Title: Quantum Quenches in Thermodynamic Limit

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Abstract: Studies of the quantum dynamics of isolated systems are currently providing fundamental insights into how statistical mechanics emerges under unitary time evolution. Thermalization seems ubiquitous, but experiments with ultracold gases have shown that it need not always occur, particularly near an integrable point. Unfortunately, computational studies of generic (nonintegrable) models are limited to small systems, for which arbitrarily long times can be calculated, or short times, for which large or infinite system sizes can be solved. Consequently, what happens in the thermodynamic limit after long times has been inaccessible to theoretical studies. In this talk, we introduce a linked-cluster based computational approach that allows one to address the latter question in lattice systems. We provide numerical evidence that, in the thermodynamic limit, thermalization occurs in the nonintegrable regime but fails at integrability. A phase transition-like behavior separates the two regimes.

Quantum quenches in the thermodynamic limit

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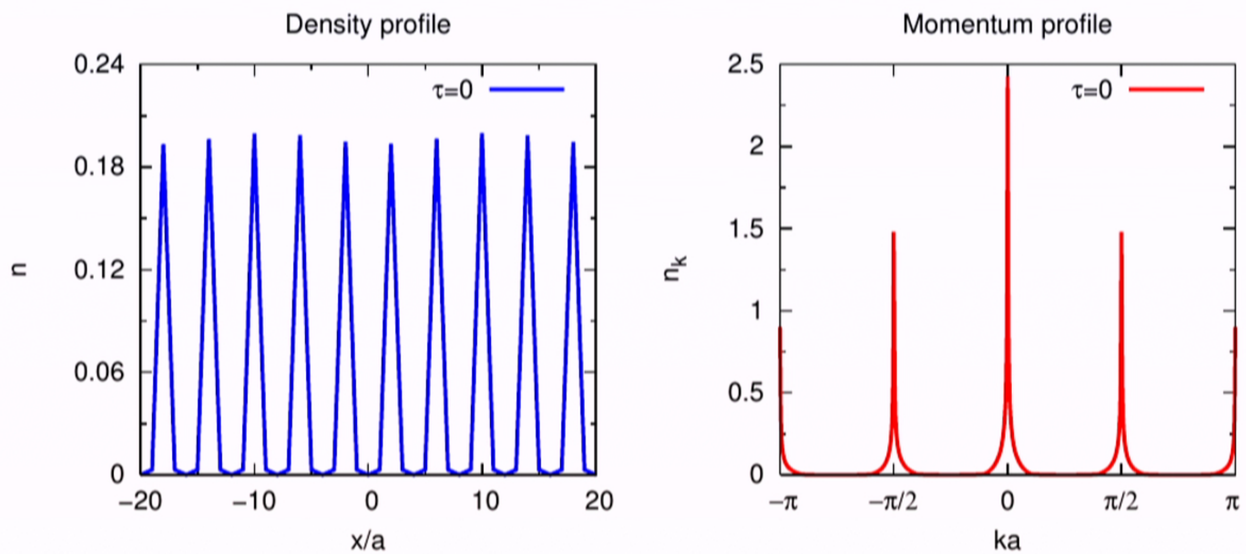
Quantum Many-Body Dynamics

Perimeter Institute for Theoretical Physics
May 12, 2014

Relaxation dynamics after turning off a superlattice



MR, A. Muramatsu, and M. Olshanii, PRA **74**, 053616 (2006).

