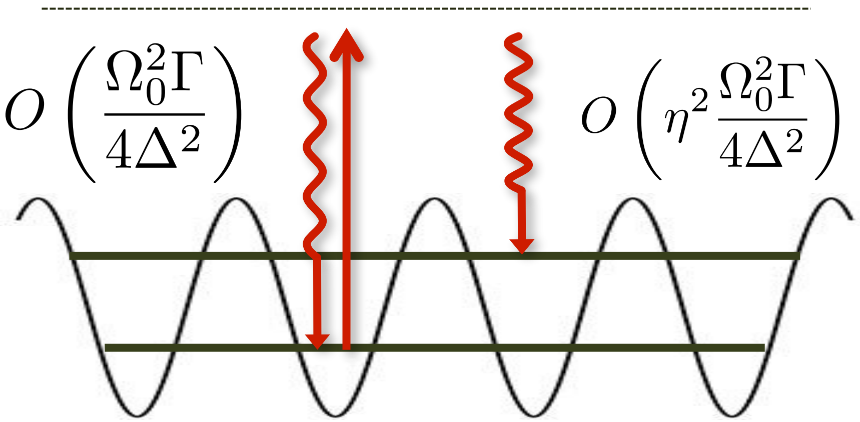
- Transfer to higher bands [measurement within site] suppressed by Lamb-Dicke factor

$$\Gamma_{\rm eff} = \frac{\Omega_0^2}{4\Delta^2}\Gamma \qquad \eta = \frac{\pi a_0}{a} = \left(\frac{1}{4V/E_R}\right)^{1/4}$$



H. Pichler, A. J. Daley, P. Zoller, PRA **82**, 063605 (2010)

Role of thermalisation in heating



- Total rate of energy increase

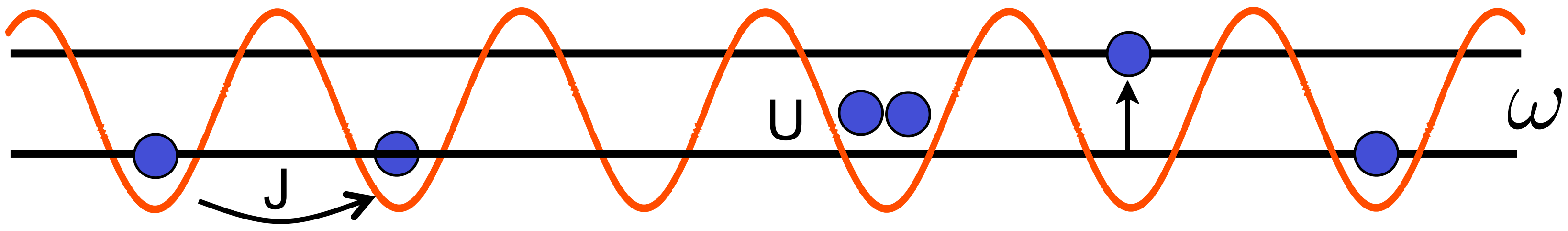
$$\frac{d\langle\hat{H}\rangle}{dt} = \frac{\Omega_0^2\Gamma}{4\Delta^2}E_R N_{tot} = \gamma E_R N_{tot}$$

