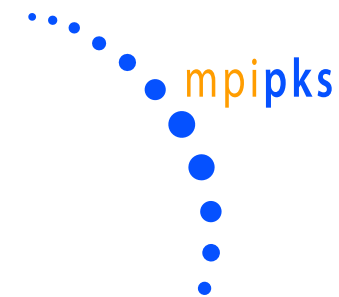


Numerical Simulations of Quenches in Bose Hubbard models

Andreas Läuchli,
 “New states of quantum matter”
 MPI für Physik komplexer Systeme - Dresden

<http://www.pks.mpg.de/~aml>



C. Kollath, AML, E. Altman, PRL 2007
 AML and C. Kollath, JSTAT 2008
 G. Biroli, C. Kollath, and AML, arXiv:0907.3731

Disentangling Quantum Many-Body Systems, KITP, November 1, 2010

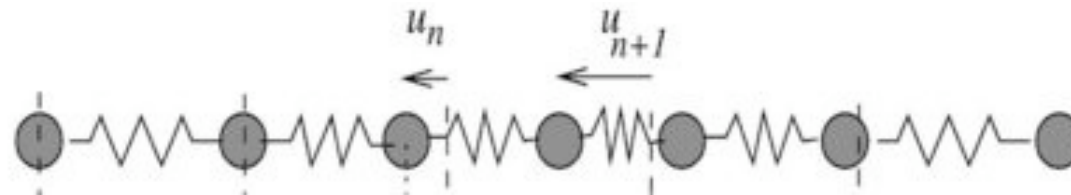


Fermi Pasta Ulam Tsingou Paradox (1953)



Fermi Pasta Ulam Tsingou Paradox (1953)

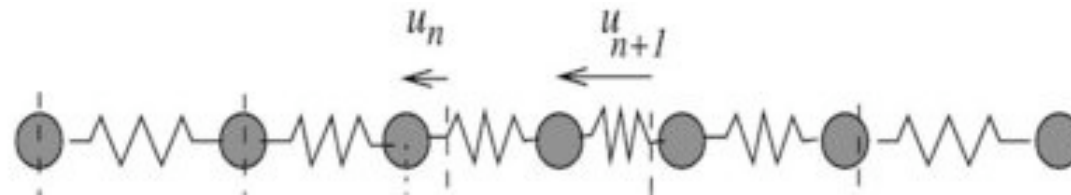
- A chain of harmonic oscillators, coupled with nonlinear couplings





Fermi Pasta Ulam Tsingou Paradox (1953)

- A chain of harmonic oscillators, coupled with nonlinear couplings

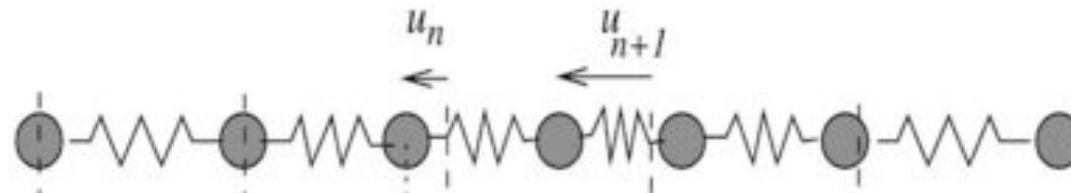


- A nonintegrable system, should thus approach thermal equilibrium



Fermi Pasta Ulam Tsingou Paradox (1953)

- A chain of harmonic oscillators, coupled with nonlinear couplings



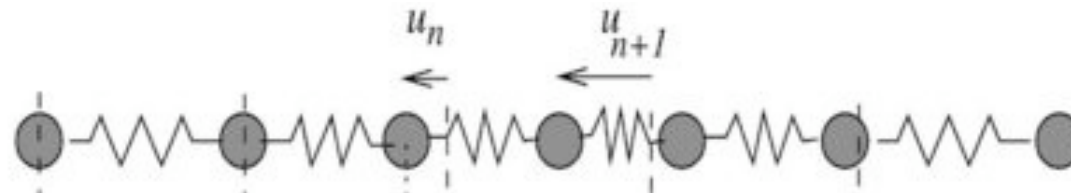
- A nonintegrable system, should thus approach thermal equilibrium
- One of the first computer experiments in history





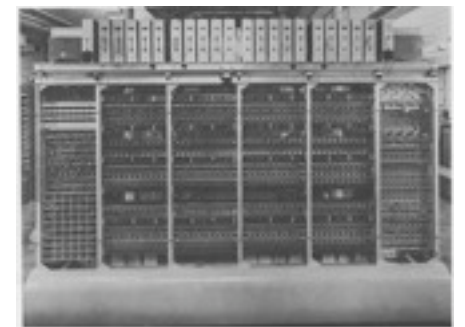
Fermi Pasta Ulam Tsingou Paradox (1953)

- A chain of harmonic oscillators, coupled with nonlinear couplings



- A nonintegrable system, should thus approach thermal equilibrium

- One of the first computer experiments in history



- Big surprise: The system does not thermalize, despite the nonintegrability



Fermi Pasta Ulam Tsingou Paradox (1953)

- A chain of harmonic oscillators, coupled with nonlinear couplings

- A nonintegrable

- One of the first

- Big surprise: T

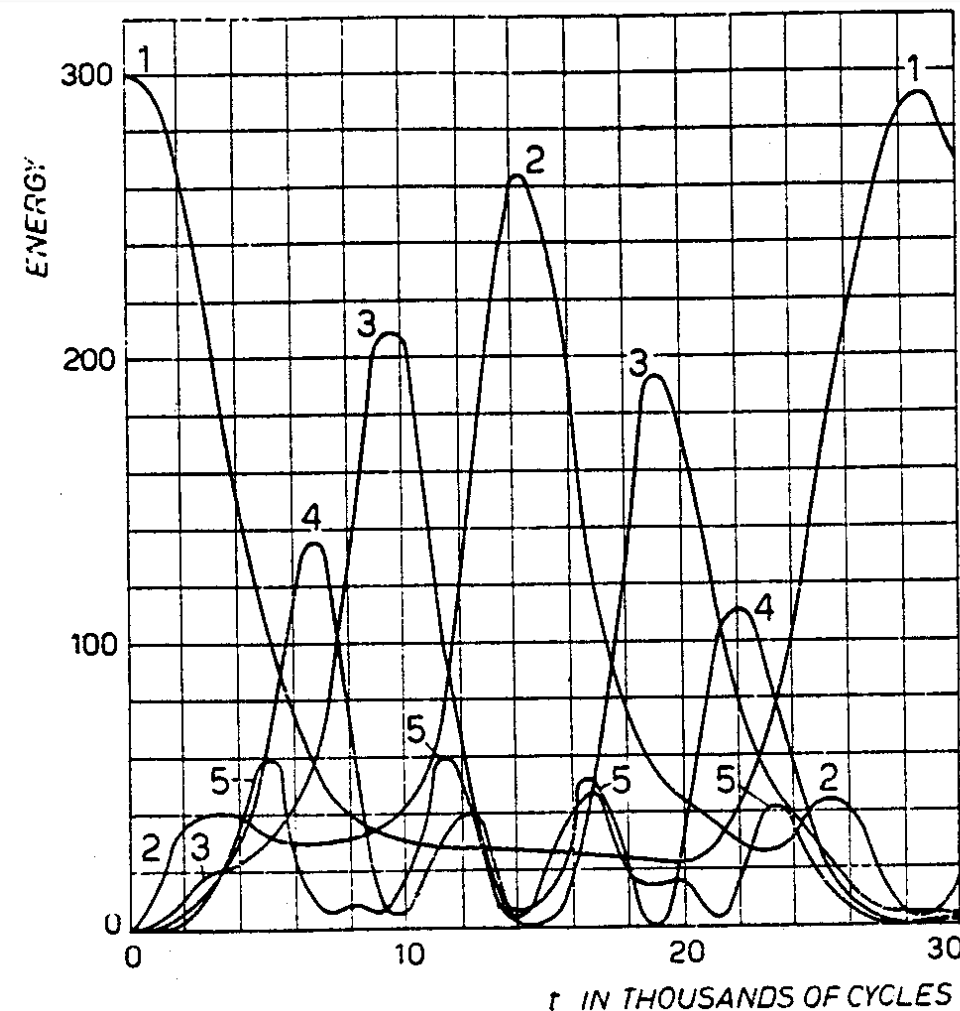
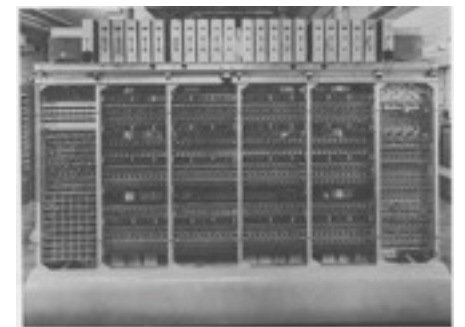


Fig. 1. – The quantity plotted is the energy (kinetic plus potential in each of the first five modes). The units for energy are arbitrary. $N = 32$; $\alpha = 1/4$; $\delta t^2 = 1/8$. The initial form of the string was a single sine wave. The higher modes never exceeded in energy 20 of our units. About 30,000 computation cycles were calculated.

um

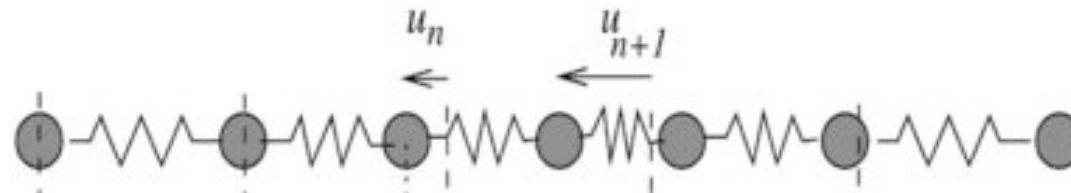


integrability



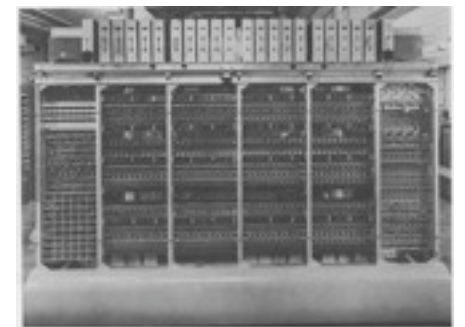
Fermi Pasta Ulam Tsingou Paradox (1953)

- A chain of harmonic oscillators, coupled with nonlinear couplings



- A nonintegrable system, should thus approach thermal equilibrium

- One of the first computer experiments in history

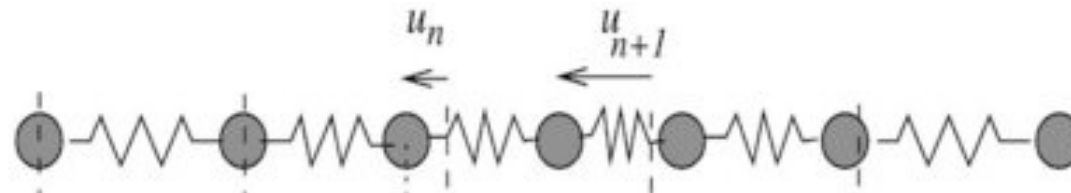


- Big surprise: The system does not thermalize, despite the nonintegrability



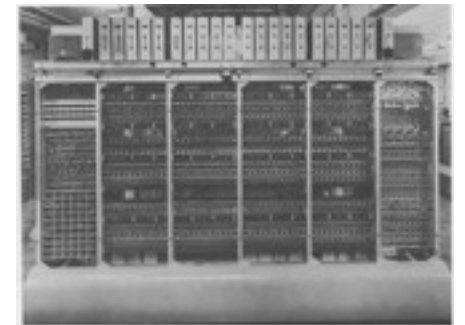
Fermi Pasta Ulam Tsingou Paradox (1953)

- A chain of harmonic oscillators, coupled with nonlinear couplings



- A nonintegrable system, should thus approach thermal equilibrium

- One of the first computer experiments in history



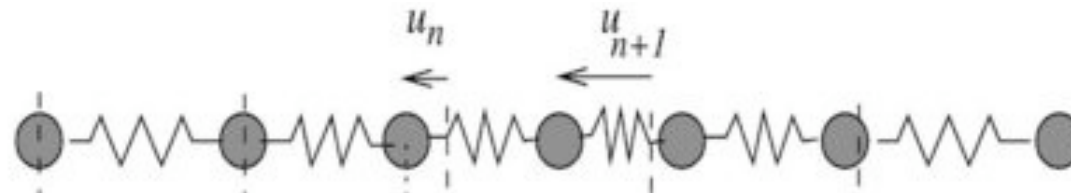
- Big surprise: The system does not thermalize, despite the nonintegrability

- Seminal work leading KAM Theory etc, ...



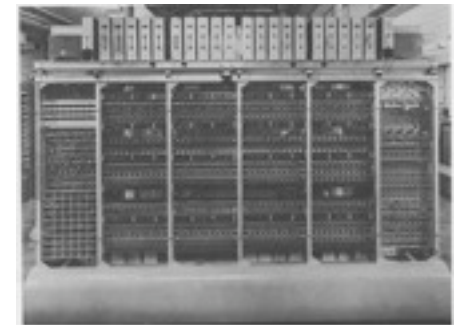
Fermi Pasta Ulam Tsingou Paradox (1953)

- A chain of harmonic oscillators, coupled with nonlinear couplings



- A nonintegrable system, should thus approach thermal equilibrium

- One of the first computer experiments in history



- Big surprise: The system does not thermalize, despite the nonintegrability

- Seminal work leading KAM Theory etc, ...

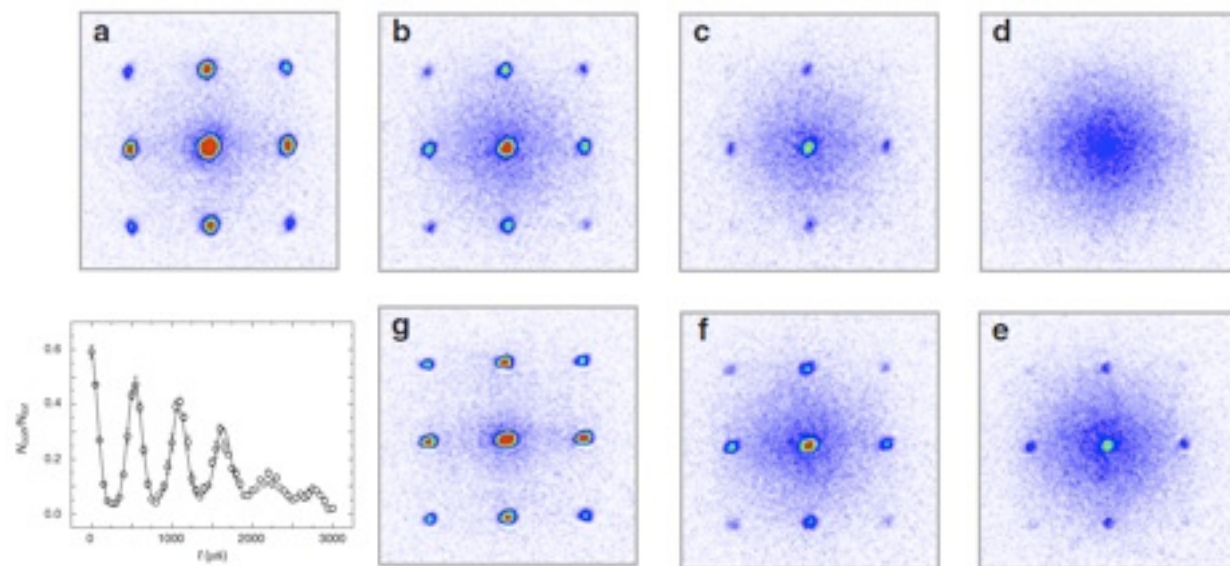
- Quantum world ?



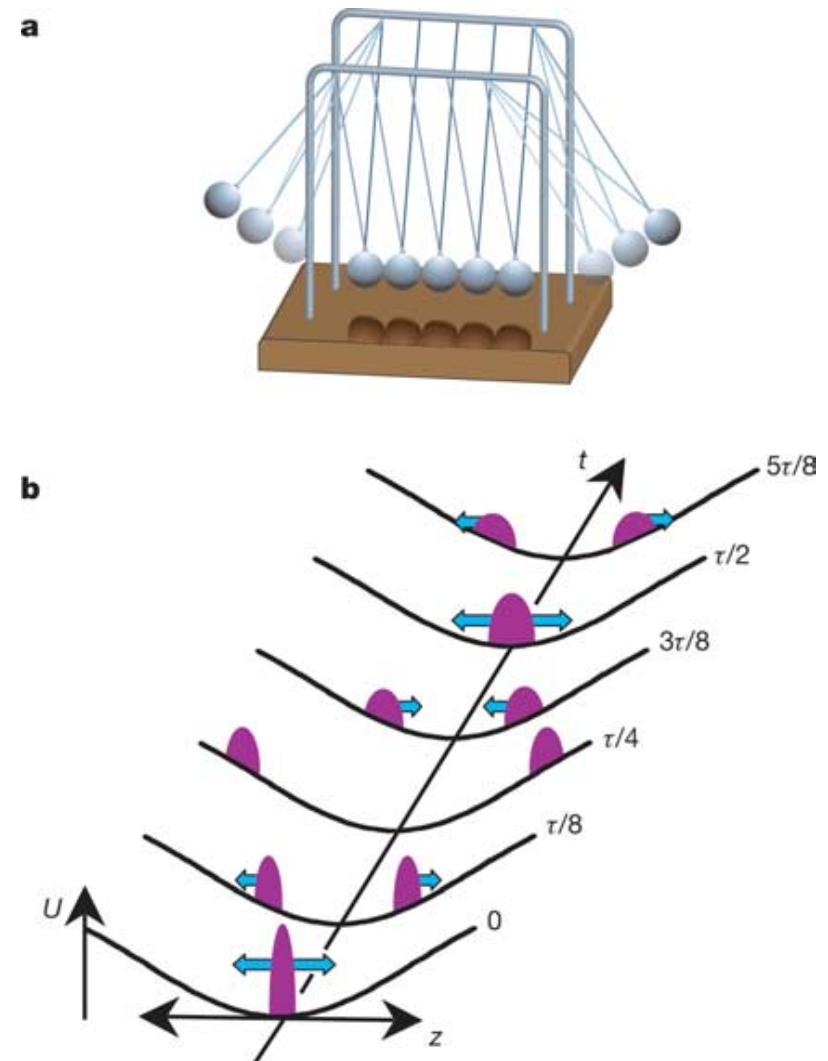
Quantum World: Two experimental examples

● Collapse and Revival of a superfluid

● Quantum Newton's cradle



Greiner et al, Nature 2002



Kinoshita et al, Nature 2006



Outline

- Experimental Motivation: Ultracold bosons in an optical lattice
- Short time behavior
 - Light-cone effect:
spreading of correlations
entanglement entropy
- Long time behavior
 - Properties of steady state ?
 - Is the steady state already “thermal” ?



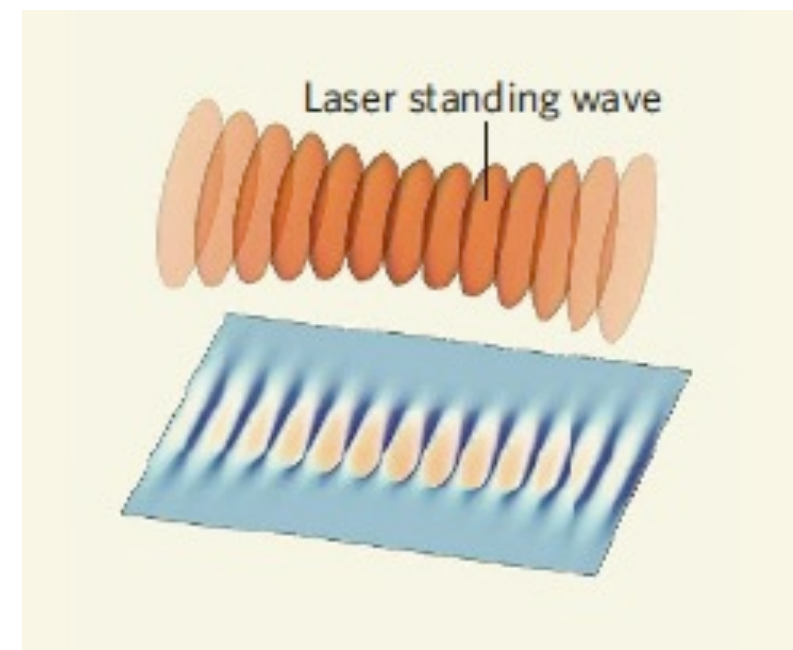
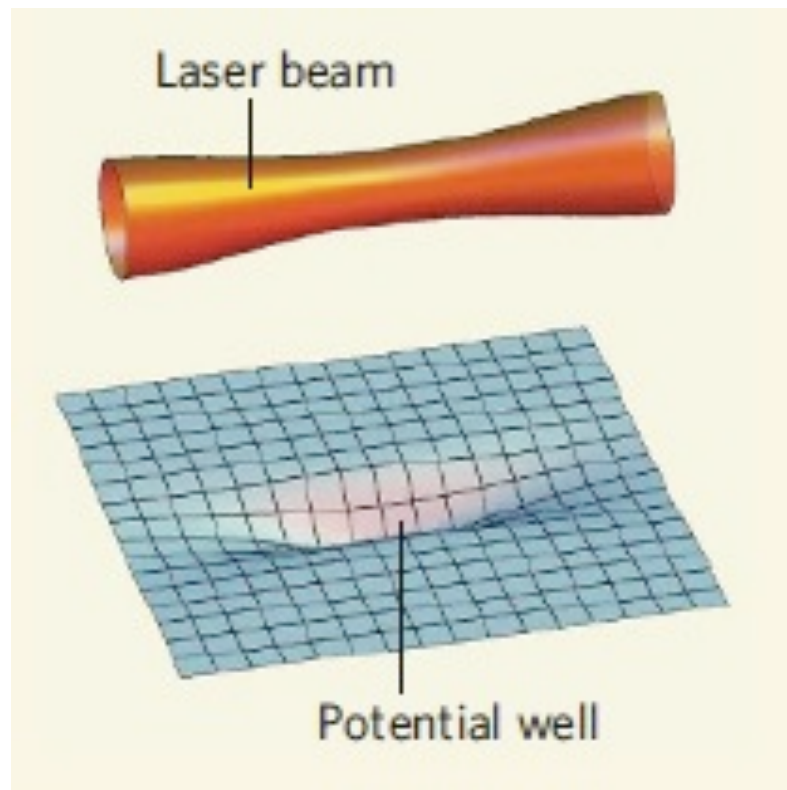
Outline

- Experimental Motivation: Ultracold bosons in an optical lattice
- Short time behavior
 - Light-cone effect:
spreading of correlations
entanglement entropy
- Long time behavior
 - Properties of steady state ?
 - Is the steady state already “thermal” ?