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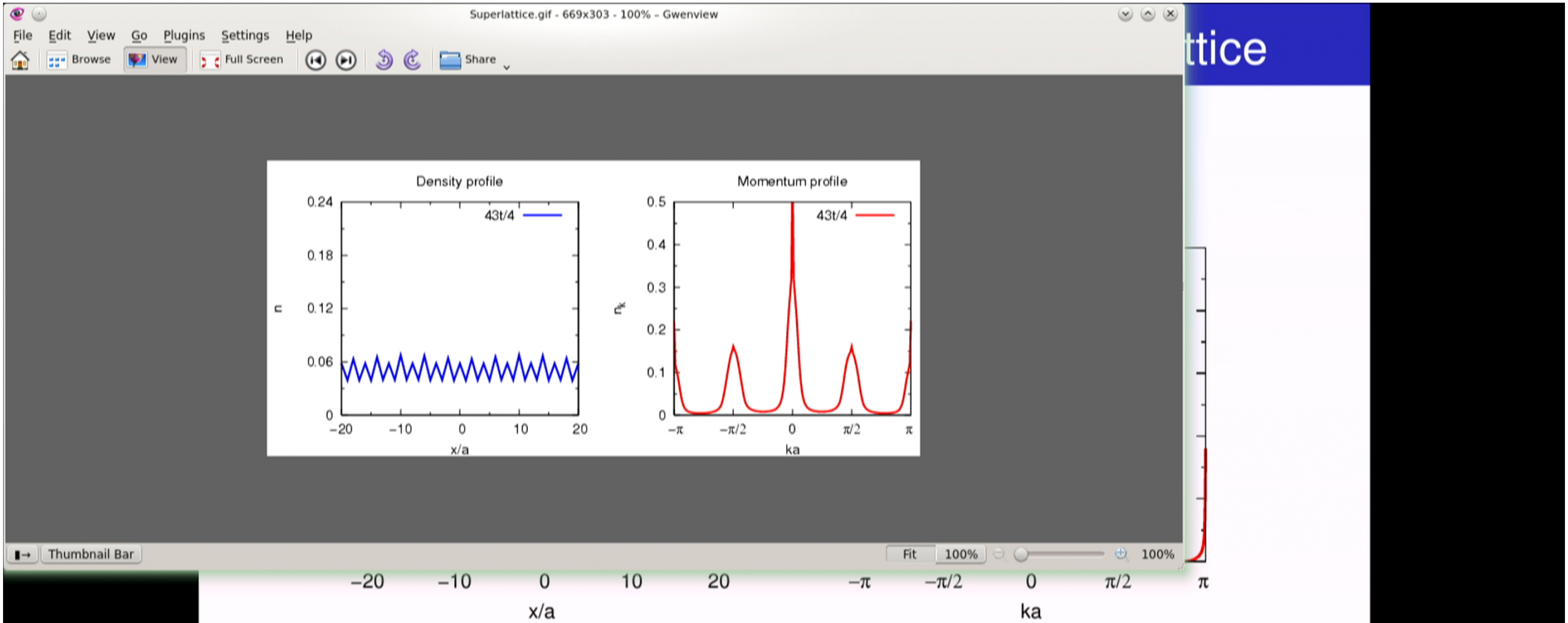

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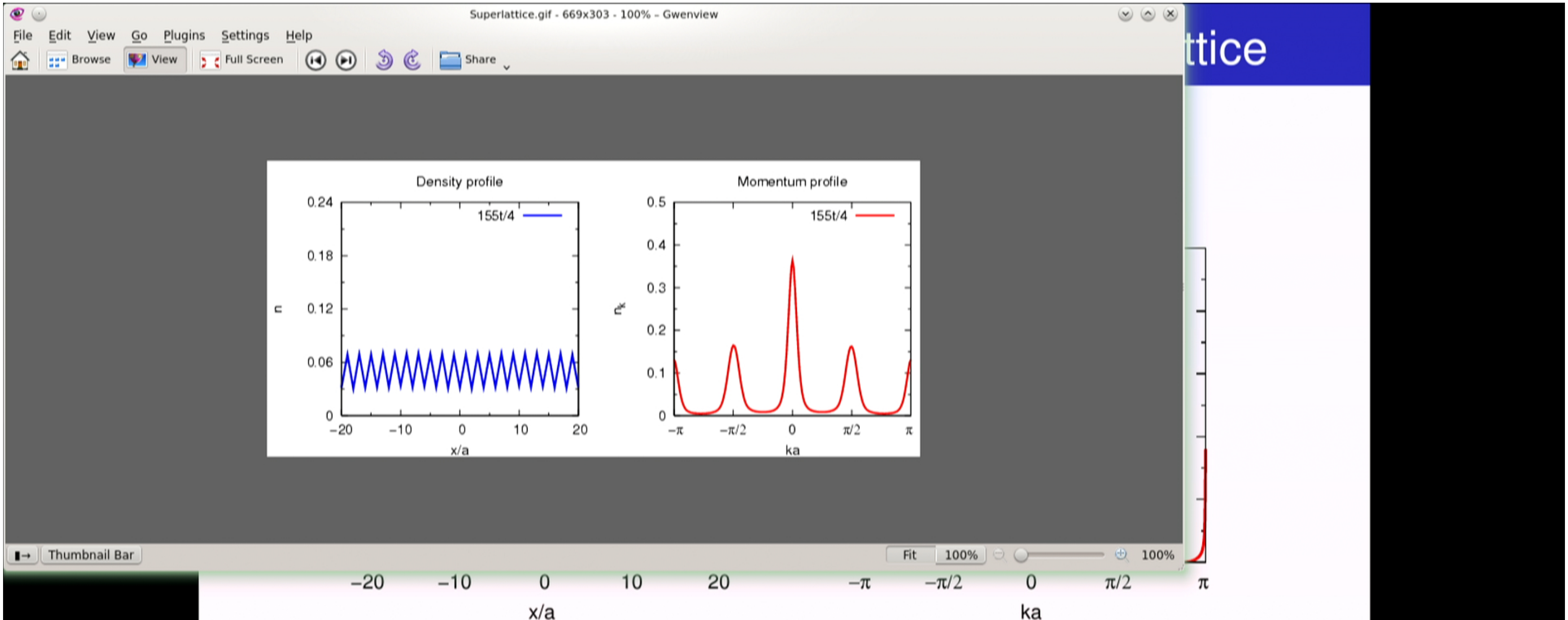