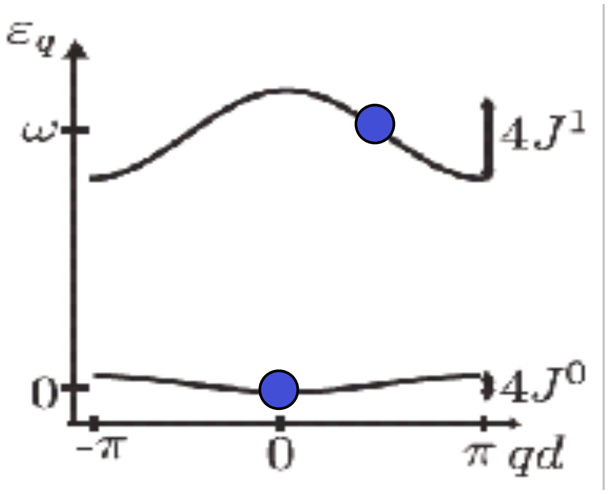
recoil energy

number of atoms

- But the system will **not thermalise on experimental timescales**

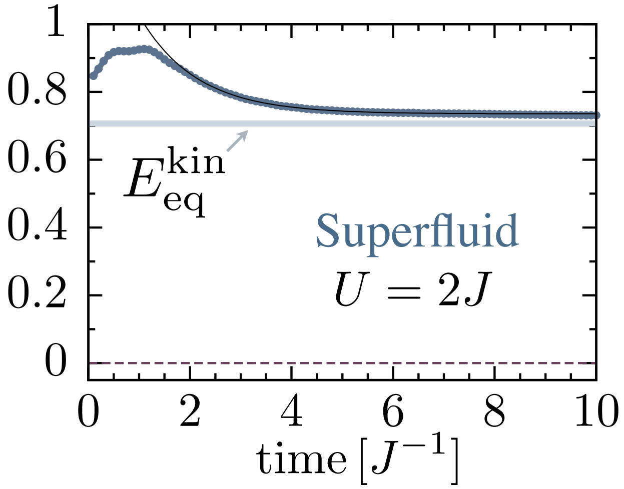
$$\omega \gg U, J$$

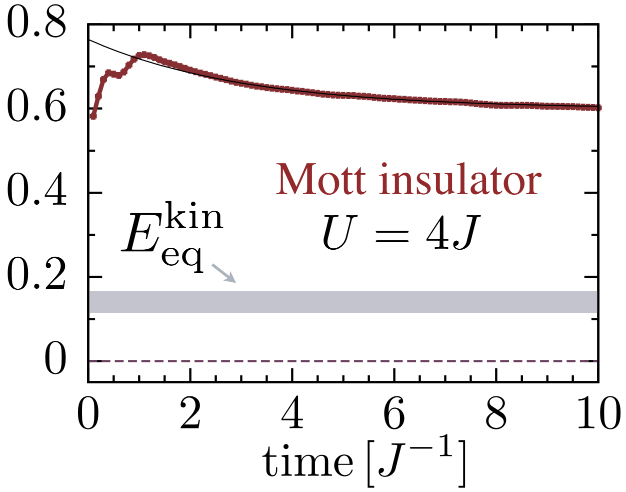




- Within a band, thermalises sometimes

J. Schachenmayer, L. Pollet, M. Troyer,
and A. J. Daley, PRA **89**, 011601(R) (2014)





- Need to consider full time-dependent dynamics

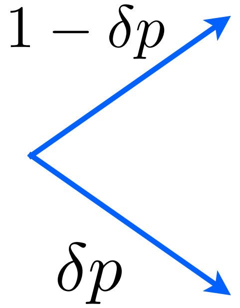
Time-dependent dynamics in 1D: t-DMRG + Quantum Trajectories

$$\dot{\rho} = -i[H,\rho] - \frac{\Gamma}{2}\sum_m \left[c_m^\dagger c_m \rho + \rho c_m^\dagger c_m - 2 c_m \rho c_m^\dagger\right]$$

- Quantum trajectories (or the Monte-Carlo Wavefunction method) was developed to compute dynamics described by master equations via propagation of pure states

H. Carmichael, *An Open Systems Approach to Quantum Optics*
K. Mølmer, J. Dalibard, Y. Castin, JOSA B **10**, 524 (1993)
R. Dum *et al.*, PRA **46**, 4382 (1992)

- Simple (first-order) version [arbitrary-order possible]:
  Evolve stochastic trajectories (states) with two possible operations per timestep:



- Evolution under

$$H_{\text{eff}} = H - i\frac{\Gamma}{2}\sum_m c_m^\dagger c_m$$

$$\begin{aligned}\delta p &= \delta t\langle\phi(t)|i(H_{\text{eff}} - H_{\text{eff}}^\dagger)|\phi(t)\rangle \\ &= \delta t\sum_m \langle\phi(t)|c_m^\dagger c_m|\phi(t)\rangle = \sum_m \delta p_m\end{aligned}$$