Optical lattices and Hamiltonian

Greiner and Fölling, Nature 2008



- Bosonic atoms: tunneling between wells and interaction within the same well:

$$H = -J \sum_{\langle i,j \rangle} (b_i^\dagger b_j + h.c.) + \frac{U}{2} \sum_i n_i (n_i - 1)$$

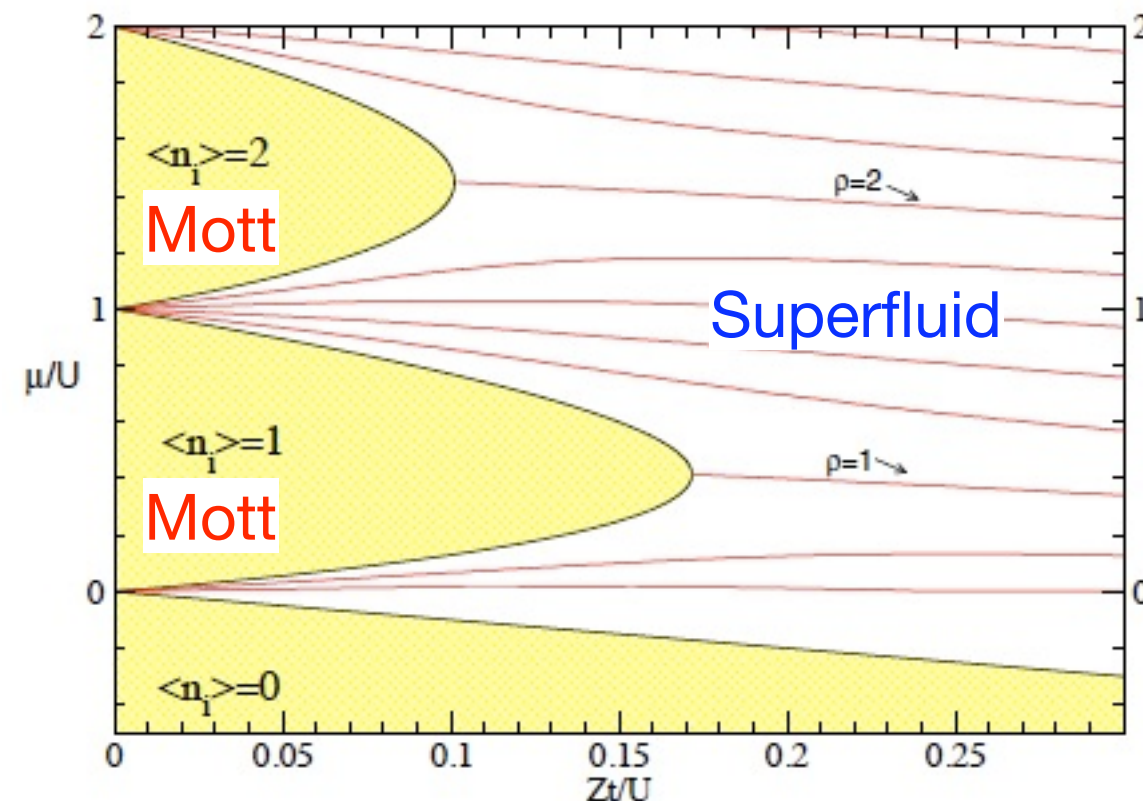
M.P.A. Fisher et al, PRB '89
D. Jaksch et al. PRL '98



Bose-Hubbard model

$$H = -J \sum_{\langle i,j \rangle} (b_i^\dagger b_j + h.c.) + \frac{U}{2} \sum_i n_i (n_i - 1)$$

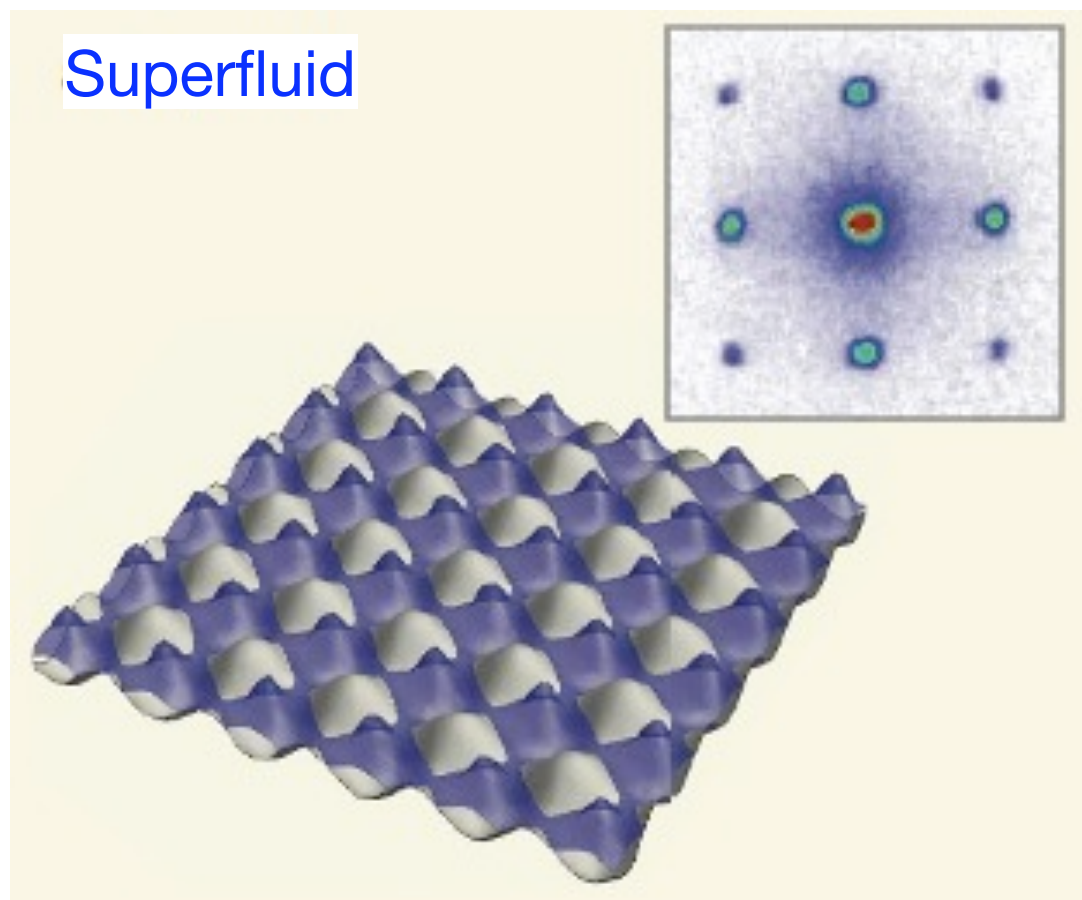
- Transition from **Superfluid** at large J/U to **Mott Insulator** at small J/U (Integer filling)



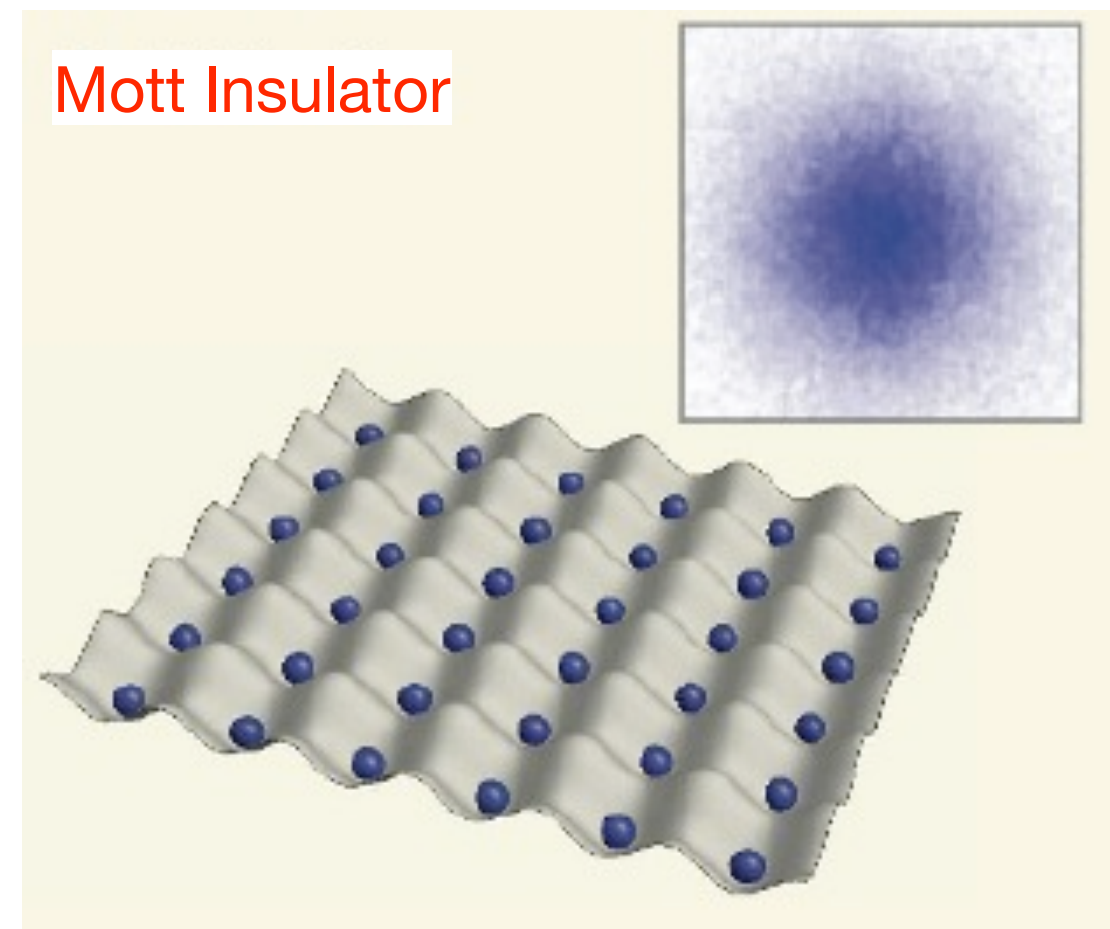


Superfluid versus Mott-Insulator

- Quantum states of bosons and their fingerprint in “time-of-flight” images



$$\langle b_i^\dagger b_j \rangle \rightarrow \langle b_i^\dagger \rangle \langle b_j \rangle$$

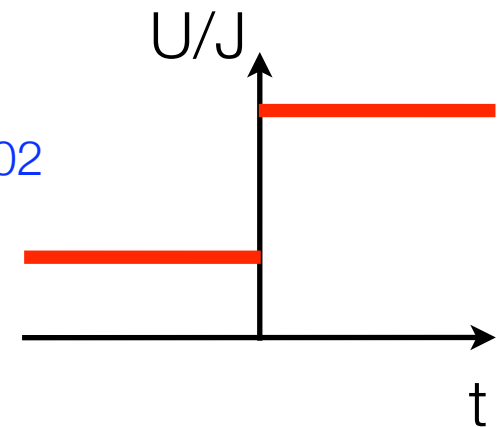


$$\langle b_i^\dagger b_j \rangle \rightarrow 0$$



Quench from the Superfluid to Mott Insulator

Greiner et al, Nature 2002

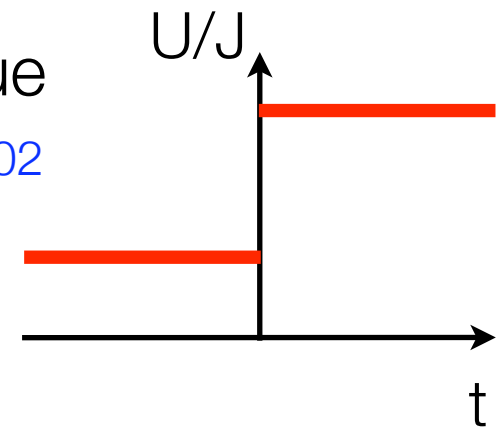




Quench from the Superfluid to Mott Insulator

- Sudden increase of the interaction strength from small to large value

Greiner et al, Nature 2002



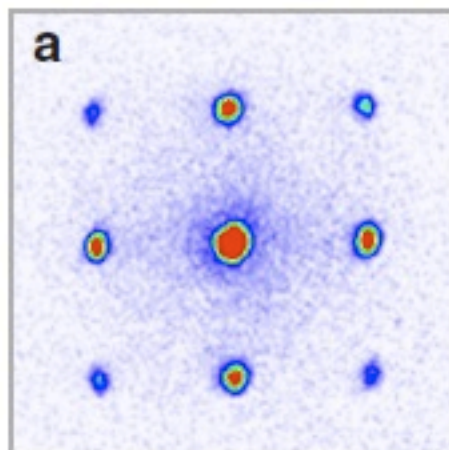
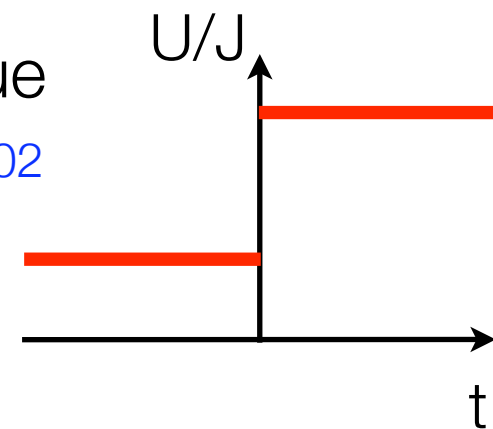


Quench from the Superfluid to Mott Insulator

- Sudden increase of the interaction strength from small to large value

Greiner et al, Nature 2002

- Time dependence of time-of-flight images:



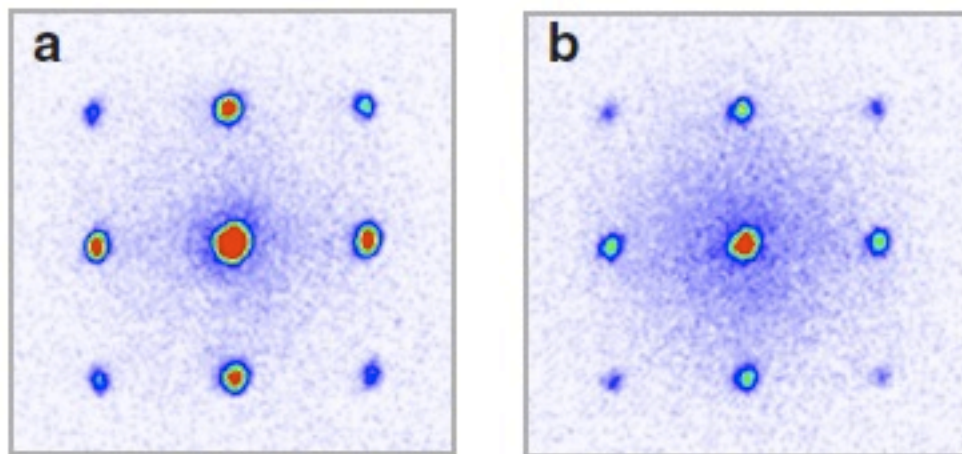
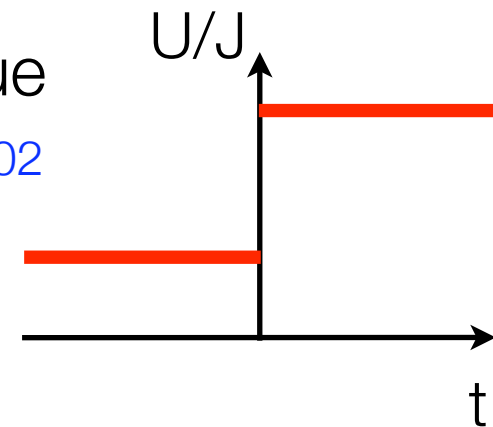


Quench from the Superfluid to Mott Insulator

- Sudden increase of the interaction strength from small to large value

Greiner et al, Nature 2002

- Time dependence of time-of-flight images:



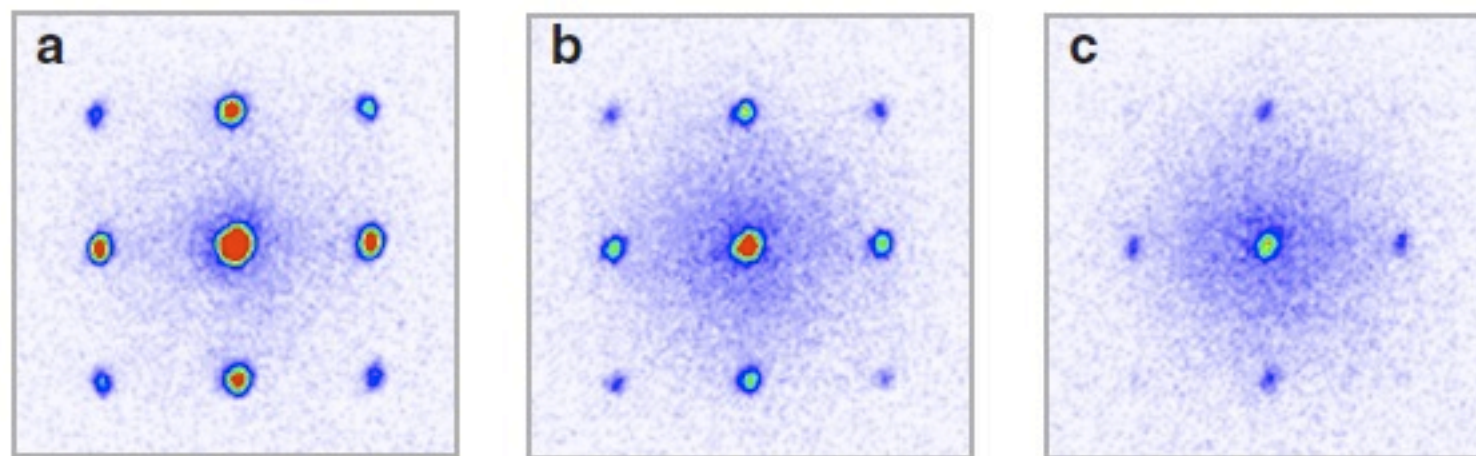
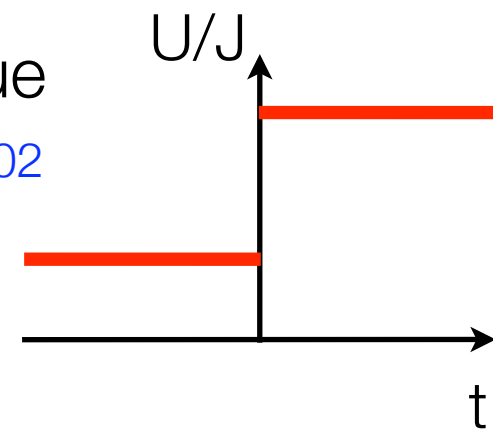


Quench from the Superfluid to Mott Insulator

- Sudden increase of the interaction strength from small to large value

Greiner et al, Nature 2002

- Time dependence of time-of-flight images:



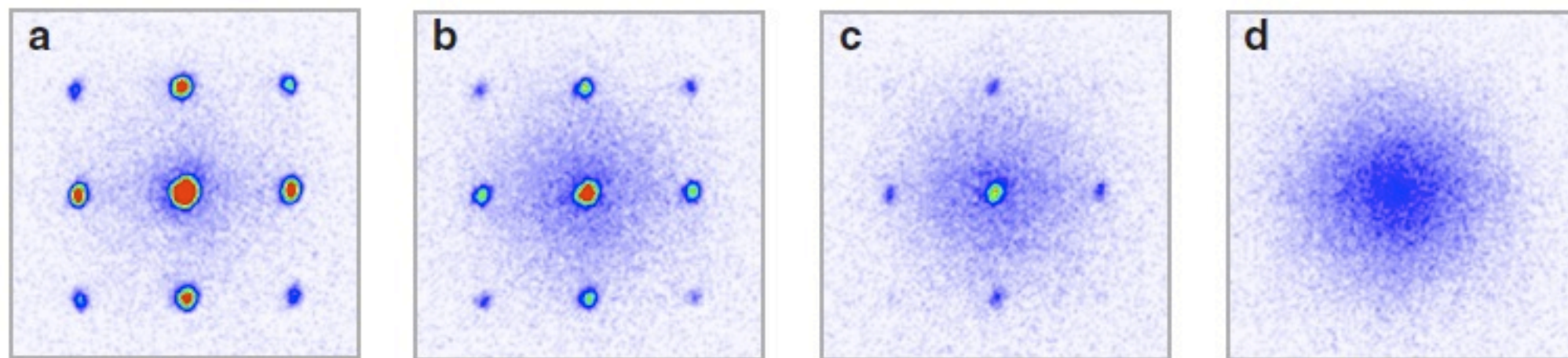
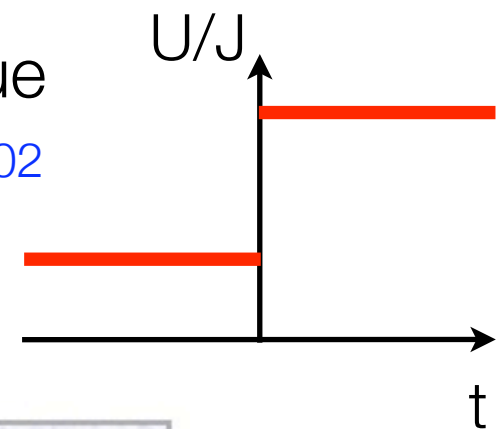