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Unitary dynamics after a sudden quench

If the initial state is not an eigenstate of $\widehat{H}$

$$|\psi_0\rangle \neq |\alpha\rangle \quad \text{where} \quad \widehat{H}|\alpha\rangle = E_\alpha|\alpha\rangle \quad \text{and} \quad E_0 = \langle\psi_0|\widehat{H}|\psi_0\rangle,$$

then a few-body observable O will evolve following

$$O(\tau) \equiv \langle\psi(\tau)|\widehat{O}|\psi(\tau)\rangle \quad \text{where} \quad |\psi(\tau)\rangle = e^{-i\widehat{H}\tau/\hbar}|\psi_0\rangle.$$

What is it that we call thermalization?

$$\overline{O(\tau)} = O(E_0) = O(T) = O(T,\mu).$$

Width of the energy density after a sudden quench

Initial state $|\psi_0\rangle = \sum_\alpha C_\alpha |\alpha\rangle$ is an eigenstate of $\widehat{H}_0$. At $\tau = 0$

$$\widehat{H}_0 \to \widehat{H} = \widehat{H}_0 + \widehat{W} \quad \text{with} \quad \widehat{W} = \sum_j \hat{w}(j) \quad \text{and} \quad \widehat{H}|\alpha\rangle = E_\alpha|\alpha\rangle.$$

The width of the weighted energy density ΔE is then

$$\Delta E = \sqrt{\sum_\alpha E_\alpha^2 |C_\alpha|^2 - (\sum_\alpha E_\alpha |C_\alpha|^2)^2} = \sqrt{\langle\psi_0|\widehat{W}^2|\psi_0\rangle - \langle\psi_0|\widehat{W}|\psi_0\rangle^2},$$

or

$$\Delta E = \sqrt{\sum_{j_1, j_2 \in \sigma} [\langle\psi_0|\hat{w}(j_1)\hat{w}(j_2)|\psi_0\rangle - \langle\psi_0|\hat{w}(j_1)|\psi_0\rangle\langle\psi_0|\hat{w}(j_2)|\psi_0\rangle]} \overset{N\to\infty}{\propto} \sqrt{N},$$

where N is the total number of lattice sites.

MR, V. Dunjko, and M. Olshanii, Nature **452**, 854 (2008).

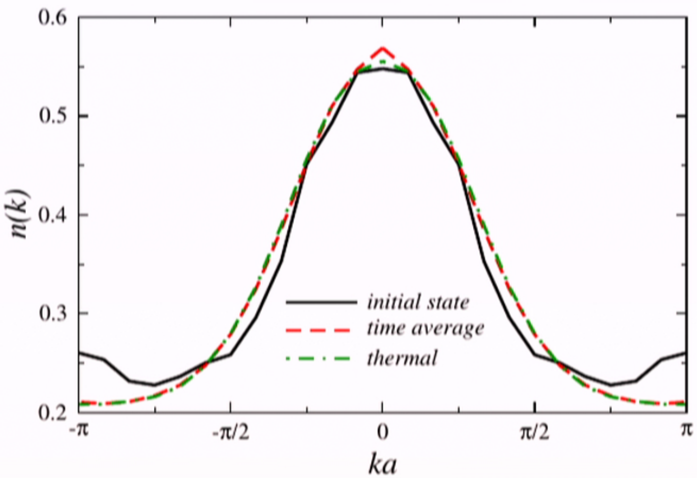
Description after relaxation (lattice models)