- Quantum Jumps (after appropriate stochastic sampling of *m*)

$$|\psi\rangle = \frac{c_m|\psi\rangle}{||c_m|\psi\rangle||}$$

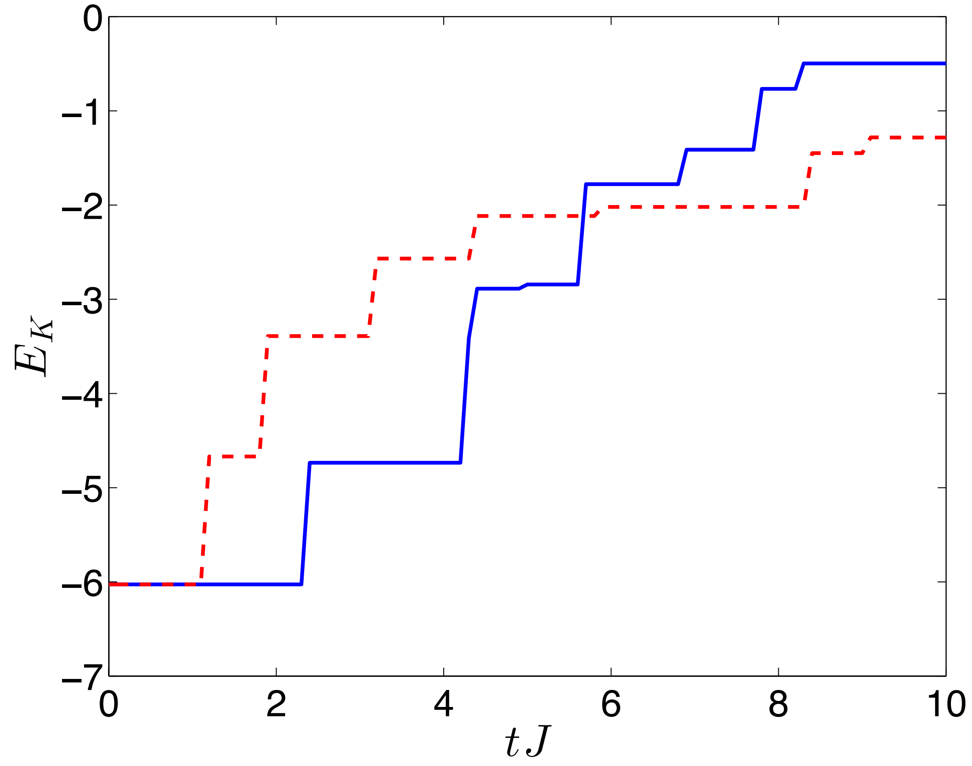
$$\Pi_m = \delta p_m/\delta p$$

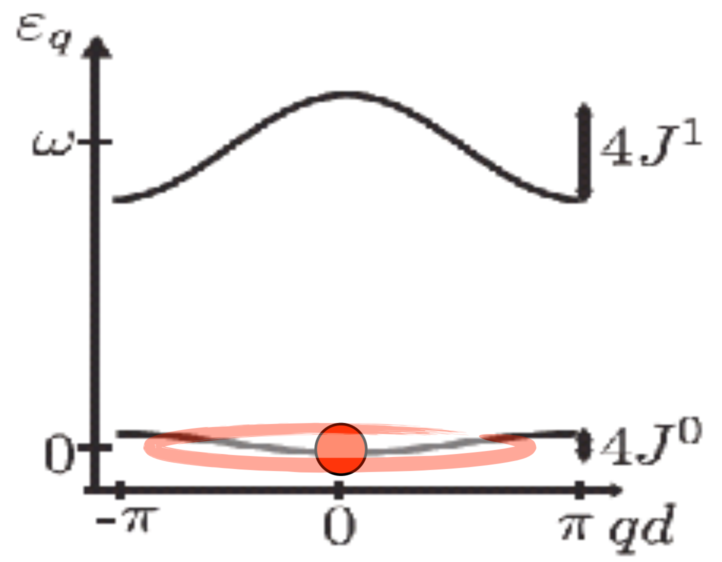
- Expectation values by stochastic average.
- Trade-off: Smaller local Hilbert space vs. trajectory averages