Quench from the Superfluid to Mott Insulator

- Sudden increase of the interaction strength from small to large value

Greiner et al, Nature 2002

- Time dependence of time-of-flight images:



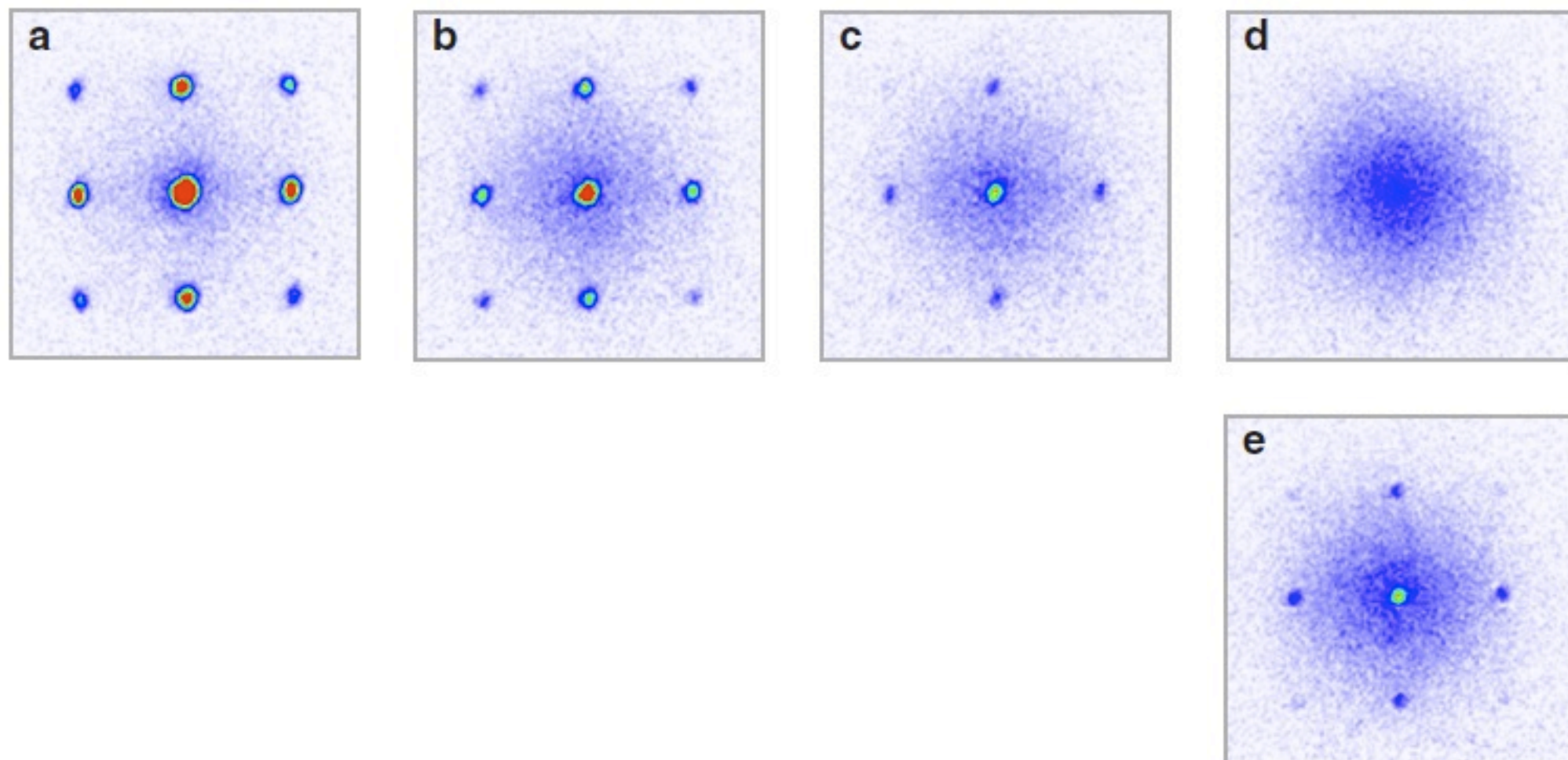
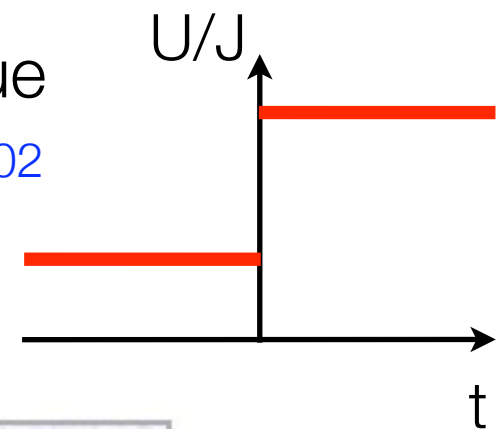


Quench from the Superfluid to Mott Insulator

- Sudden increase of the interaction strength from small to large value

Greiner et al, Nature 2002

- Time dependence of time-of-flight images:



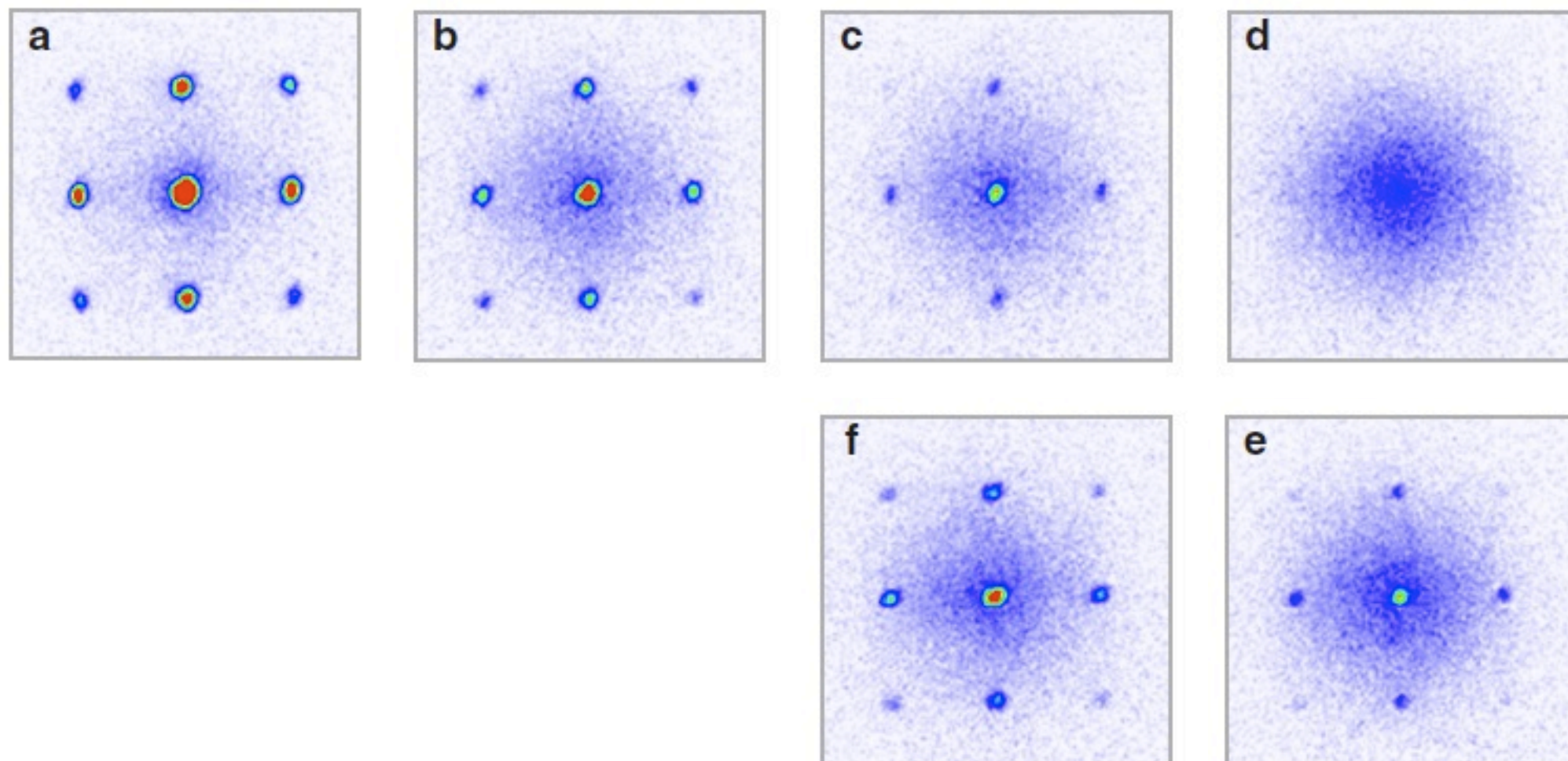
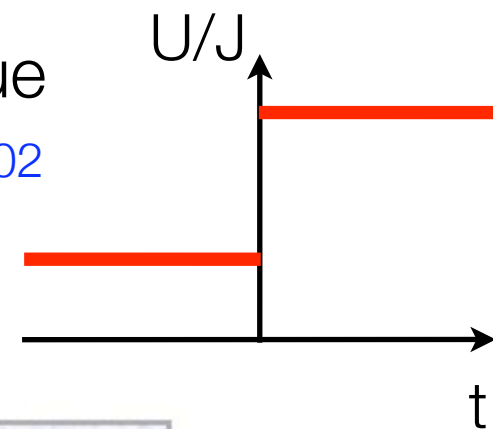


Quench from the Superfluid to Mott Insulator

- Sudden increase of the interaction strength from small to large value

Greiner et al, Nature 2002

- Time dependence of time-of-flight images:



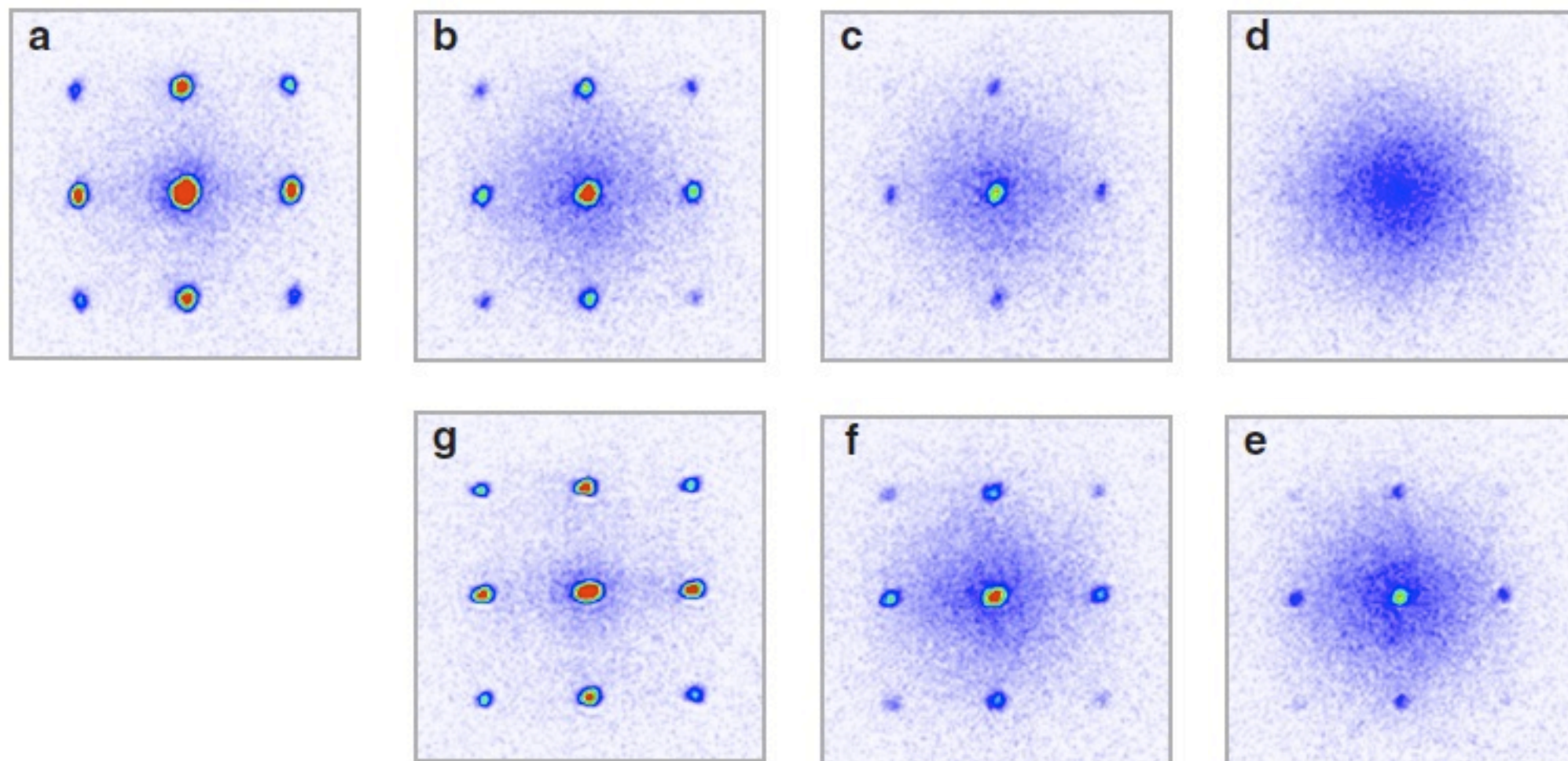
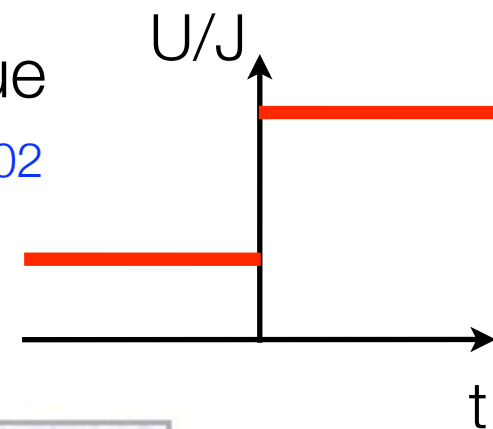


Quench from the Superfluid to Mott Insulator

- Sudden increase of the interaction strength from small to large value

Greiner et al, Nature 2002

- Time dependence of time-of-flight images:



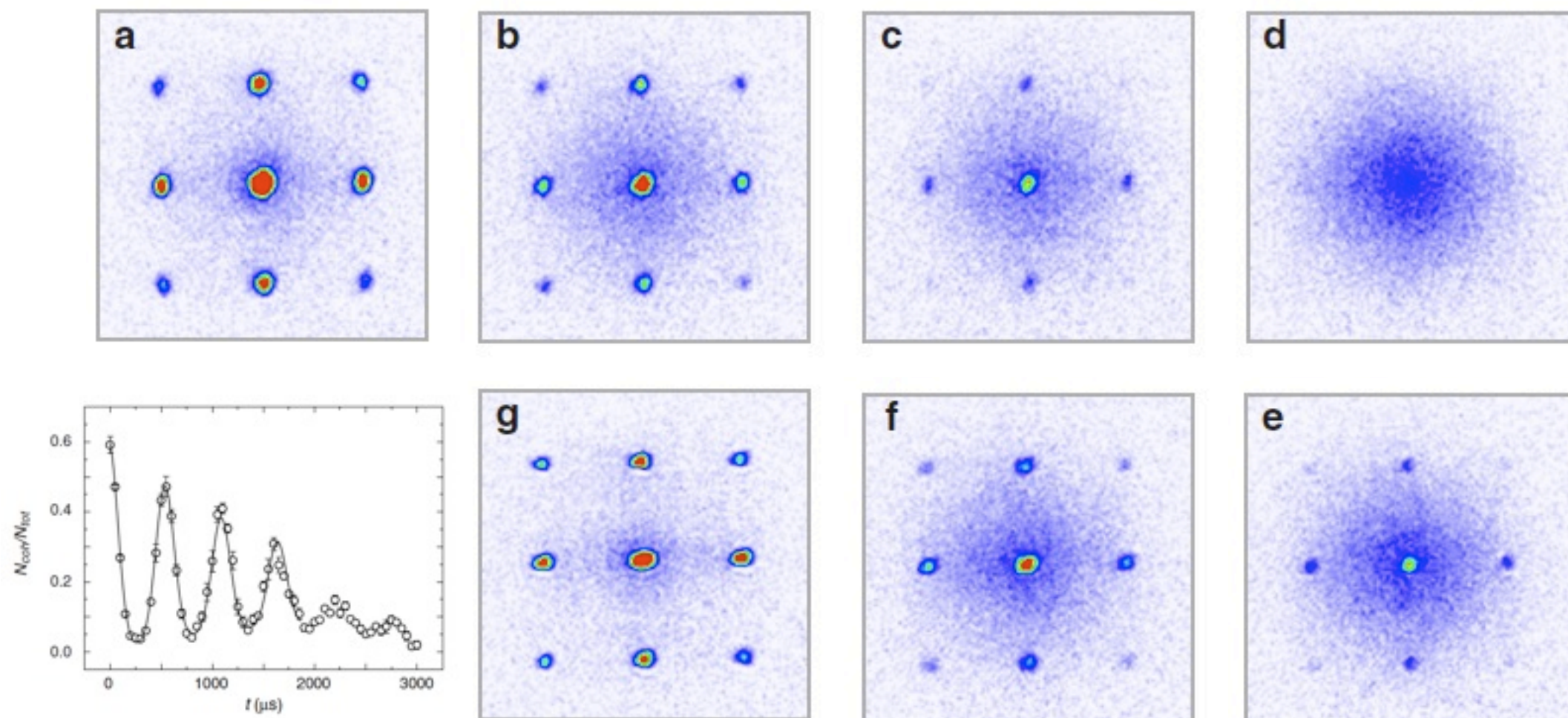
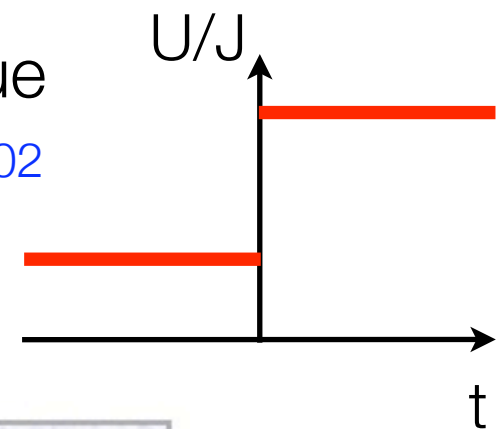


Quench from the Superfluid to Mott Insulator

- Sudden increase of the interaction strength from small to large value

Greiner et al, Nature 2002

- Time dependence of time-of-flight images:



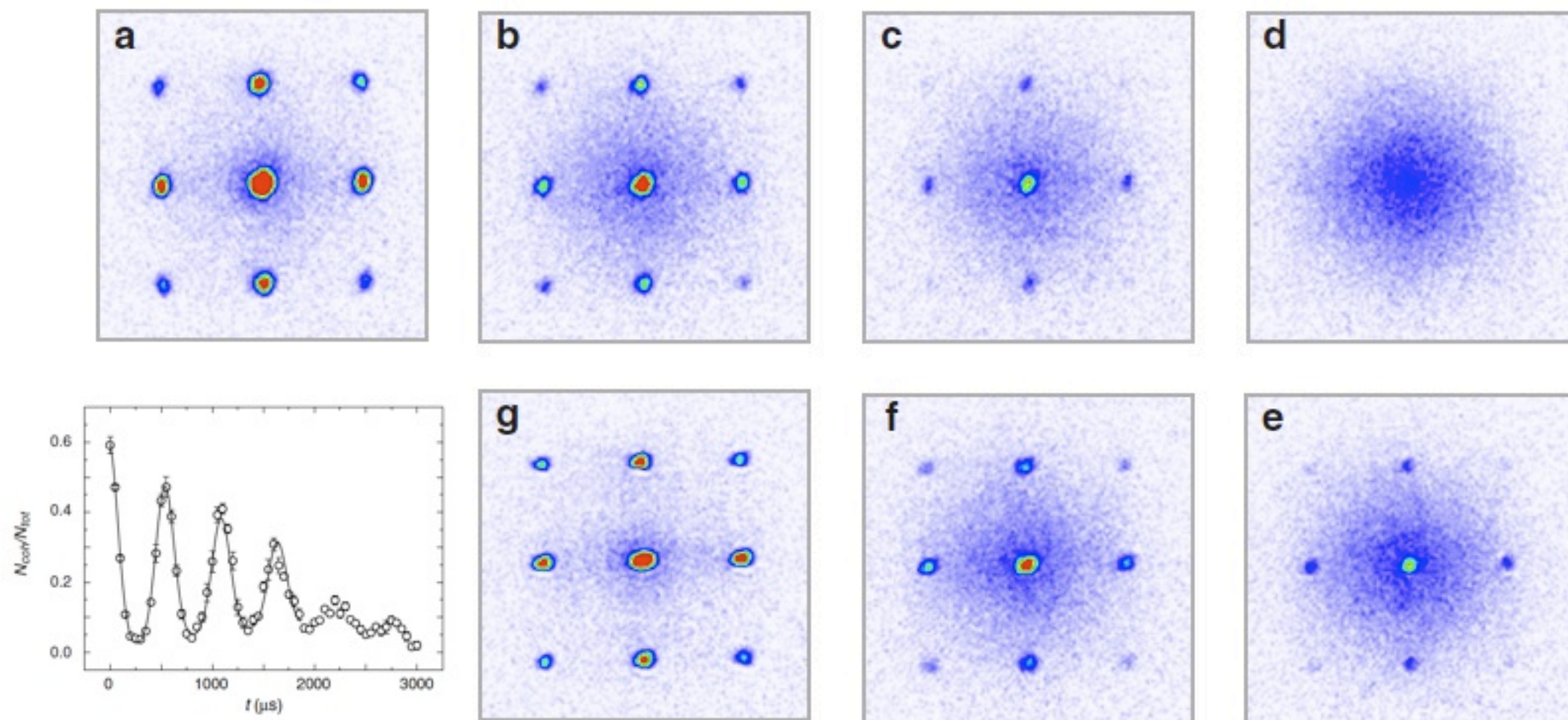
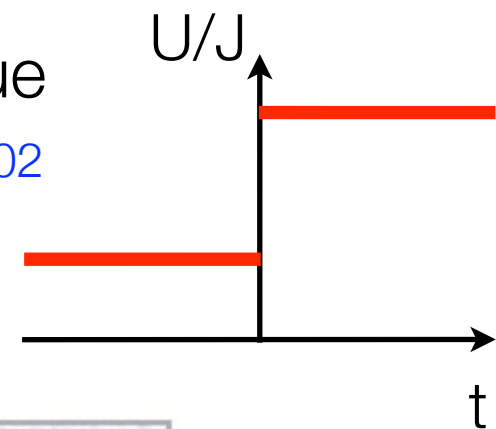


Quench from the Superfluid to Mott Insulator

- Sudden increase of the interaction strength from small to large value

Greiner et al, Nature 2002

- Time dependence of time-of-flight images:



- Collapse and Revival ! Suppressed at longer times.