A. J. Daley et al., Phys. Rev. Lett **102**, 040402 (2009).

Simple example of quantum trajectories averaging

- Example trajectories: heating of hard-core bosons, $U/J \rightarrow \infty$
  - kinetic energy:

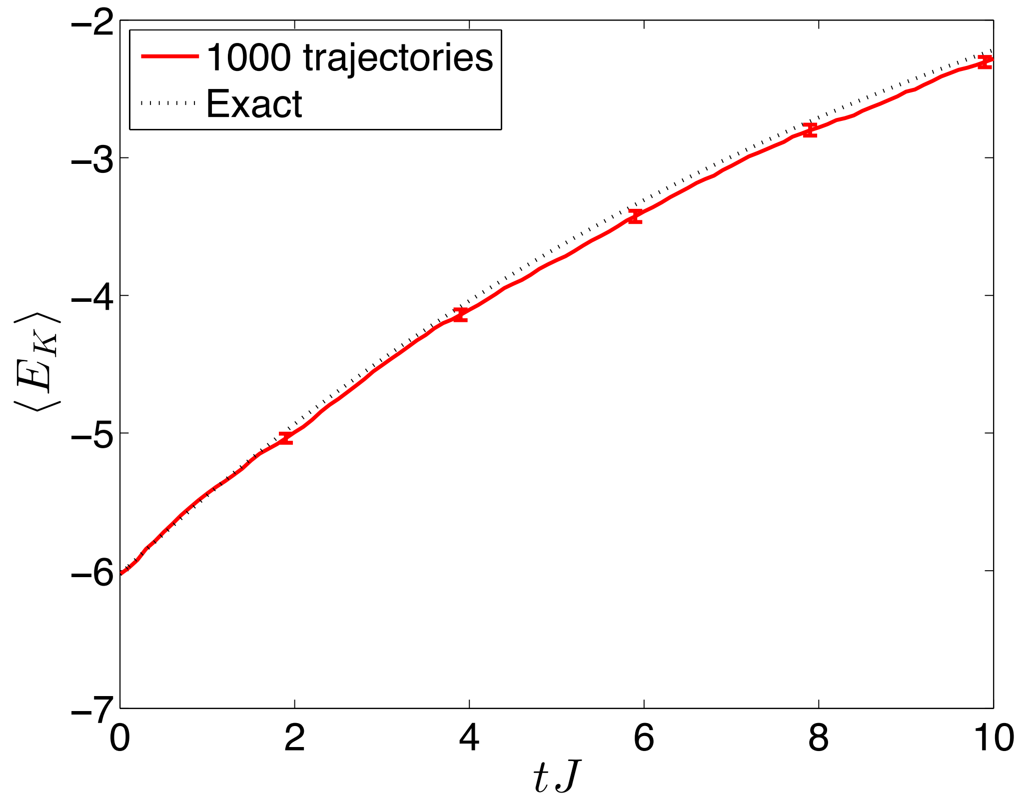




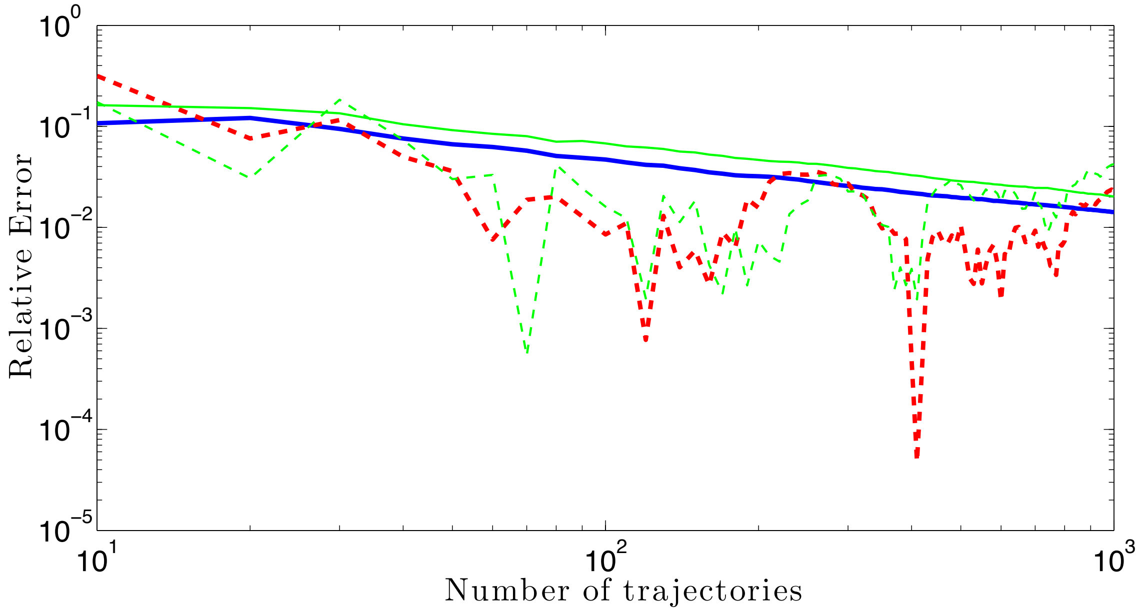
$$\dot{\rho} = -\frac{i}{\hbar}[H, \rho] + \mathcal{L}_1 \rho$$