Our Quench Setup

$$H = -J \sum_{\langle i,j \rangle} (b_i^\dagger b_j + h.c.) + \frac{U}{2} \sum_i n_i (n_i - 1)$$



Our Quench Setup

$$H = -J \sum_{\langle i,j \rangle} (b_i^\dagger b_j + h.c.) + \frac{U}{2} \sum_i n_i (n_i - 1)$$

- Linear chain (up to L=64) / occasionally square lattice



Our Quench Setup

$$H = -J \sum_{\langle i,j \rangle} (b_i^\dagger b_j + h.c.) + \frac{U}{2} \sum_i n_i (n_i - 1)$$

- Linear chain (up to $L=64$) / occasionally square lattice
- J is kept constant ($J=1$)



Our Quench Setup

$$H = -J \sum_{\langle i,j \rangle} (b_i^\dagger b_j + h.c.) + \frac{U}{2} \sum_i n_i (n_i - 1)$$

- Linear chain (up to $L=64$) / occasionally square lattice
- J is kept constant ($J=1$)
- Preparation in ground state at U_{initial} , typically in the superfluid ($U_{\text{initial}} < U_{\text{crit}}=3.37$)



Our Quench Setup

$$H = -J \sum_{\langle i,j \rangle} (b_i^\dagger b_j + h.c.) + \frac{U}{2} \sum_i n_i (n_i - 1)$$

- Linear chain (up to $L=64$) / occasionally square lattice
- J is kept constant ($J=1$)
- Preparation in ground state at U_{initial} , typically in the superfluid ($U_{\text{initial}} < U_{\text{crit}}=3.37$)
- Time evolution of this state using new Hamiltonian at U_{final}



Our Quench Setup

$$H = -J \sum_{\langle i,j \rangle} (b_i^\dagger b_j + h.c.) + \frac{U}{2} \sum_i n_i (n_i - 1)$$

- Linear chain (up to $L=64$) / occasionally square lattice
- J is kept constant ($J=1$)
- Preparation in ground state at U_{initial} , typically in the superfluid ($U_{\text{initial}} < U_{\text{crit}}=3.37$)
- Time evolution of this state using new Hamiltonian at U_{final}
- Time evolution is performed numerically using Exact Diagonalization and t-DMRG

Exact Diagonalization

Real-Time Dynamics



- It is expensive to obtain the full propagator $\exp[-itH]$
- Krylov methods exist to approximate the propagator for a given state $|\psi(0)\rangle$
One can get the time propagated state $|\psi(t)\rangle$ with only $|v\rangle = H|v\rangle$ operations.

$$\begin{aligned} |\phi'\rangle &= H|\phi_n\rangle - \beta_n|\phi_{n-1}\rangle, \\ \alpha_n &= \langle\phi_n|\phi'\rangle, \\ |\phi''\rangle &= |\phi'\rangle - \alpha_n|\phi_n\rangle, \\ \beta_{n+1} &= ||\phi''|| = \sqrt{\langle\phi''|\phi''\rangle}, \\ |\phi_{n+1}\rangle &= |\phi''\rangle/\beta_{n+1}, \end{aligned} \quad \tilde{H}_N = \begin{bmatrix} \alpha_0 & \beta_1 & 0 & \dots\dots\dots & 0 \\ \beta_1 & \alpha_1 & \beta_2 & 0 & \dots\dots & 0 \\ 0 & \beta_2 & \alpha_2 & \beta_3 & 0 & 0 \\ & & \ddots & \ddots & \ddots & \\ 0 & \dots & 0 & \beta_{N-2} & \alpha_{N-2} & \beta_{N-1} \\ 0 & \dots\dots\dots & 0 & \beta_{N-1} & \alpha_{N-1} \end{bmatrix}$$

- Calculate matrix exponential of H_N , instead of the full Hamiltonian

Park & Light, J. Chem. Phys 1986

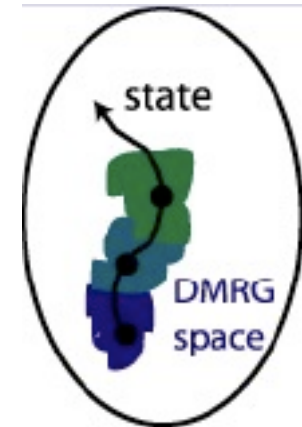
- Time evolution of quantum systems with up to 10^8 degrees of freedom (dim H)

Numerical Methods: tDMRG



- t-DMRG (large systems $L=100++$, but relatively short times)

- Adaptive control of the optimal Hilbert space as time evolves.



- Maximum time depends on entanglement growth.

G. Vidal PRL '03
A. Daley et al., JSTAT '04
S. White & A. Feiguin, PRL '04

- More refined approaches can reach larger times (however still require exponential resources):

- Light-cone MPS
- Heisenberg picture

M. Hastings, J. Math. Phys. 2009
M.C. Bañuls, et al., PRL 2009
M.C. Bañuls, et al., arXiv:1007:3957

M. Hartmann et al., PRL 2009



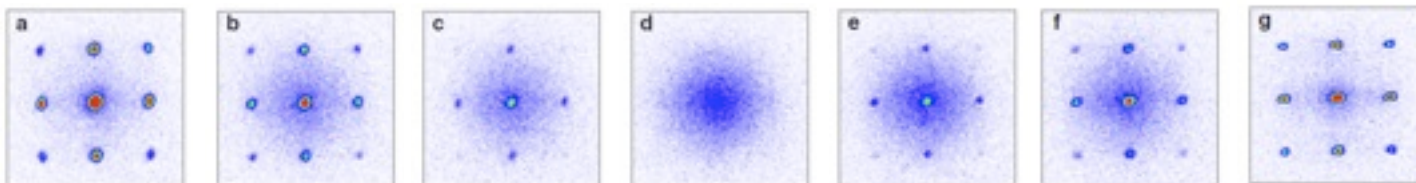
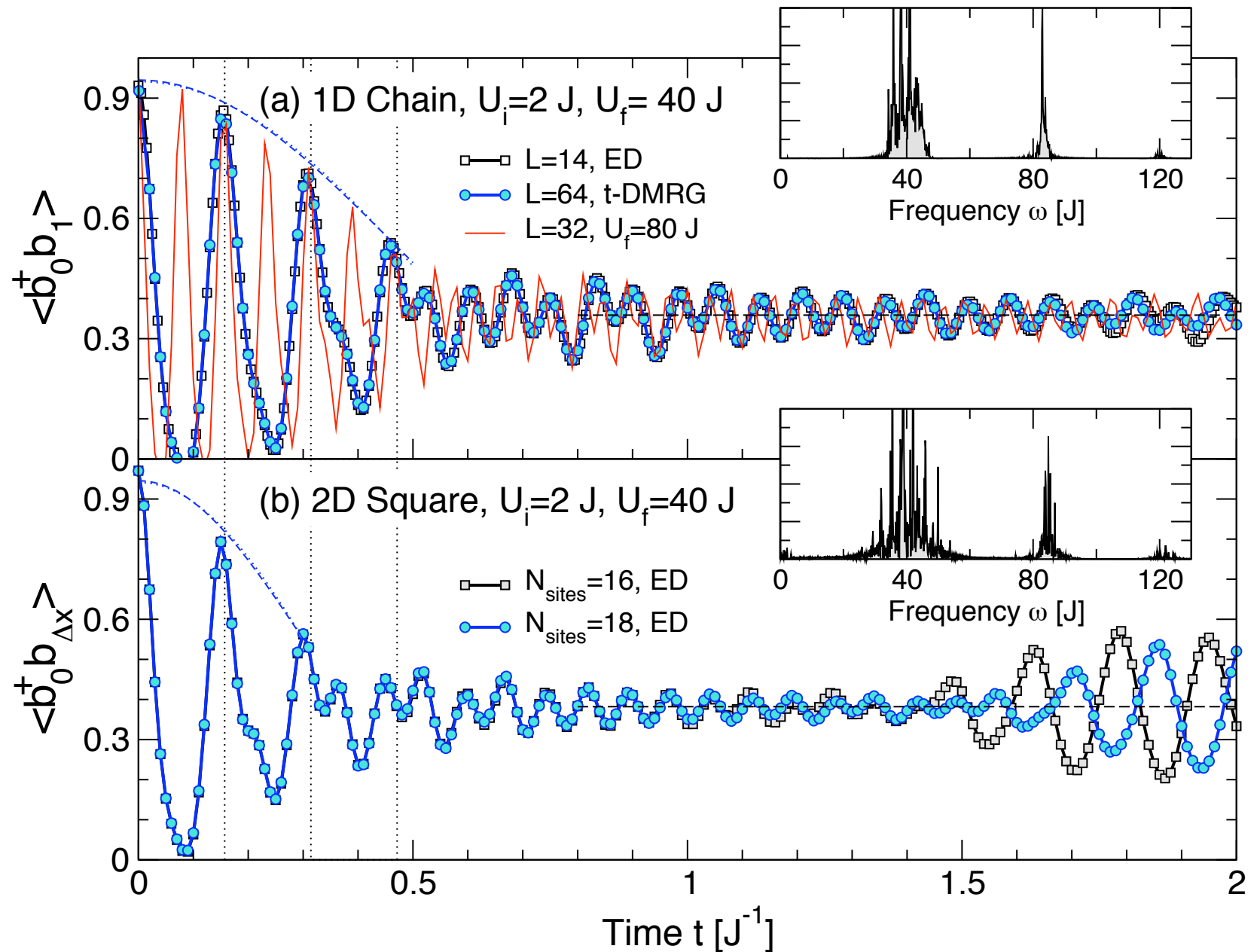
Outline

- Experimental Motivation: Ultracold bosons in an optical lattice
- Short time behavior
 - Light-cone effect:
spreading of correlations
entanglement entropy
- Long time behavior
 - Properties of steady state ?
 - Is the steady state already “thermal” ?



Superfluid correlation

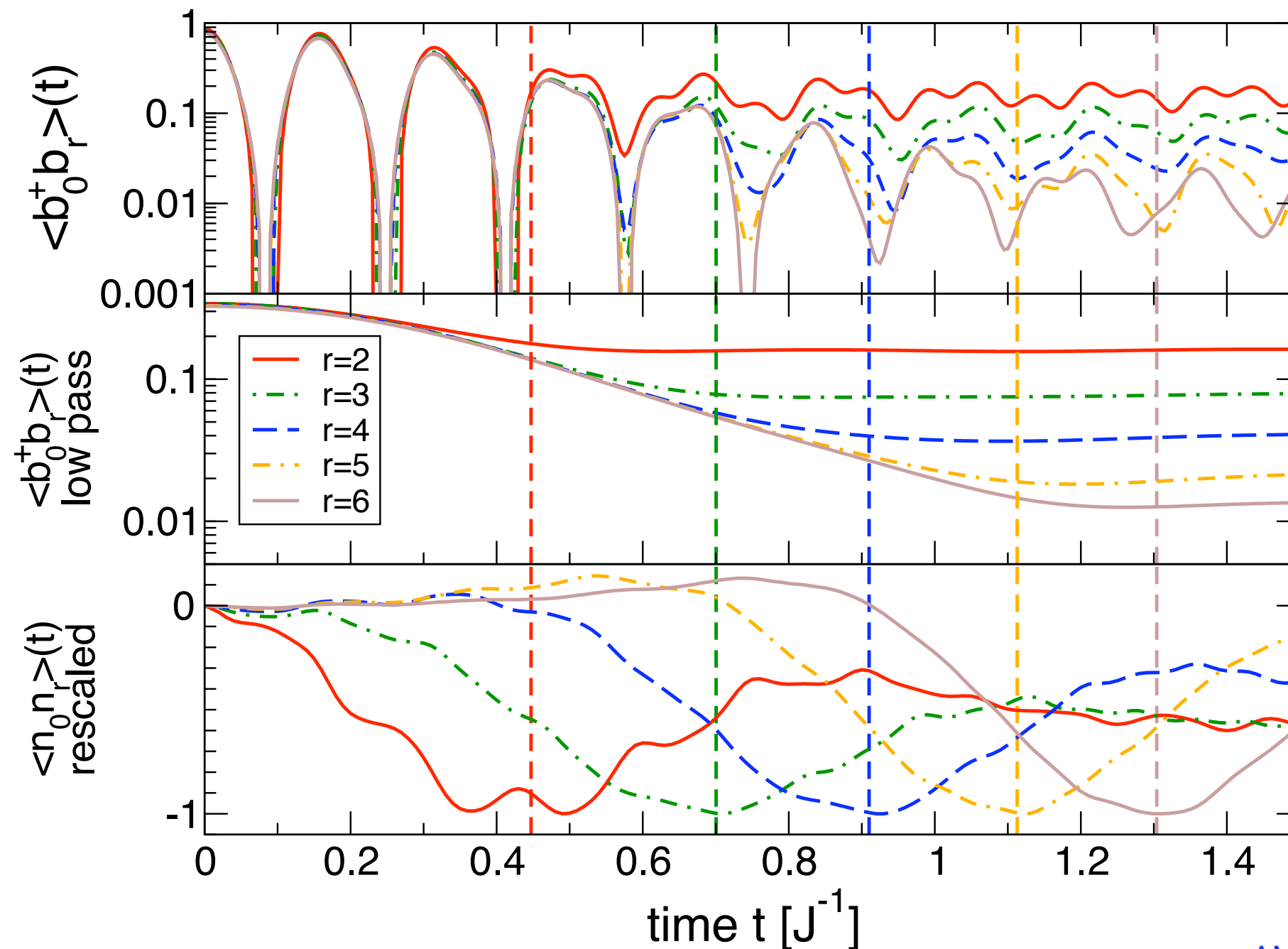
- Pronounced collapse and revival. Relaxation to steady state at later times
- Collapse and revival controlled by U
- Relaxation faster for larger bandwidth (1D/2D)





Space-time dependence of correlators

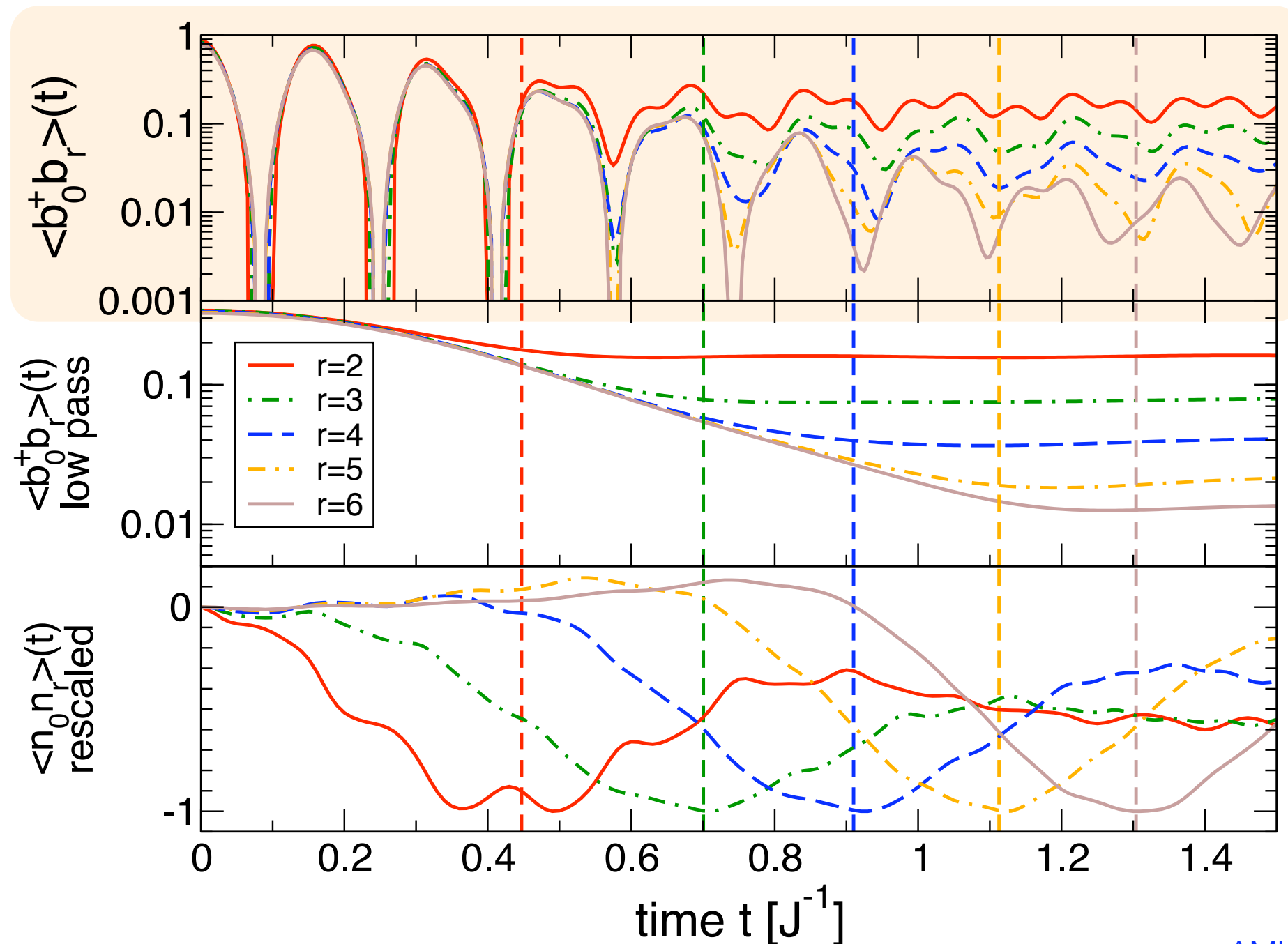
- Correlation functions at different spatial separations:





Space-time dependence of correlators

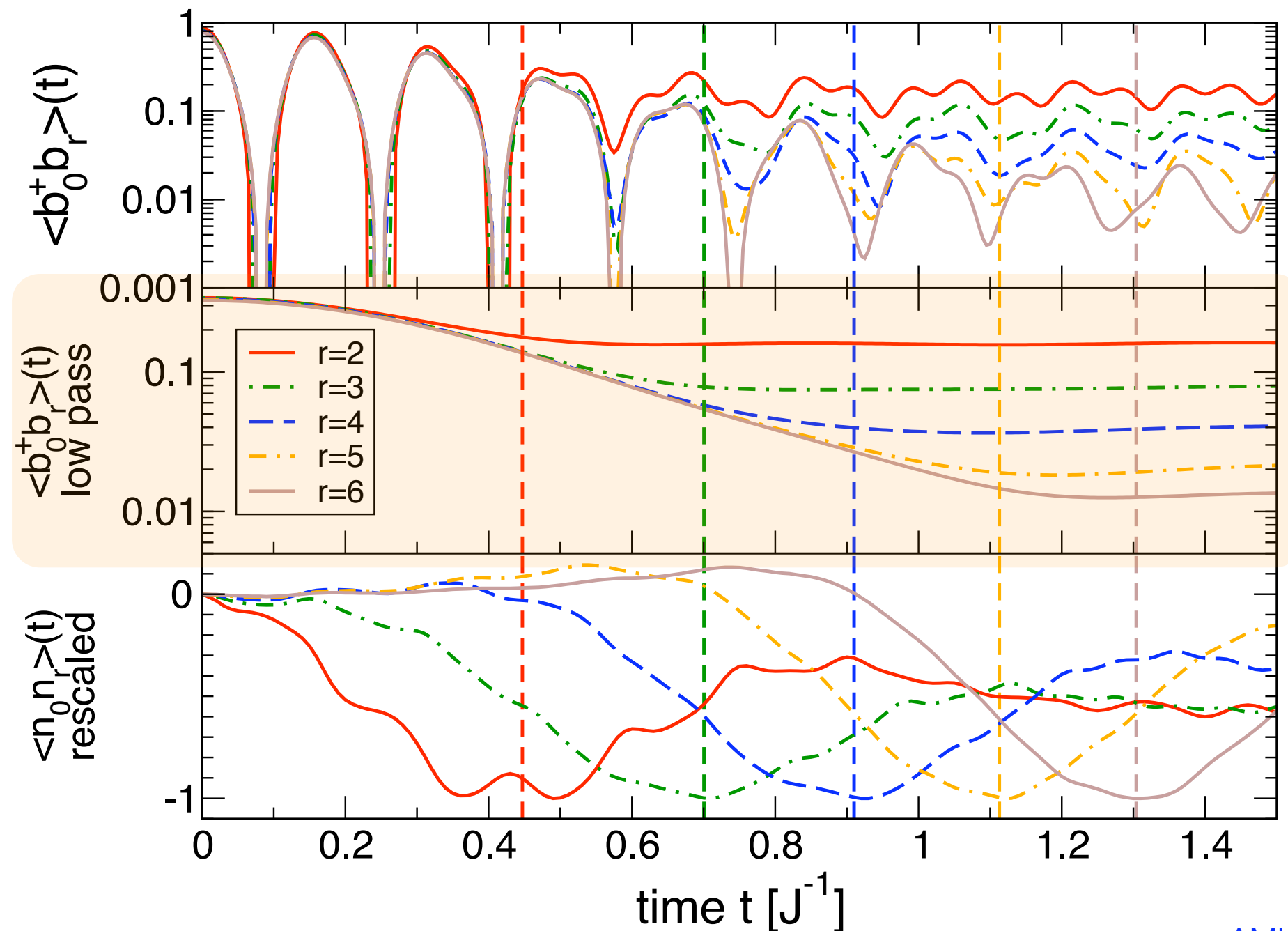
- Correlation functions at different spatial separations:





Space-time dependence of correlators

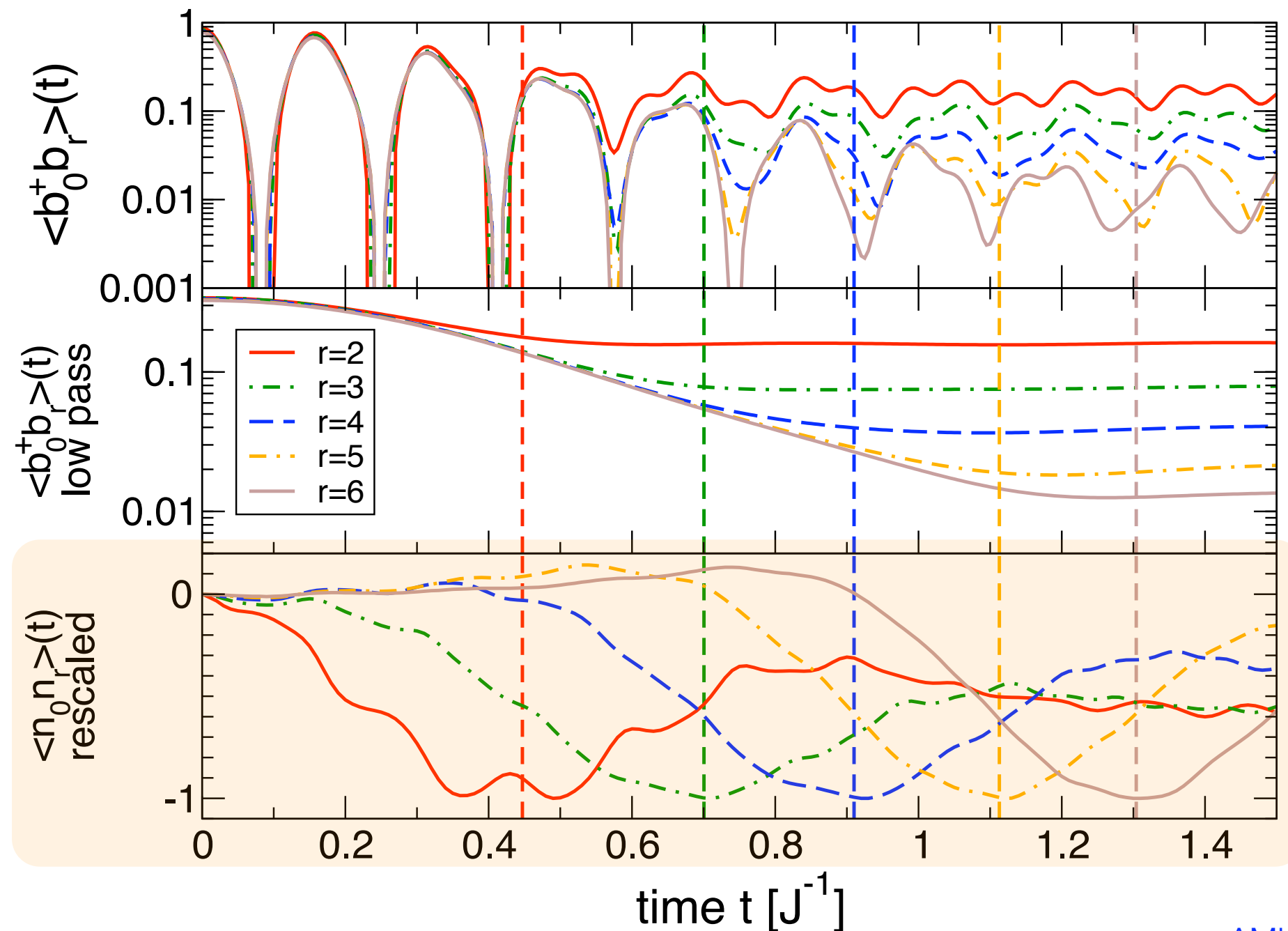
- Correlation functions at different spatial separations:





Space-time dependence of correlators

- Correlation functions at different spatial separations:

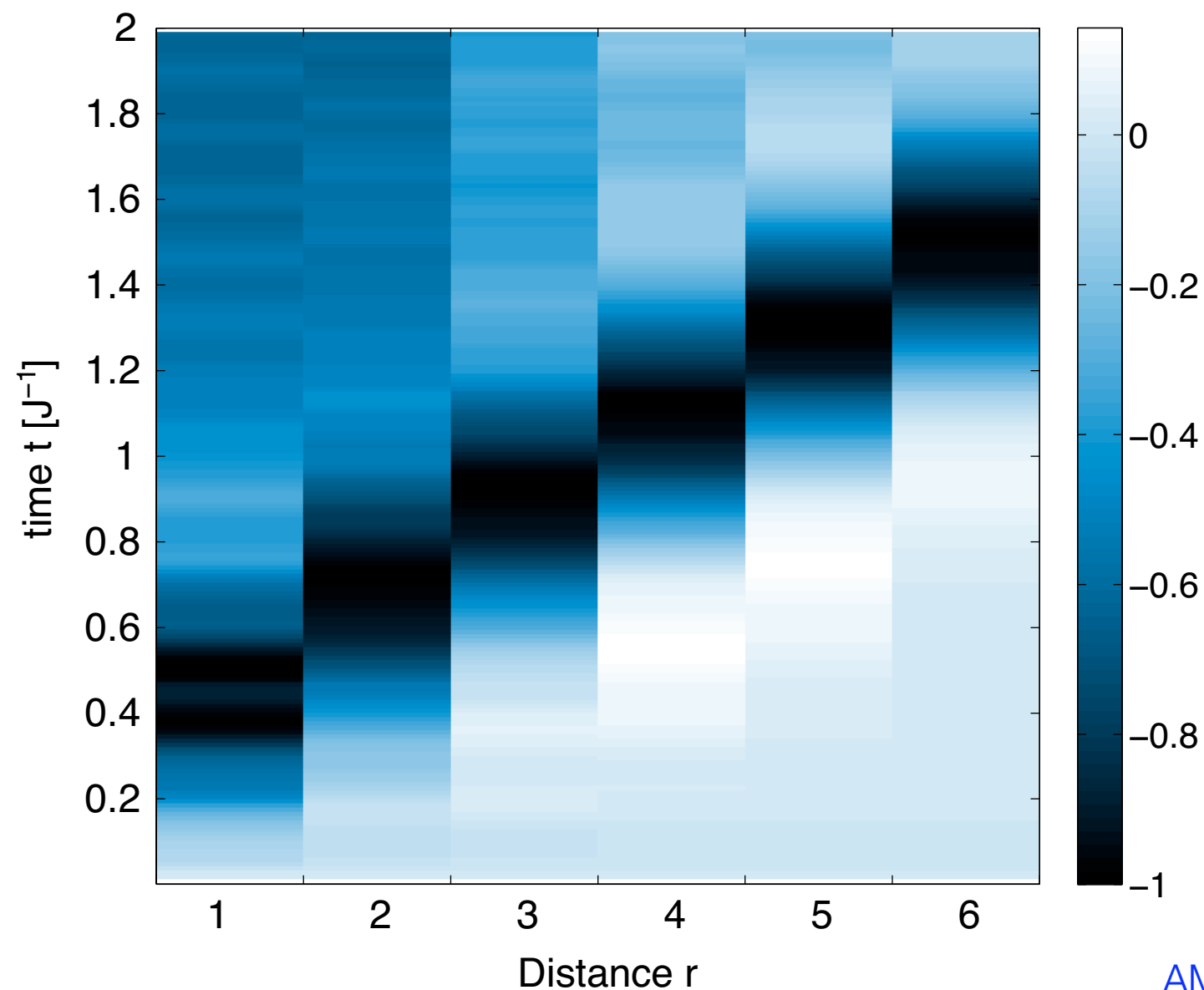




Lightcone / Horizon effect

Lieb and Robinson CMP '72

- More distant sites see correlation signal pass at later times. Linear relation.



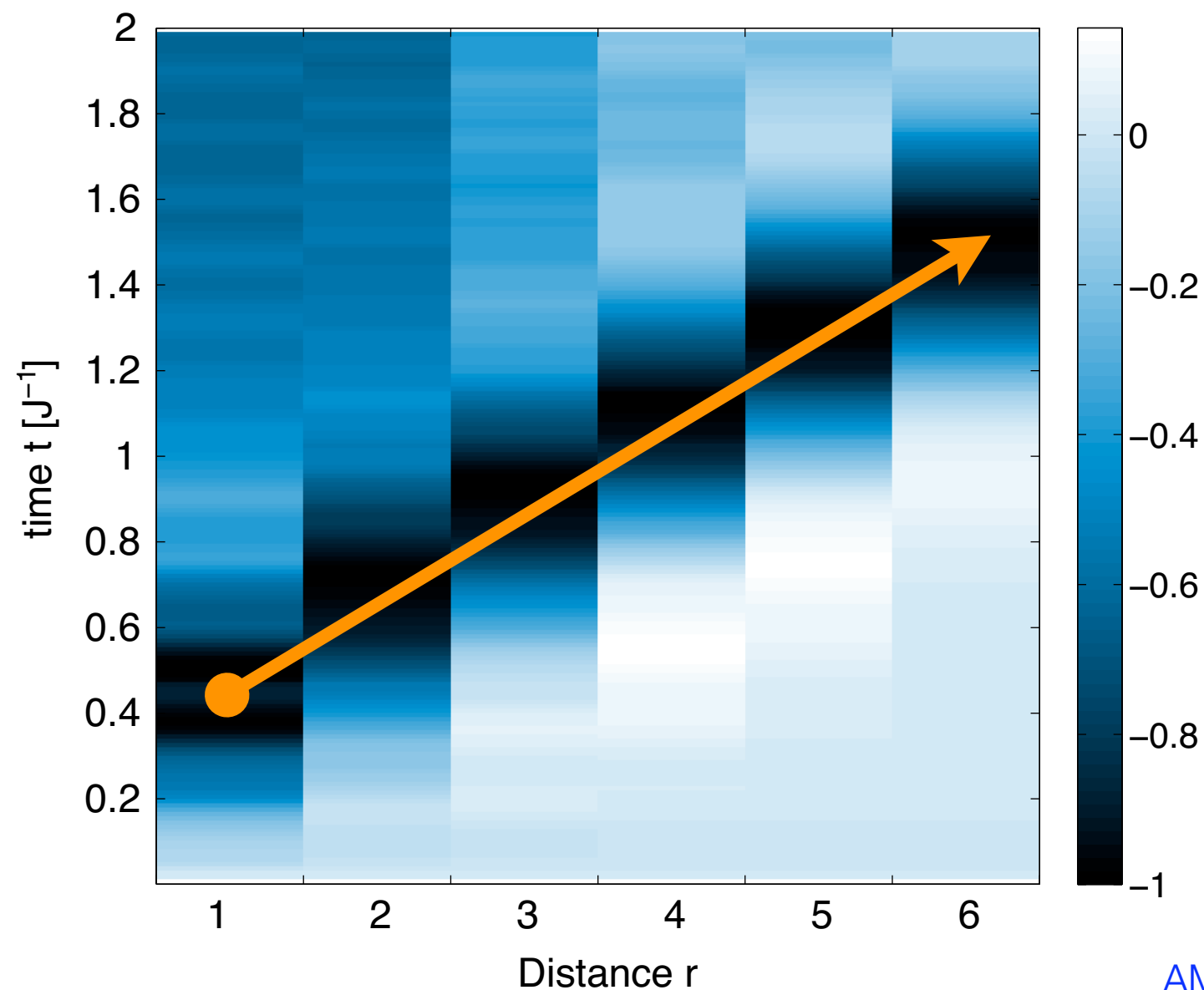
AML and Kollath, JSTAT '08



Lightcone / Horizon effect

Lieb and Robinson CMP '72

- More distant sites see correlation signal pass at later times. Linear relation.

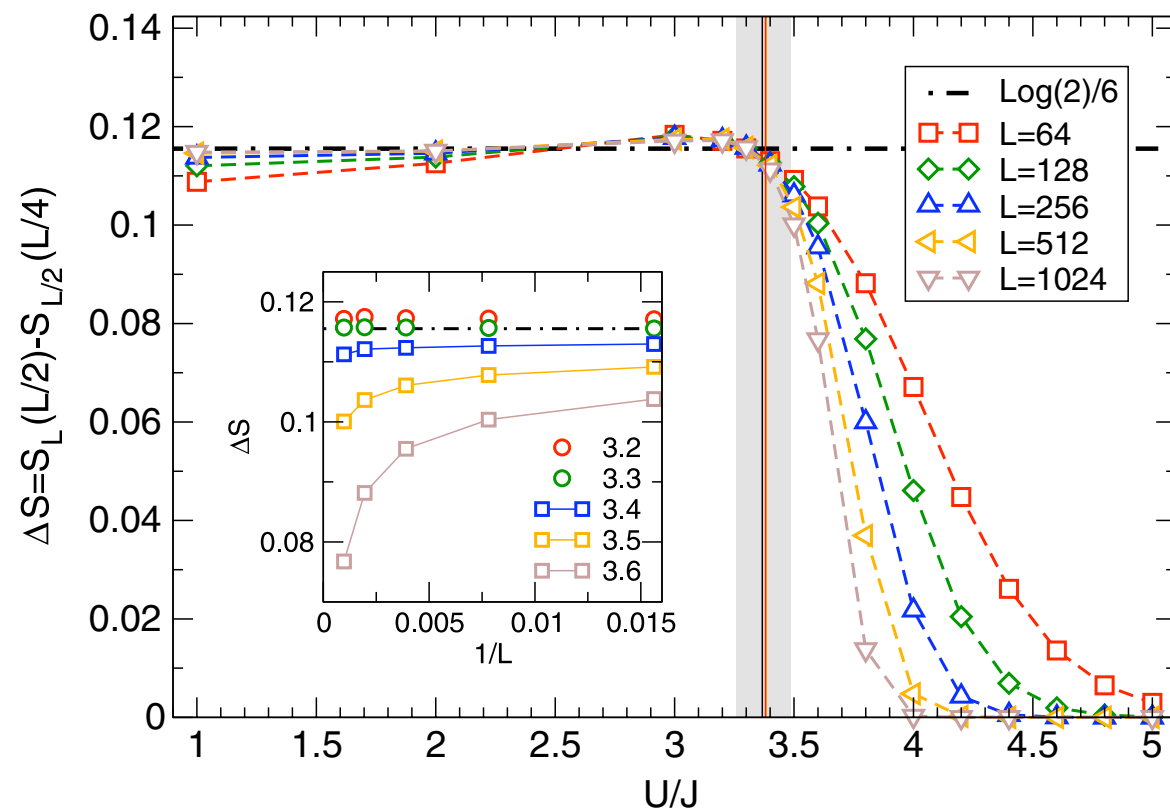


AML and Kollath, JSTAT '08

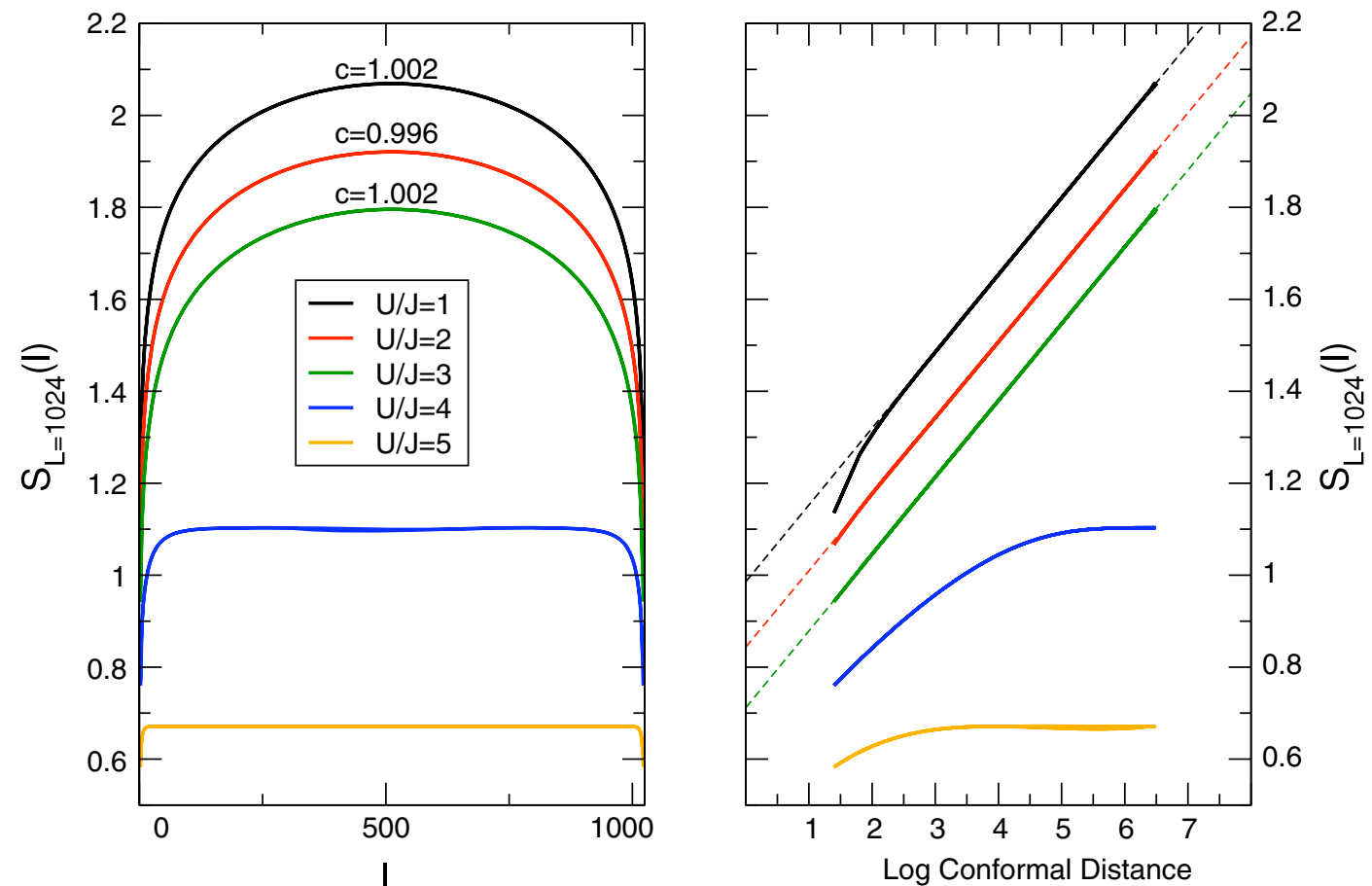


von Neumann Entanglement Entropy (first static)

- Saturation of vN EE in gapped phase
- Logarithmic divergence in critical phase (single component $c=1$)



$$S_A = \text{Tr}_A[-\rho_A \log \rho_A]$$

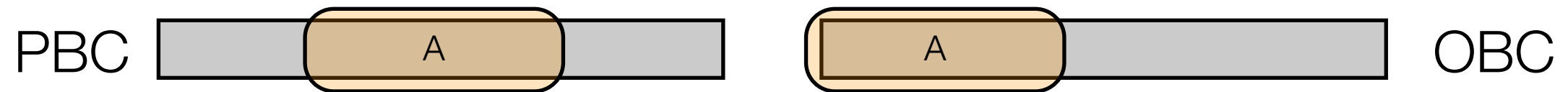


- Entropy increase upon system doubling reveals the phase transition quite accurately.