$$\mathcal{L}_1 \rho = \frac{\gamma}{2} \sum_i (2 n_i \rho n_i - n_i n_i \rho - \rho n_i n_i)$$

- Averaged trajectories vs exact solutions



- Statistical error and discrepancy to exact results ($1/\sqrt{N}$)



A. J. Daley, Advances in Physics 63, 77 (2014)

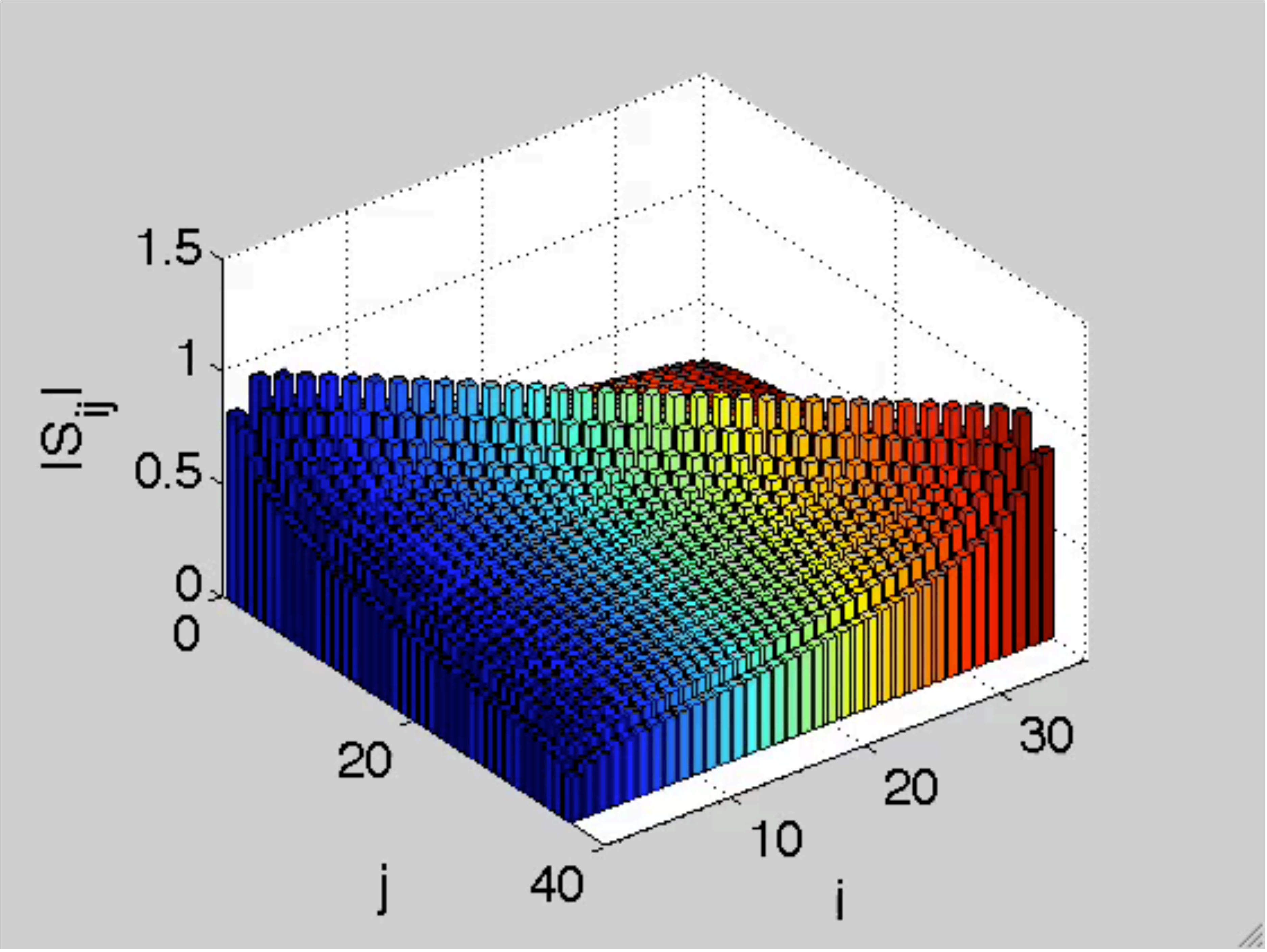
Decay of characteristic correlation functions

- Solve master equation in lowest band via t-DMRG + quantum trajectories

A. J. Daley, Advances in Physics **63**, 77 (2014)

$\langle b_i^\dagger b_j \rangle$

36 sites
36 atoms
U/J=3, Γ = 0.01J
TJ=30



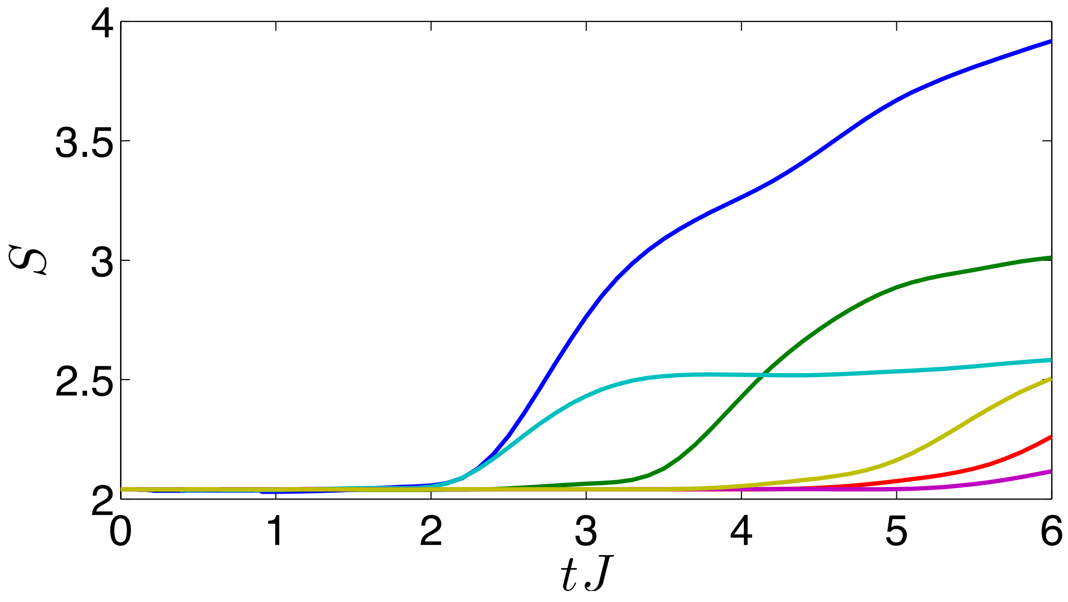
- Long-range correlations in Superfluid strongly affected, Mott Insulator relatively robust
- Decay proportional to scattering rate (worse for red detuning)

H. Pichler, A. J. Daley, P. Zoller, PRA **82**, 063605 (2010)

Computational costs

- Sampling over trajectories
- Requirement of large D to represent large entanglement
- Often mixed states can have less entanglement than pure-state trajectories