Entanglement time evolution

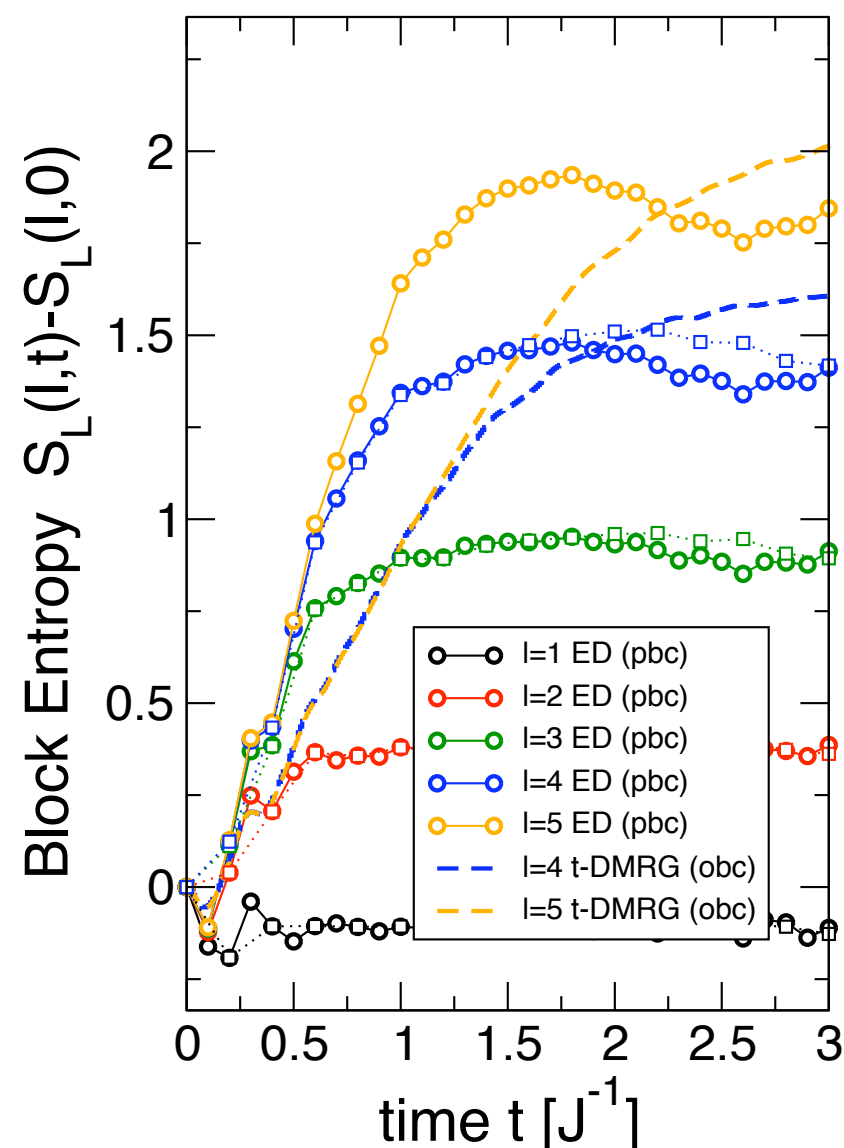
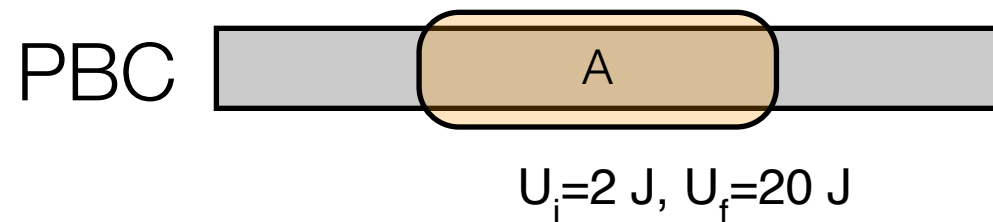
- von Neumann entropy of a block A consisting of l sites $S_A = \text{Tr}_A[-\rho_A \log \rho_A]$





Entanglement time evolution

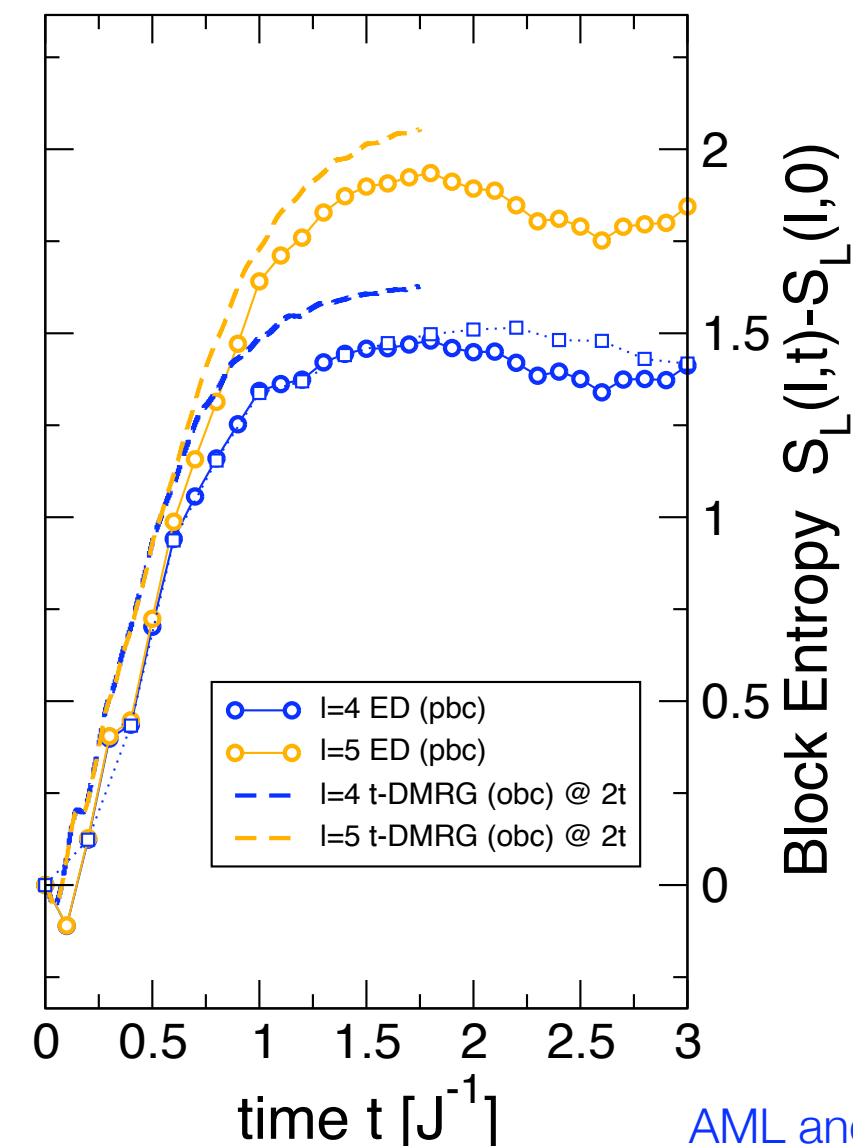
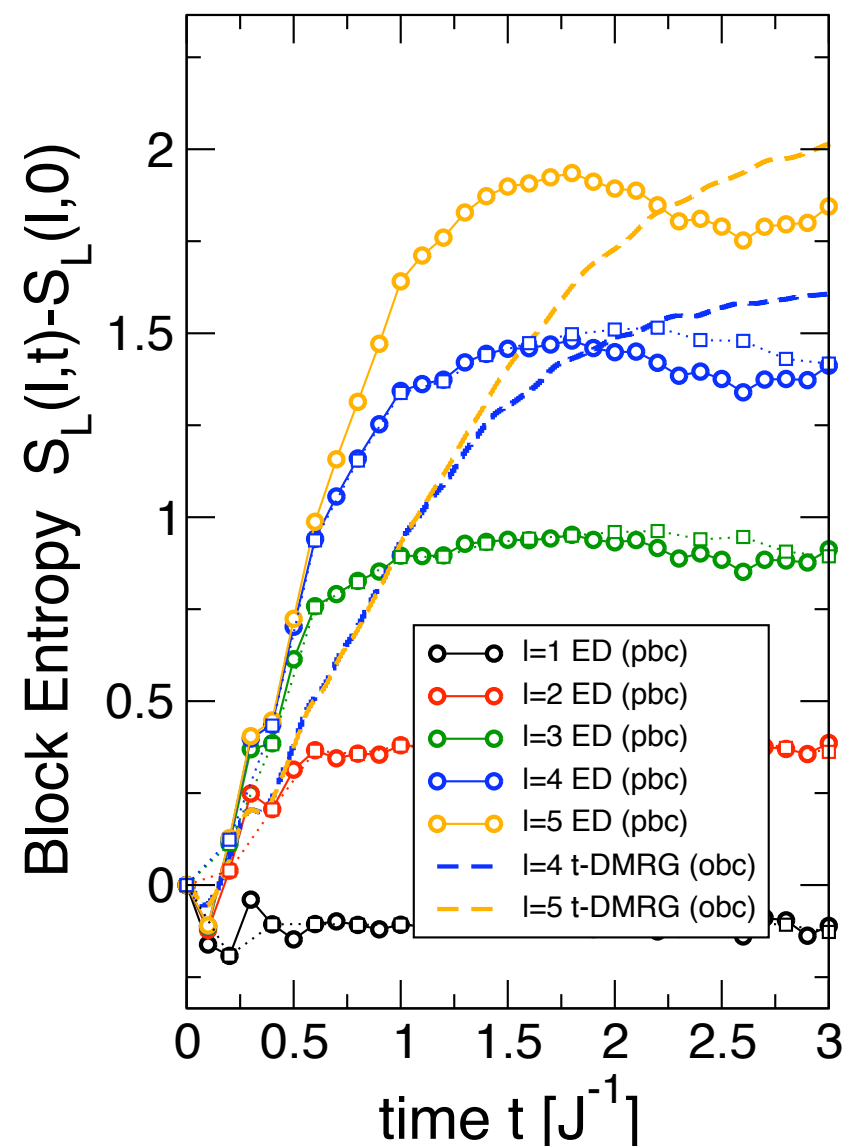
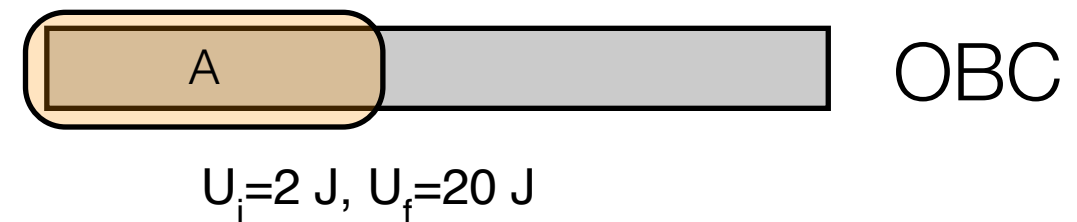
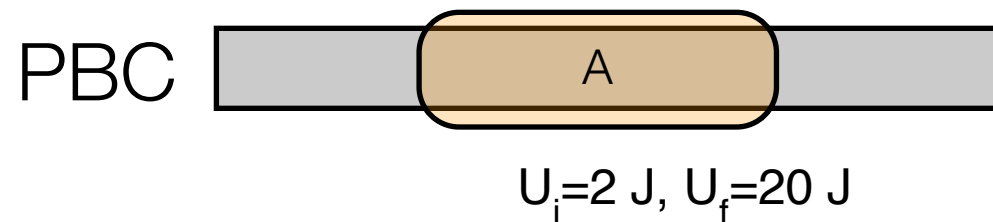
- von Neumann entropy of a block A consisting of l sites $S_A = \text{Tr}_A[-\rho_A \log \rho_A]$





Entanglement time evolution

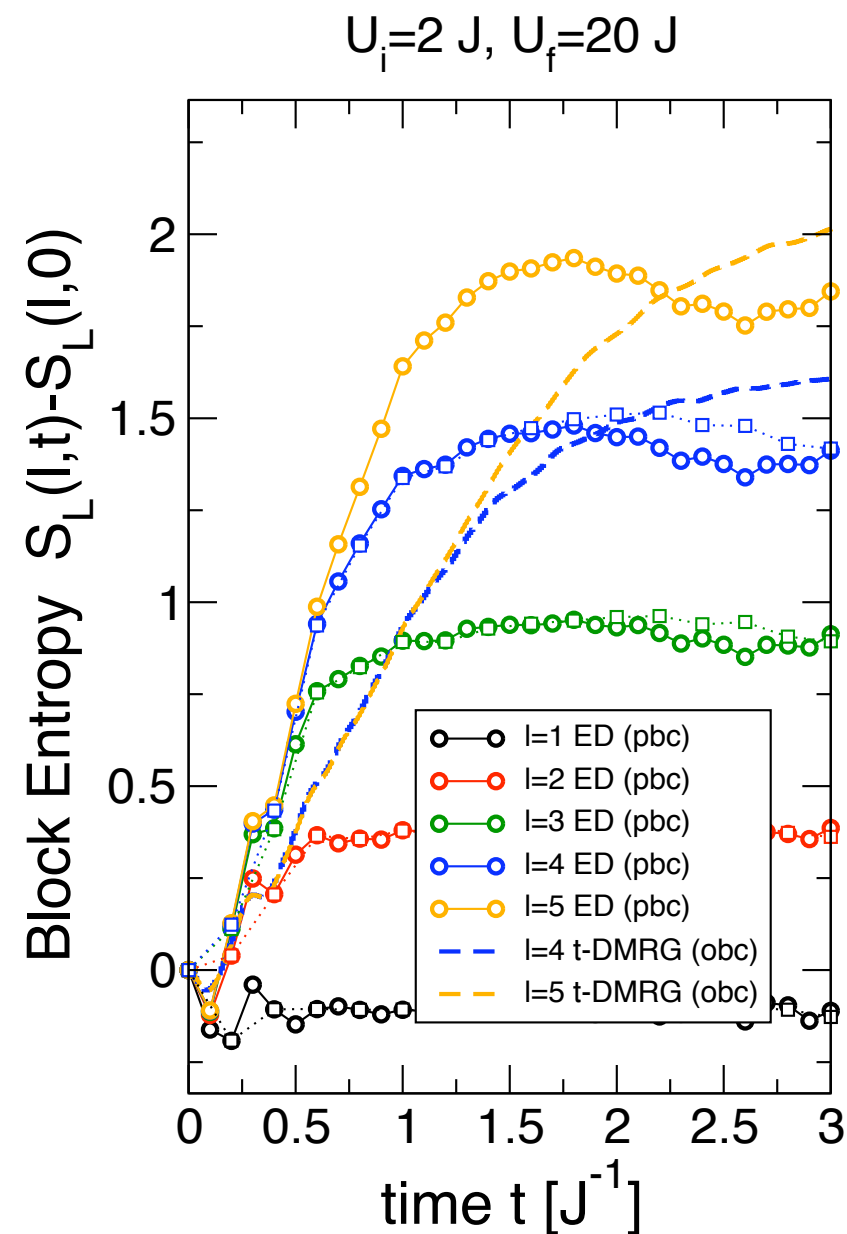
- von Neumann entropy of a block A consisting of l sites $S_A = \text{Tr}_A[-\rho_A \log \rho_A]$



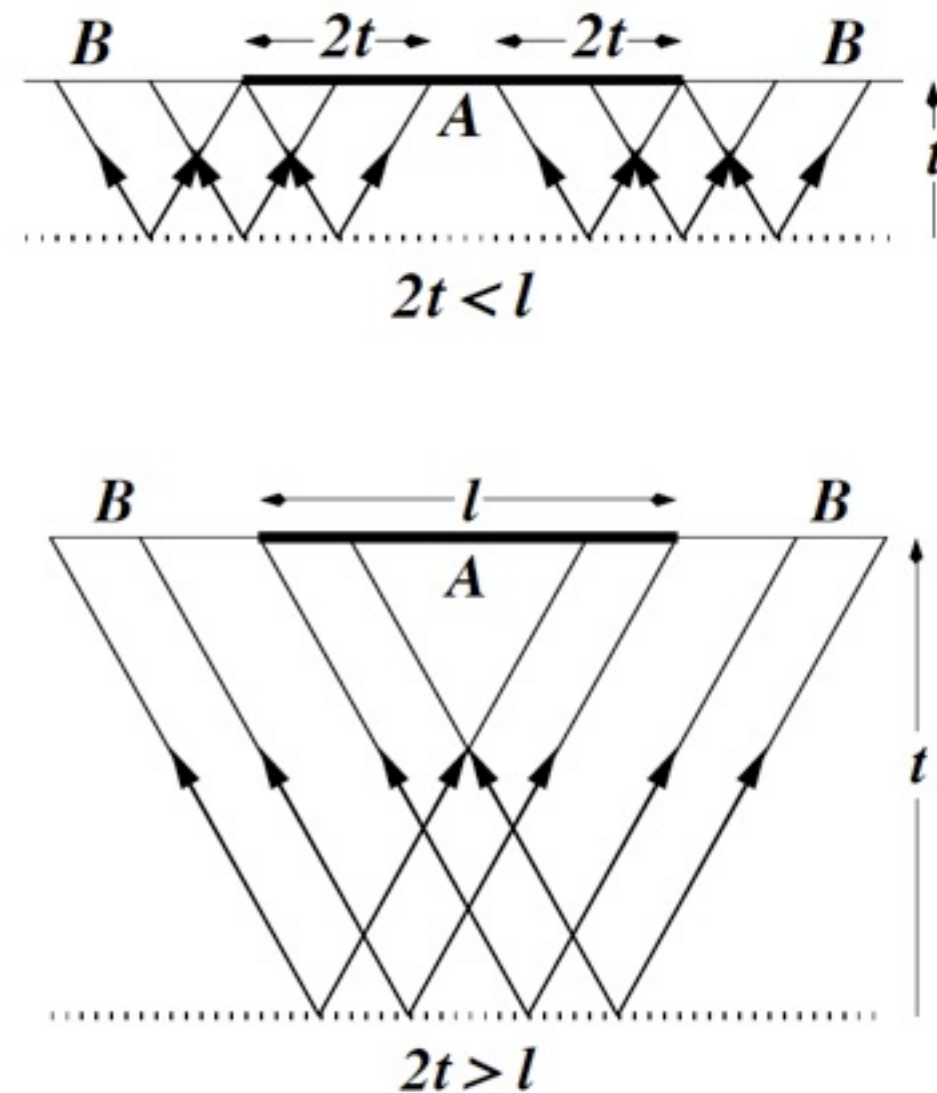


Entanglement time evolution

- Linear growth in time first, then saturation to value proportional to l



AML and Kollath, JSTAT '08



Calabrese and Cardy, JSTAT '05

G. De Chiara *et al.*, JSTAT '06

Related systems: Barmettler *et al.*, PRA 2008, Manmana *et al.* PRB 2009



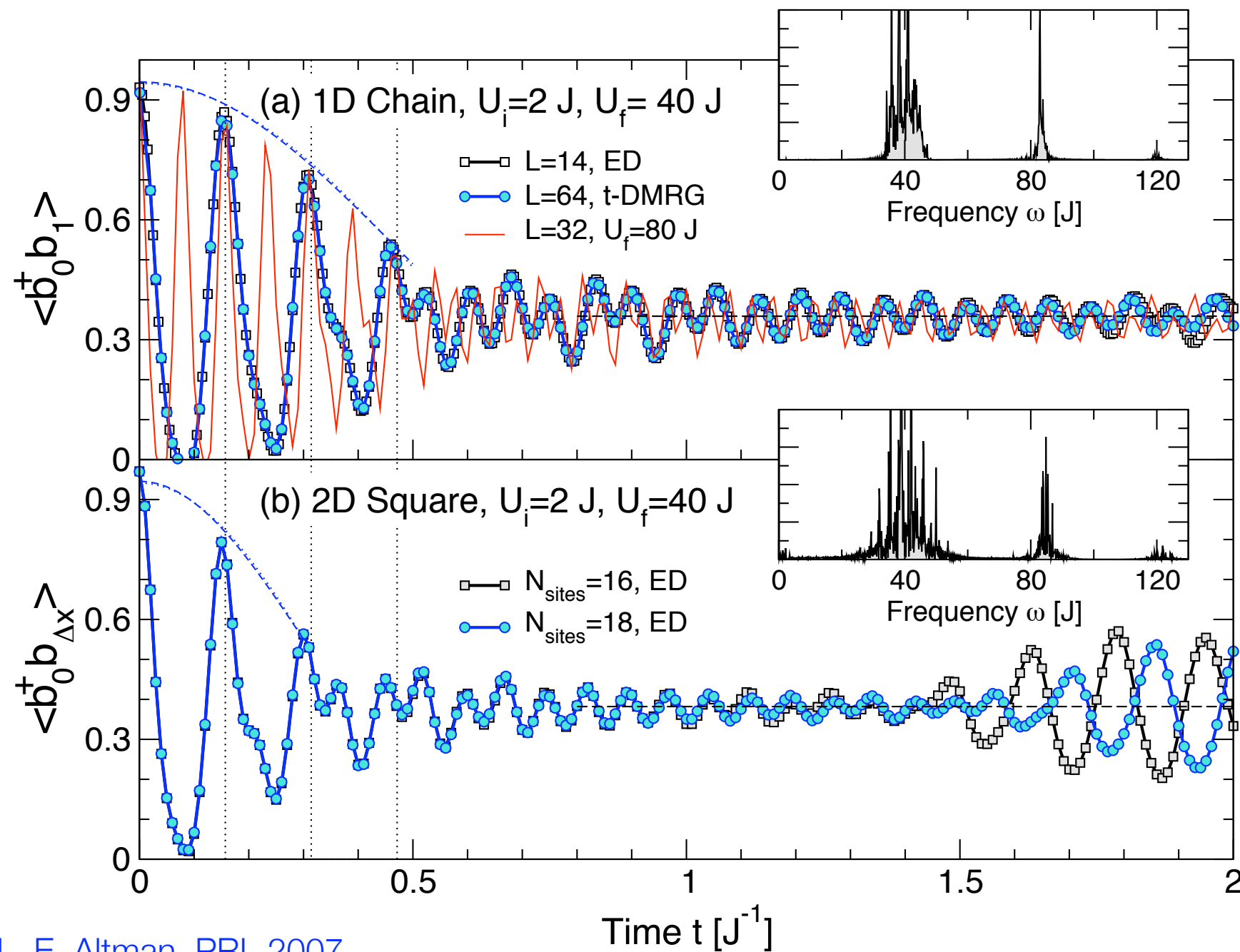
Outline

- Experimental Motivation: Ultracold bosons in an optical lattice
- Short time behavior
 - Light-cone effect:
spreading of correlations
entanglement entropy
- Long time behavior
 - Properties of steady state ?
 - Is the steady state already “thermal” ?