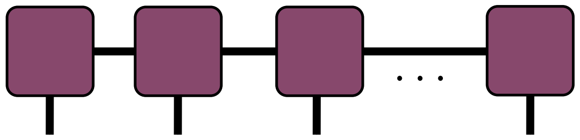
Von Neumann Entropy (split in centre), typical trajectories:



Alternative: represent the density matrix directly

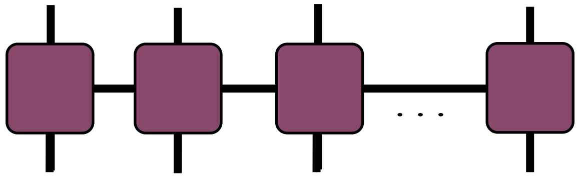
Matrix product state

$|\psi\rangle \approx$



Matrix product operator (density operator)

$\rho \approx$

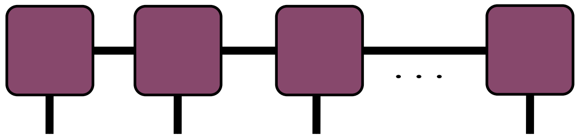
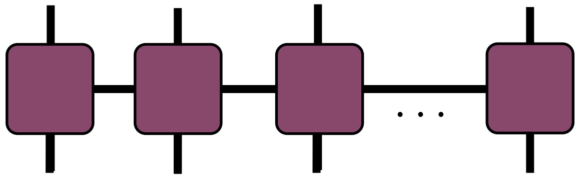


F. Verstraete, J.J. García-Ripoll, and J.I. Cirac, PRL **93**, 207204 (2004)
M. Zwolak and G. Vidal, PRL **93,** 207205 (2004)
F. Verstraete et al., Adv. Phys. **57**, 143 (2008).

S. Montangero, J. Eisert et al.,
M.-C. Banuls, J. I. Cirac et al.,
M. Plenio et al.

See the talks by P. Silvi and M.-C. Bañuls

t-DMRG + trajectories vs. Matrix Product Density Operators

$\|\psi\rangle \approx$ 	$\rho \approx$ 
• Local Hilbert space dimension *d*	• Local Hilbert space dimension d^2
• MPS bond dimension doesn't represent classical correlations (trajectory average)	• MPS bond dimension increases to represent classical correlations
• Code parallelisation with perfect scaling	• Code sometimes difficult to parallelise
• With right choice of unravelling, can exhibit symmetries not present in the density operator	• Often has more limited symmetries than the pure-state trajectories
• Local jumps can lead to entanglement growth, entanglement can be artificially enhanced [optimise?]	• Mixed states will often have smaller actual entanglement
• Need to average stochastic trajectories, statistical errors smaller for global quantities	• Answer obtained without stochastic averages
	• Questions surrounding positivity

Review: A. J. Daley, Advances in Physics 63, 77 (2014)

Anton Buyskikh
Saubhik Sarkar
Guanglei Xu
Jorge Yago
Rosaria Lena

Suzanne McEndoo
Alexandre Tacla
Araceli Venegas Gomez
Samantha Hume
Ella Wylie
Malcolm Jardine

Johannes Schachenmayer (JILA)

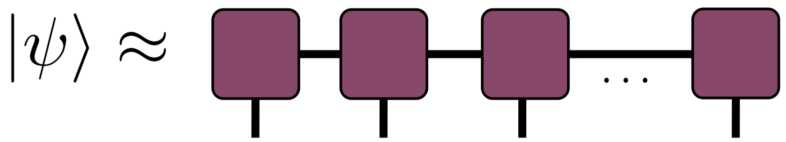
Hannes Pichler (Harvard)
Peter Zoller (Innsbruck)

Summary / Outlook

- Coherent and dissipative dynamics provide a new toolbox of techniques for controlling many-body systems of cold atoms

- Tensor networks offer controllable variational calculation of static properties and real-time dynamics

- We have two routes to compute dynamics in open many-body systems



- This has many applications to understanding many-body dynamics, and to directly modelling ongoing experiments