Relaxation

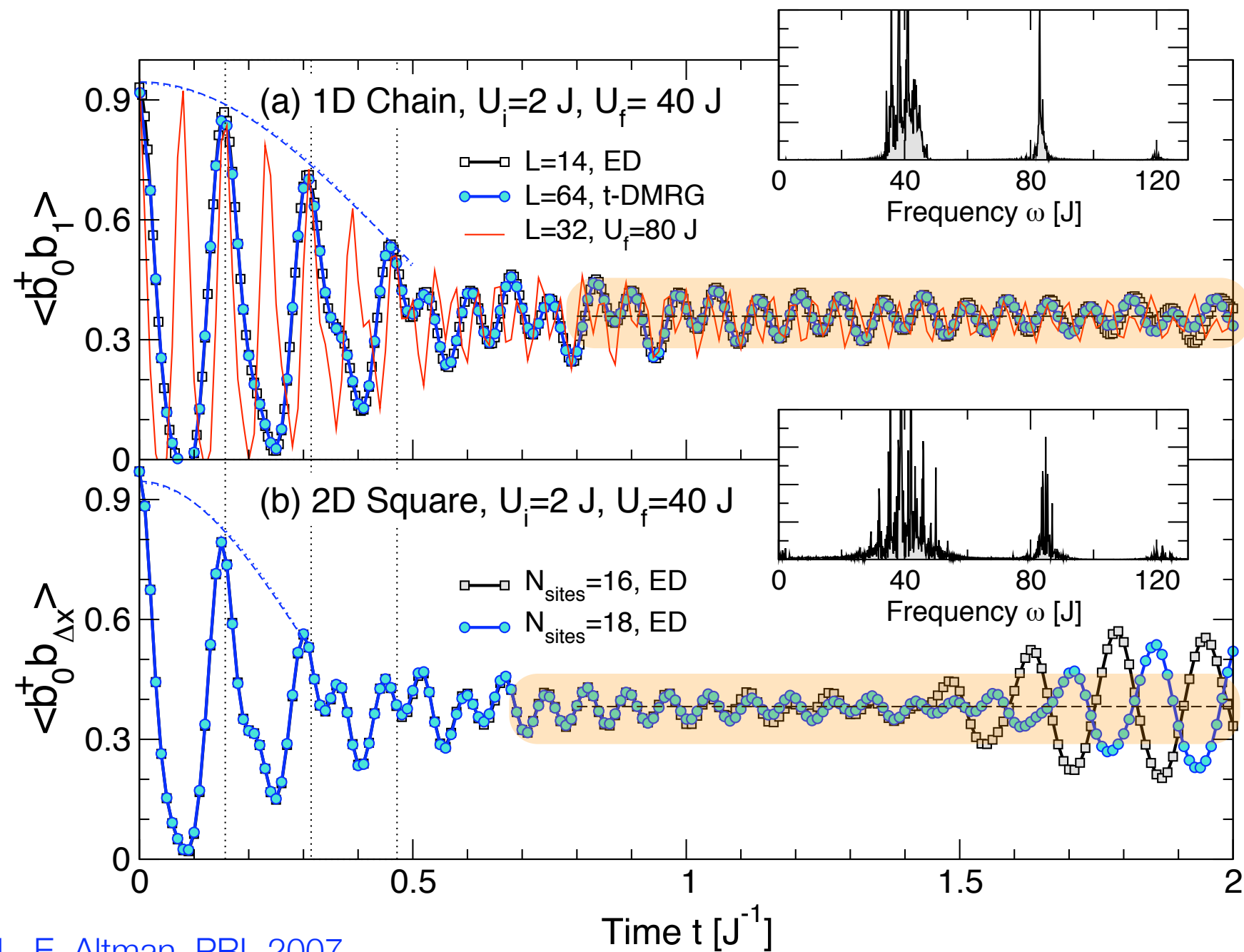
- Properties of the steady state after the relaxation





Relaxation

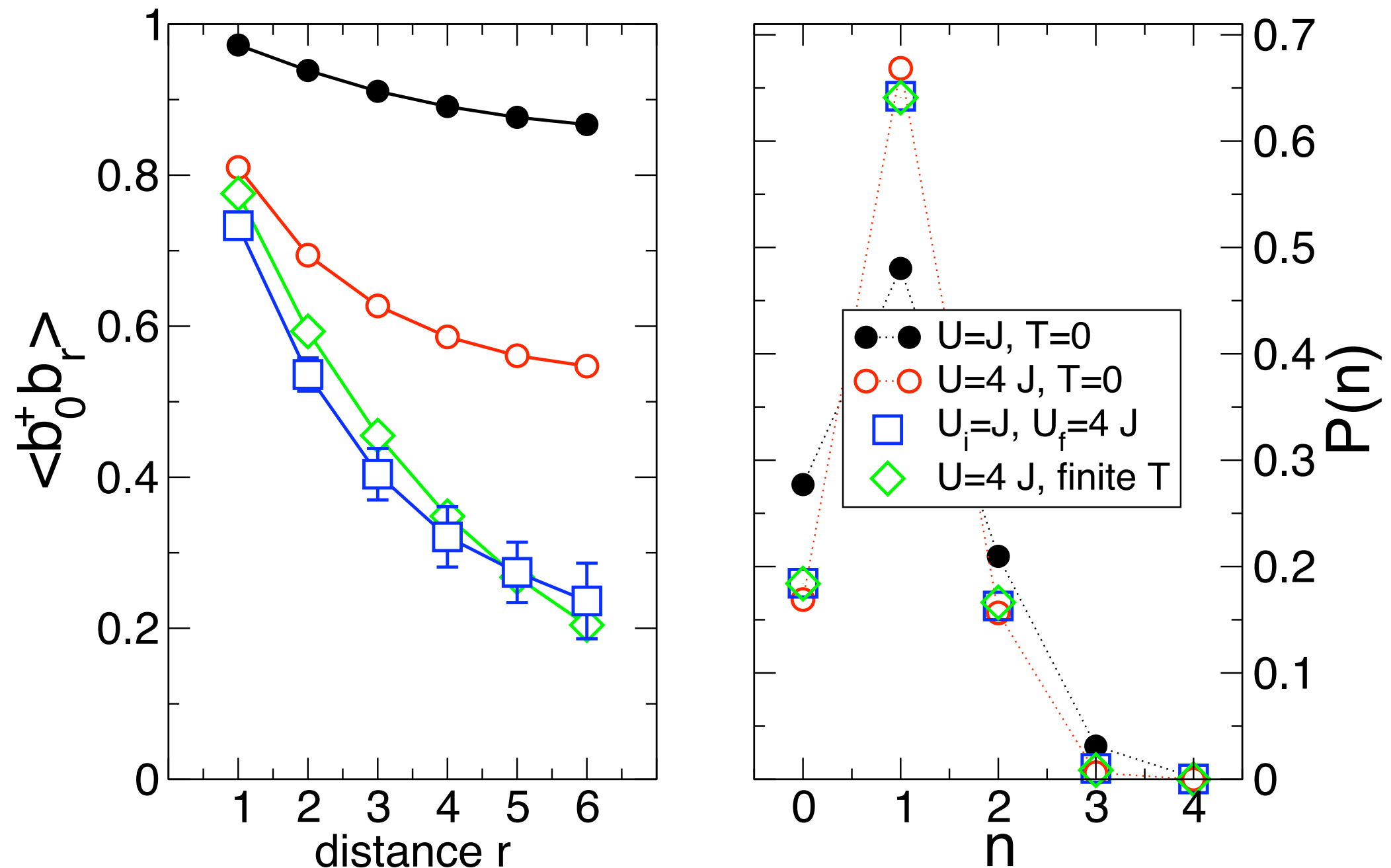
- Properties of the steady state after the relaxation





Weak Quench: Looks “thermal”

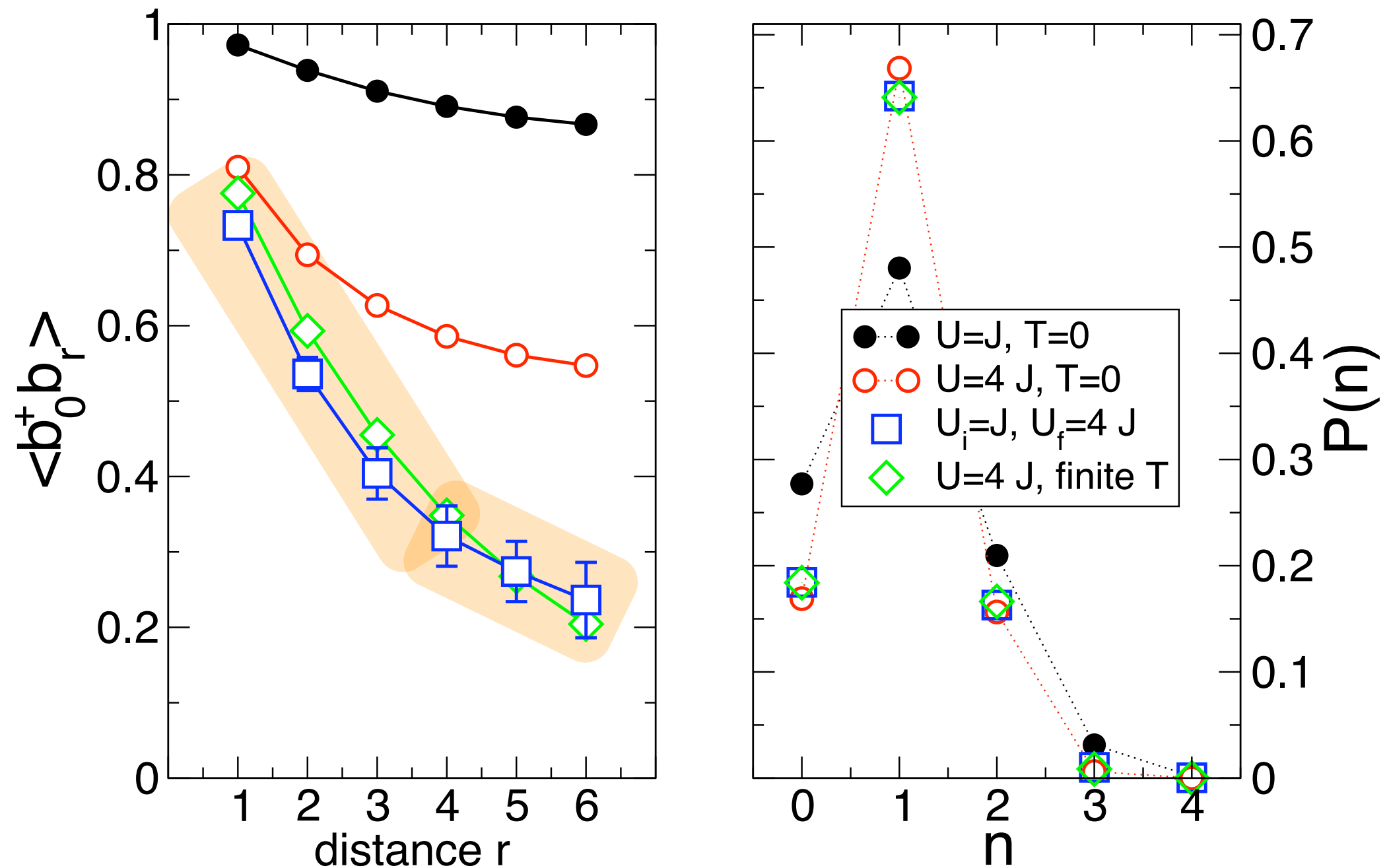
1D Chain, $U_i=J$, $U_f=4 J$





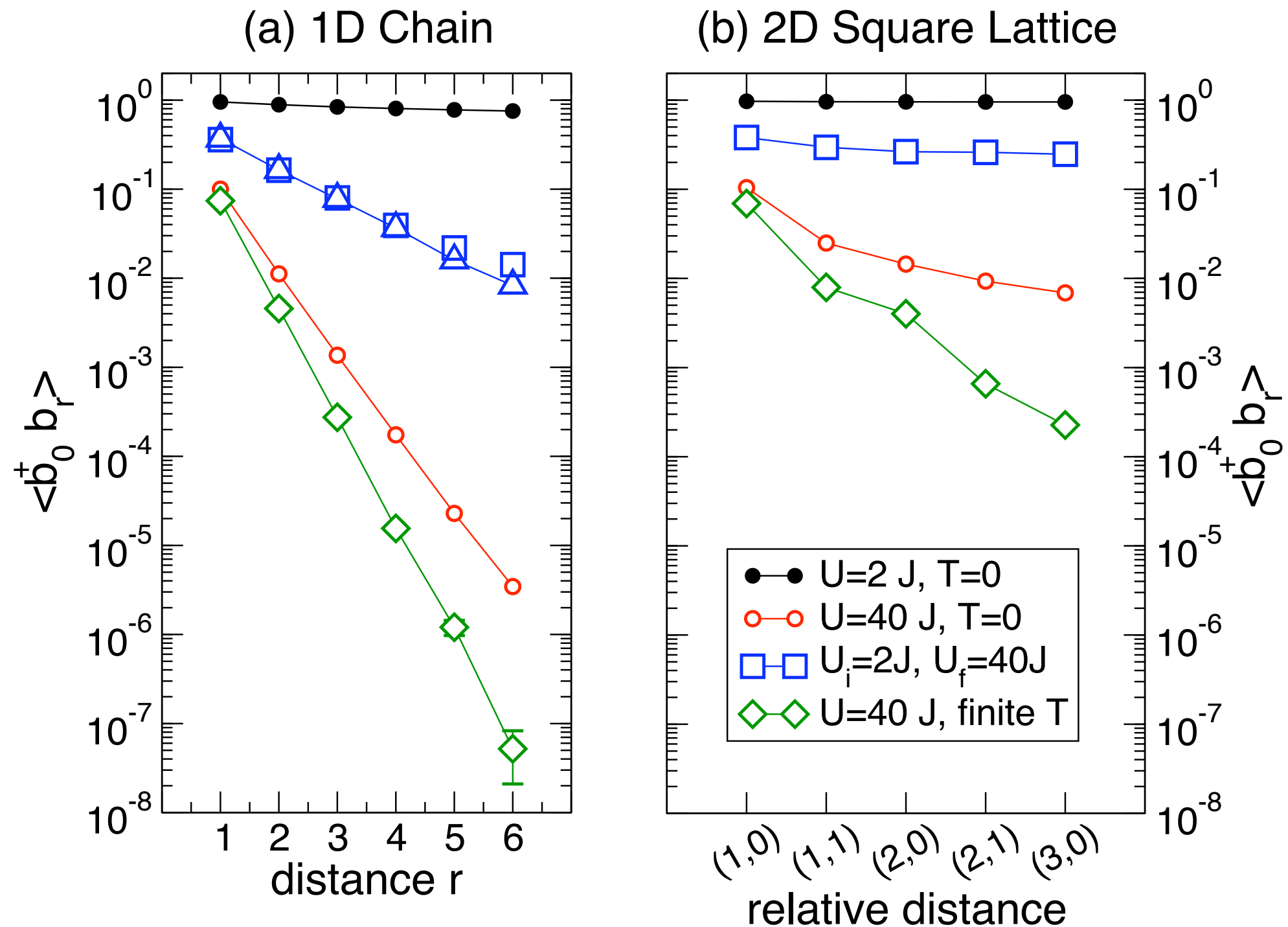
Weak Quench: Looks “thermal”

1D Chain, $U_i=J$, $U_f=4J$



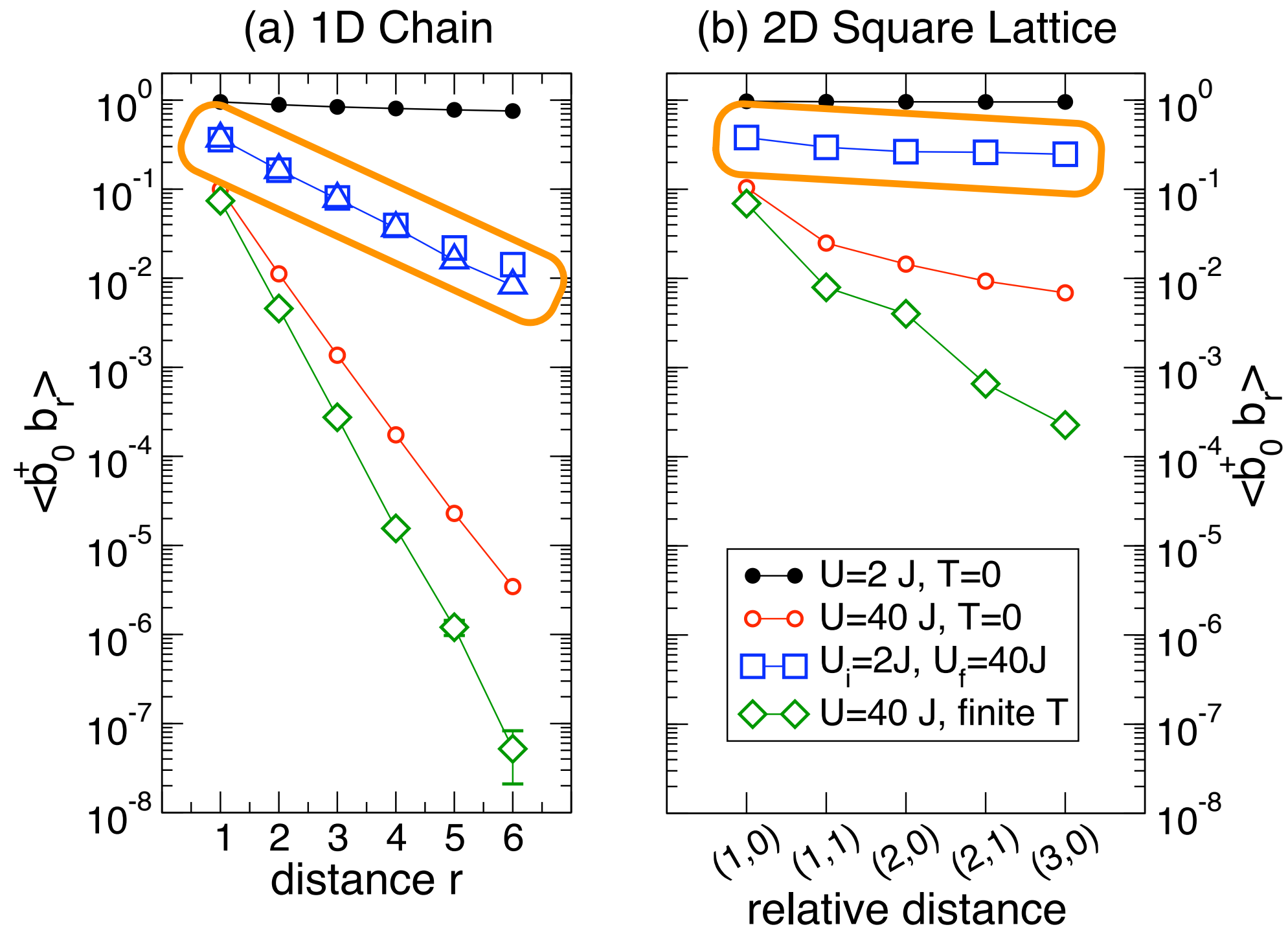


Deep Quench: non-thermal / memory effect ?



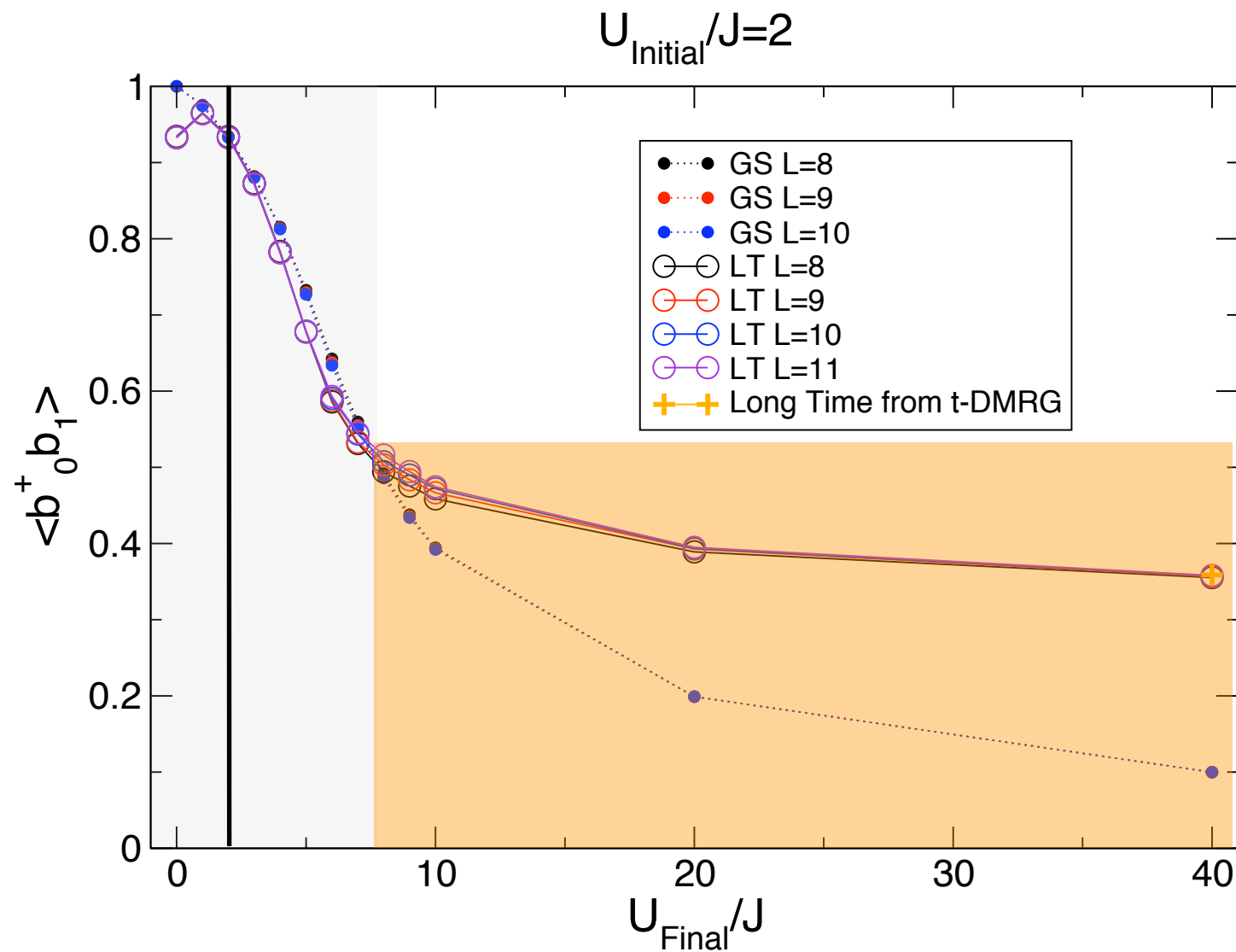


Deep Quench: non-thermal / memory effect ?



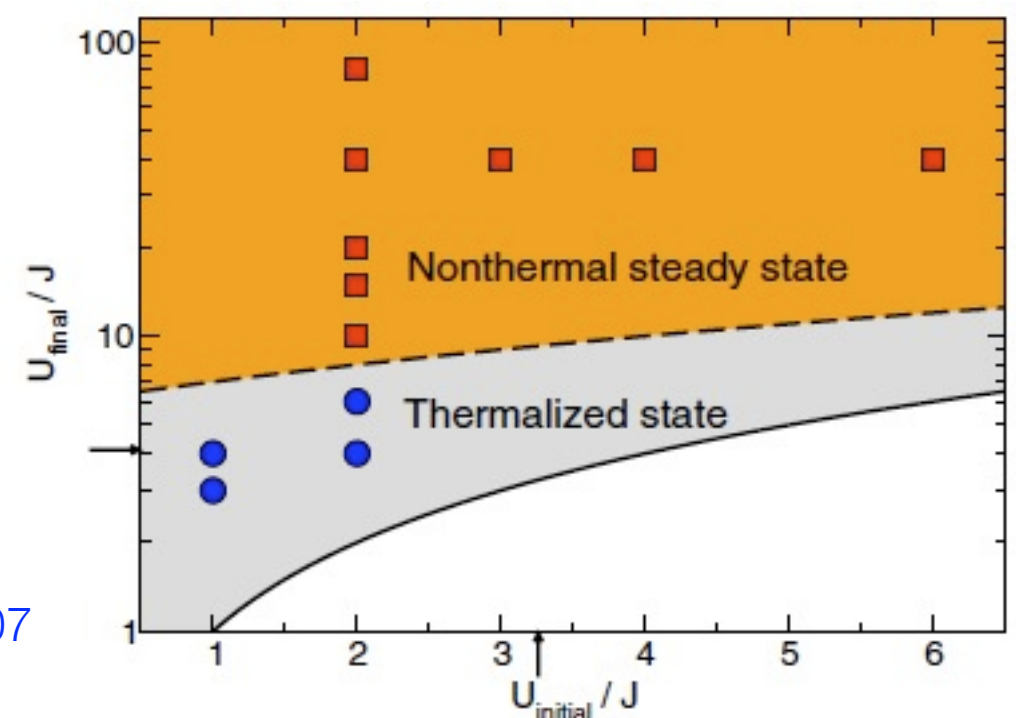


Quench depth dependence



C. Kollath, AML, E. Altman, PRL 2007

- Appearance of a seemingly non-thermal steady state at large U_{final}
- Why is this ?
(Non)-Integrability ?
atypical eigenstates targeted ?





Back to the roots

- At $t > 0$ $|\psi(t)\rangle = e^{-iHt}|\psi_0\rangle$, and long time averages are given by:

$$\langle \mathcal{O} \rangle_{\infty} = \frac{1}{T} \int_0^T dt \langle \psi(t) | \mathcal{O} | \psi(t) \rangle = \frac{1}{T} \int_0^T dt \sum_{\alpha, \beta} c_{\alpha} c_{\beta}^* e^{-it(E_{\alpha} - E_{\beta})} \langle \beta | \mathcal{O} | \alpha \rangle$$

$$\langle \mathcal{O} \rangle_{\infty} = \sum_{\alpha} |c_{\alpha}|^2 \langle \alpha | \mathcal{O} | \alpha \rangle = \text{Tr}[\rho_D \mathcal{O}]$$
$$c_{\alpha} = \langle \alpha | \psi_0 \rangle$$
$$\rho_D = \sum_{\alpha} |c_{\alpha}|^2 |\alpha\rangle \langle \alpha|$$

- Thermalization:
von Neumann 1929

$$\sum_{\alpha} |c_{\alpha}|^2 \langle \alpha | \mathcal{O} | \alpha \rangle = \langle \mathcal{O} \rangle_{E, N}$$

\updownarrow *dependent* \updownarrow *independent*
on the initial state



Eigenstate thermalization hypothesis (ETH)

- Deutsch (91), Srednicki (94)

The expectation value $\langle \alpha | \mathcal{O} | \alpha \rangle$ of a few body observable in an eigenstate $|\alpha\rangle$ of a large interacting many body system equals the thermal micro-canonical average at the intensive energy E_α/N .

- Rigol, Dunjiko, Olshanii, Nature 2008

In the diagonal ensemble the intensive energy does not fluctuate and is equal (by definition) to the micro-canonical one

$$\left(\sum (E_\alpha/N)^2 |c_\alpha|^2 - \left(\sum (E_\alpha/N) |c_\alpha|^2 \right)^2 \right) \rightarrow 0 \quad \text{for } N \rightarrow \infty$$

● Thermalization:

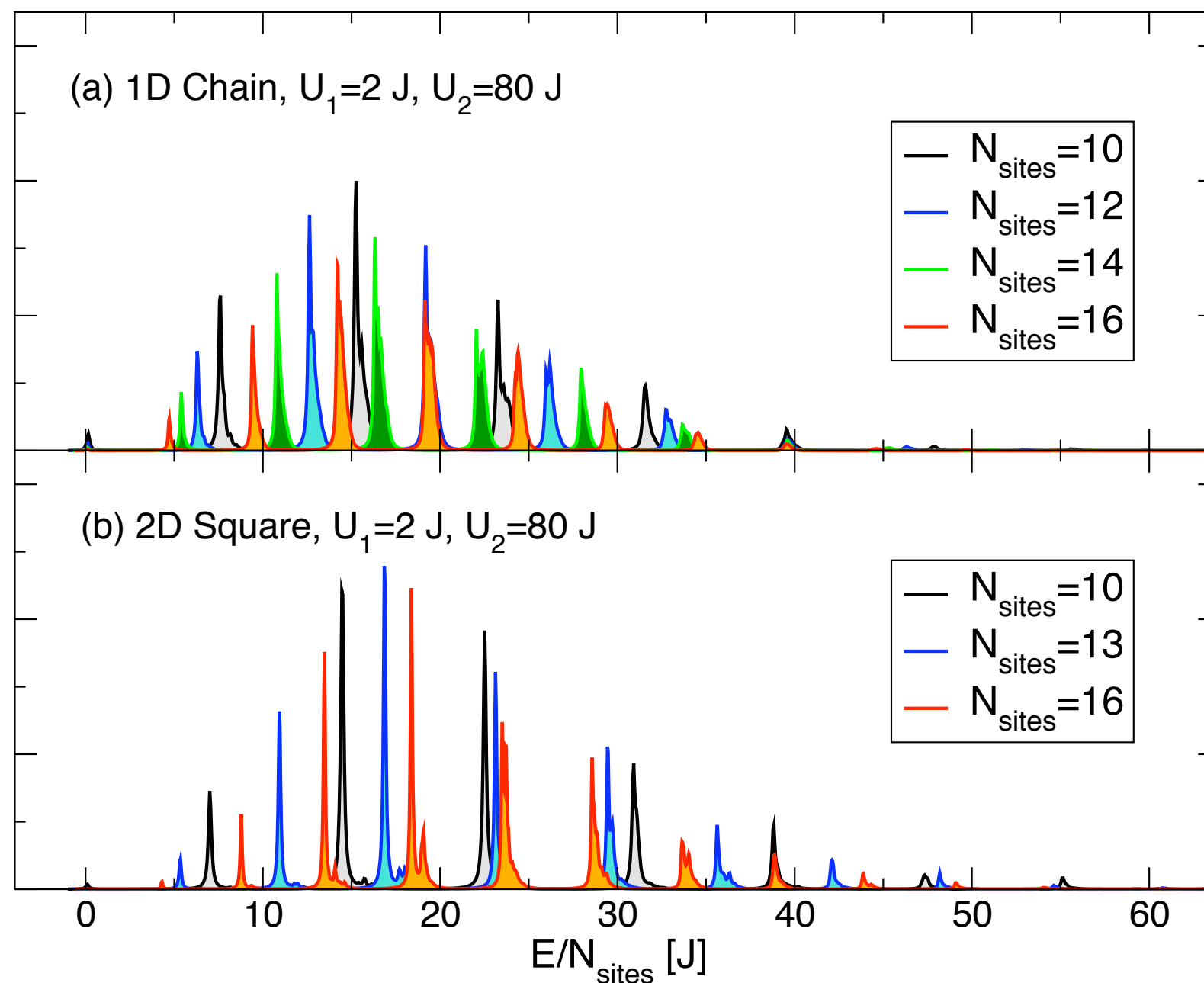
$$\sum_{\alpha} |c_{\alpha}|^2 \langle \alpha | \mathcal{O} | \alpha \rangle = \sum_{\alpha} |c_{\alpha}|^2 \langle \mathcal{O} \rangle_{E_{\alpha}, N} = \langle \mathcal{O} \rangle_{E, N}$$



Quench: Overlap with U_f eigenbasis

- Extensive amount of energy pumped into the system through the quench

$$f(\omega) = \sum_{\alpha} |c_{\alpha}|^2 \times \delta(N\omega - E_{\alpha})$$

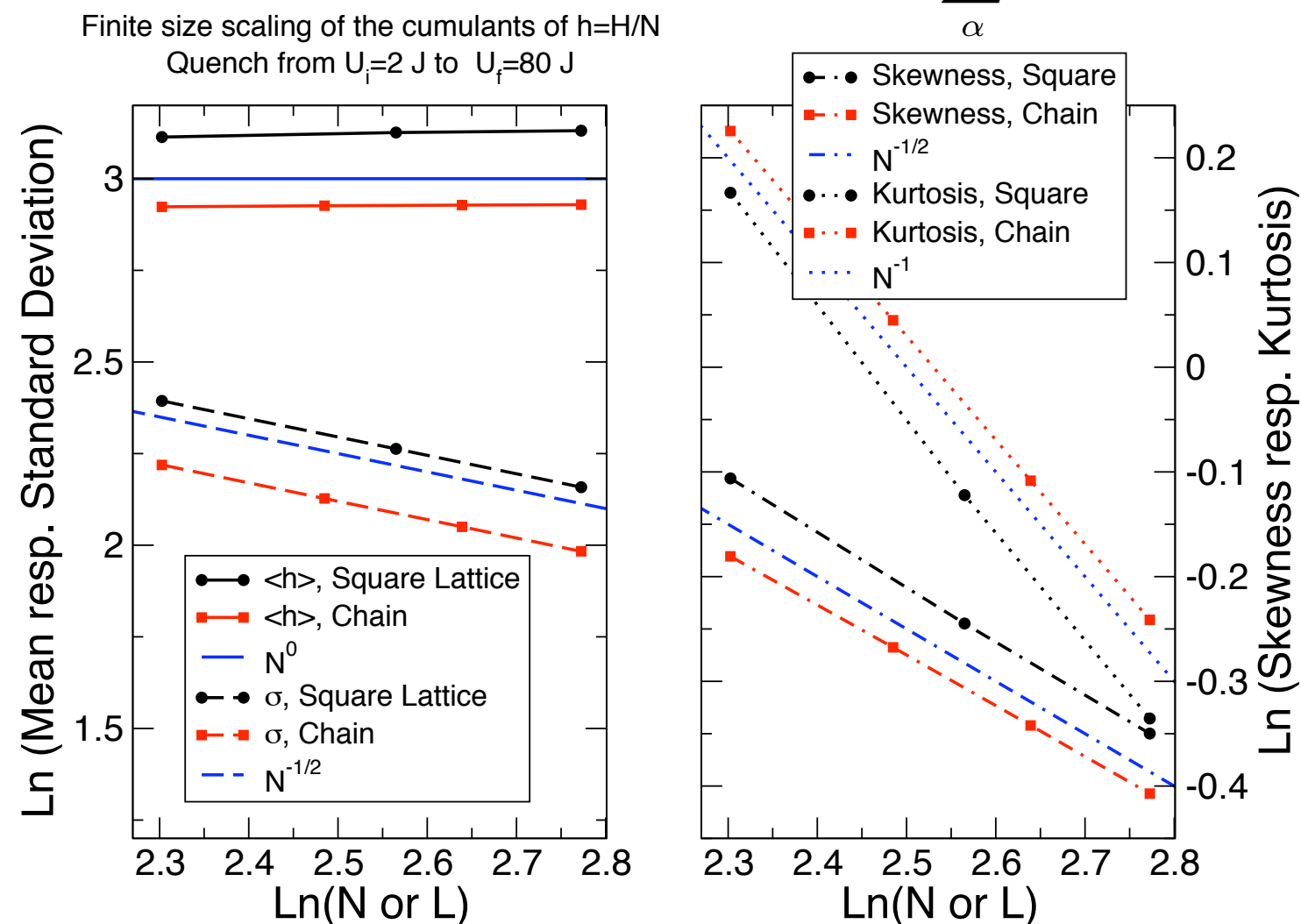




Quench: Cumulants of overlaps

- Cumulants of Quench distribution: low cumulants approach Gaussian values (as in CLT)

$$f(\omega) = \sum_{\alpha} |c_{\alpha}|^2 \times \delta(N\omega - E_{\alpha})$$



see also S. Manmana *et al.*, PRL 2007; M. Rigol *et al.*, Nature 2008

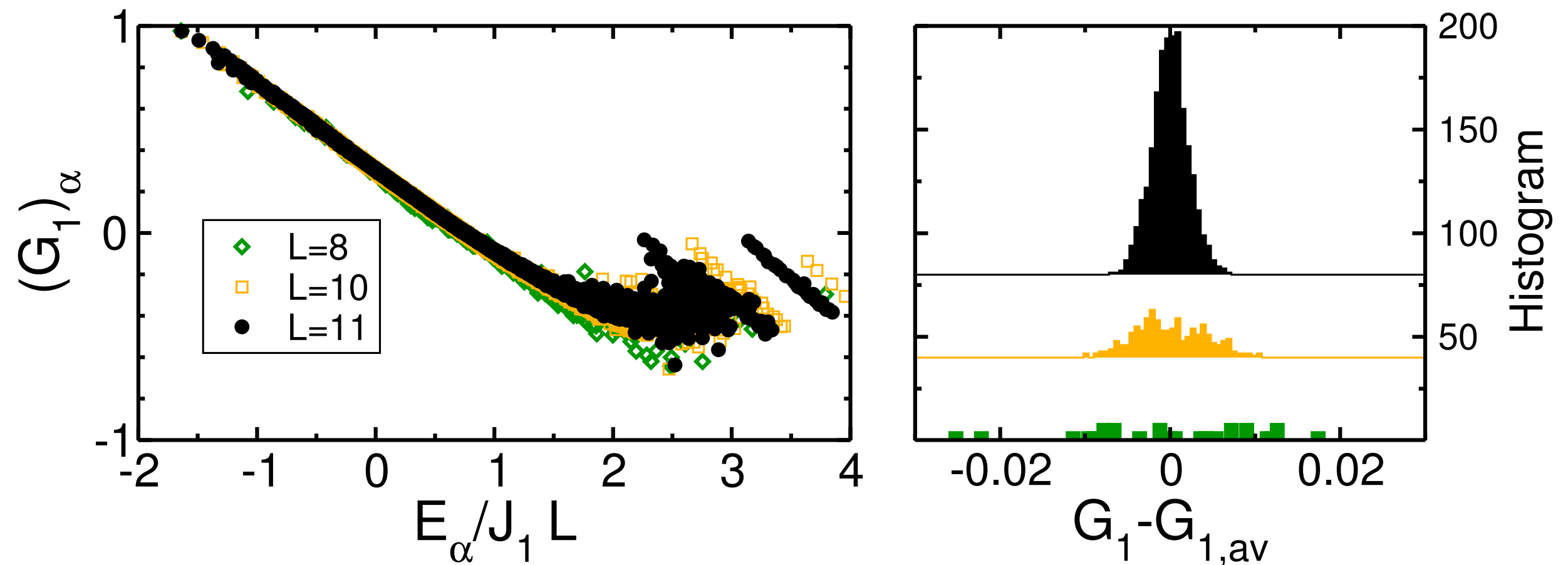
- What do very high moments do ? Does some structure survive ?



ETH: G_1 of eigenstates at $U/J=1$

- at small U rare states seem to be absent already for small system sizes.

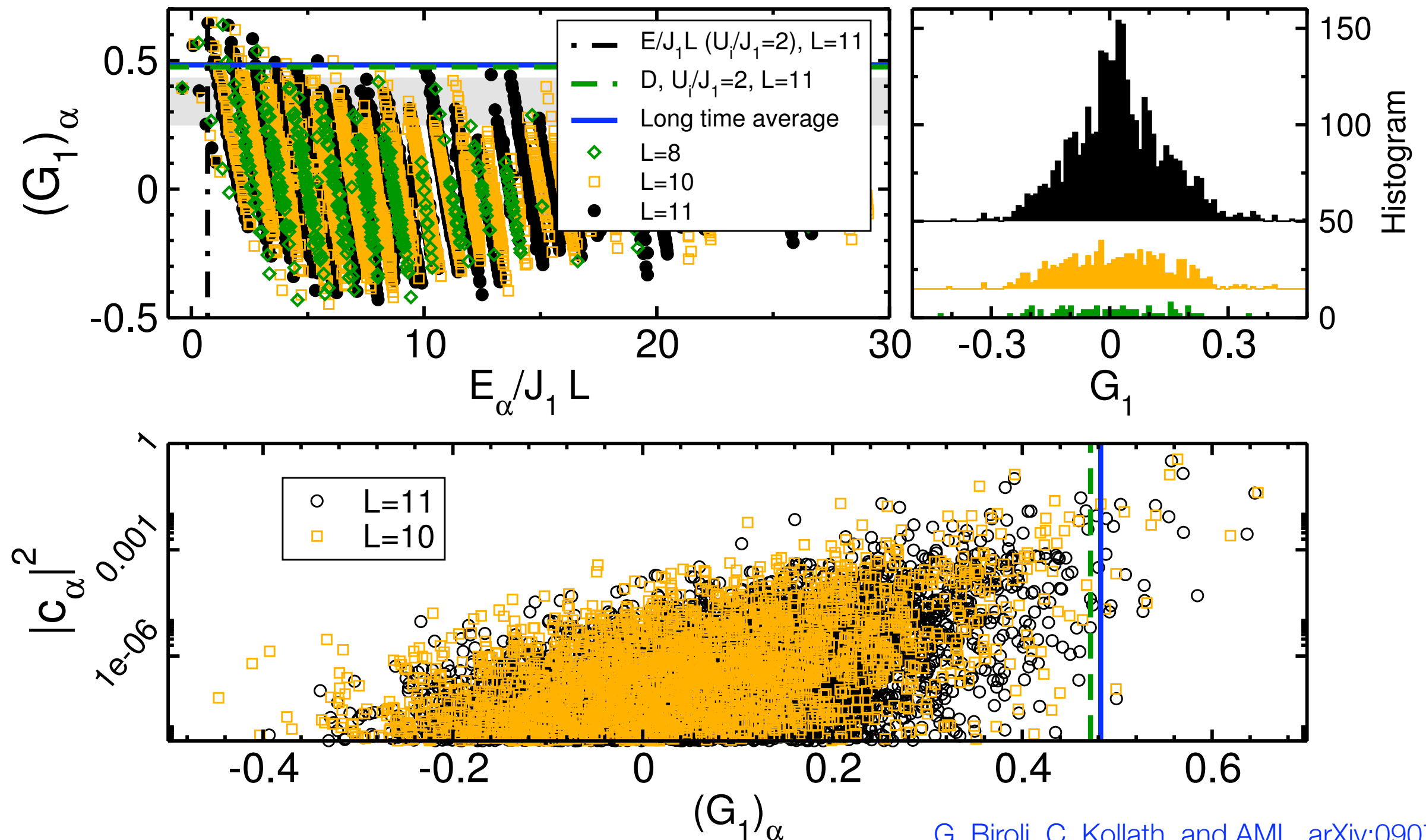
$$(\mathcal{G}_1)_\alpha = \langle \alpha | b_j^\dagger b_{j+1} | \alpha \rangle$$





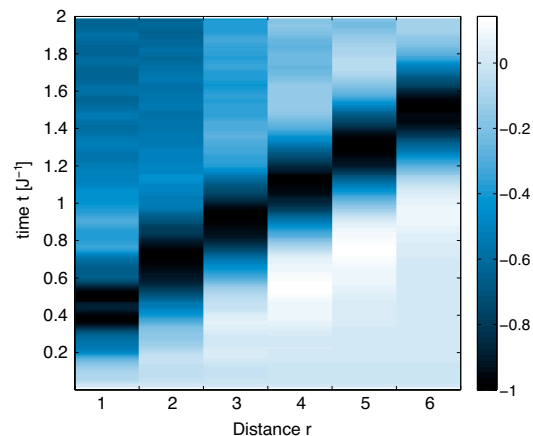
ETH ? : G_1 of eigenstates at $U/J=10$

- Full diagonalization results for small systems $(\mathcal{G}_1)_\alpha = \langle \alpha | b_j^\dagger b_{j+1} | \alpha \rangle$

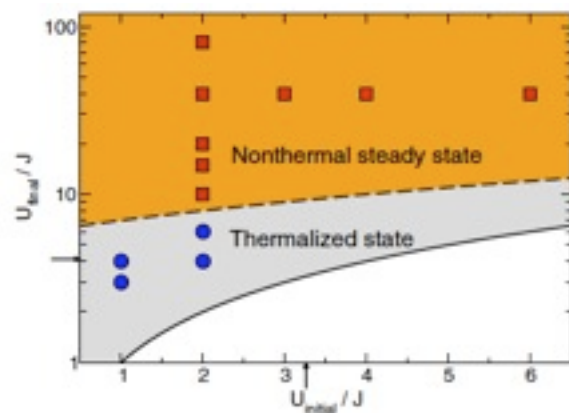




Conclusions



- “Causal” horizon evidenced in the spreading of correlations and entanglement growth
- Nice agreement with theoretical predictions



- Small quenches in this model lead to “thermal” state w.r.t. the observables we checked.
- Deep quenches lead to apparently non-thermal steady state. Importance of rare states for finite systems
- Experimentally relevant for ultracold atomic systems, which are typically much smaller than Avogadro’s number.

Thank you !