Hard-core boson (spinless fermion) Hamiltonian

$$\hat{H} = \sum_{i=1}^{L} -t\left(\hat{b}_i^\dagger \hat{b}_{i+1} + \text{H.c.}\right) + V\hat{n}_i\hat{n}_{i+1} - t'\left(\hat{b}_i^\dagger \hat{b}_{i+2} + \text{H.c.}\right) + V'\hat{n}_i\hat{n}_{i+2}$$

Dynamics vs statistical ensembles

Nonintegrable: $t' = V' \neq 0$



MR, PRL **103**, 100403 (2009), PRA **80**, 053607 (2009), . . .

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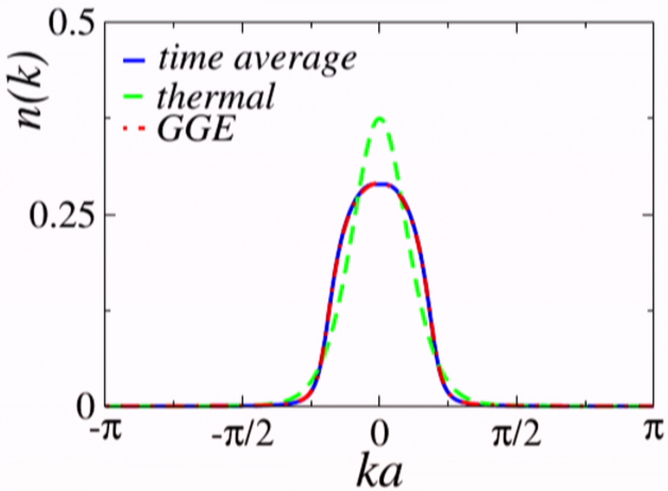

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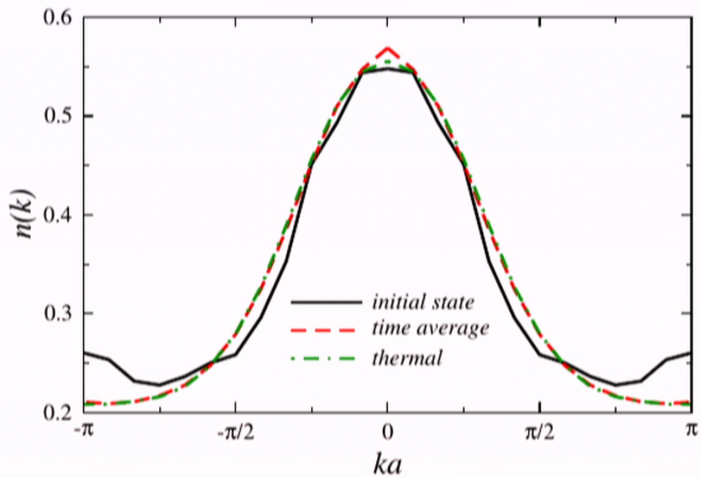

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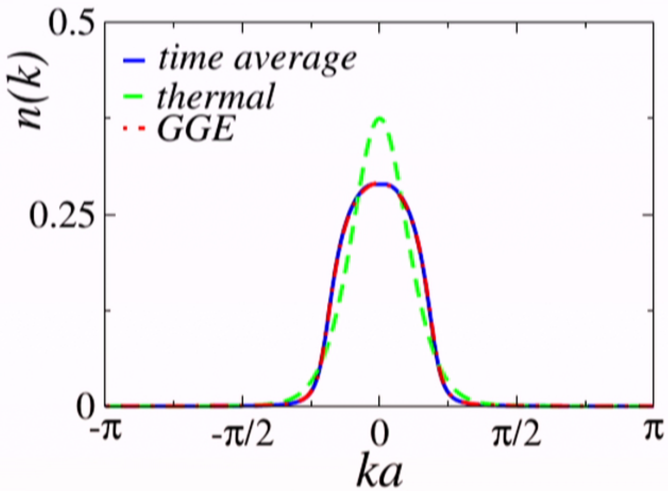

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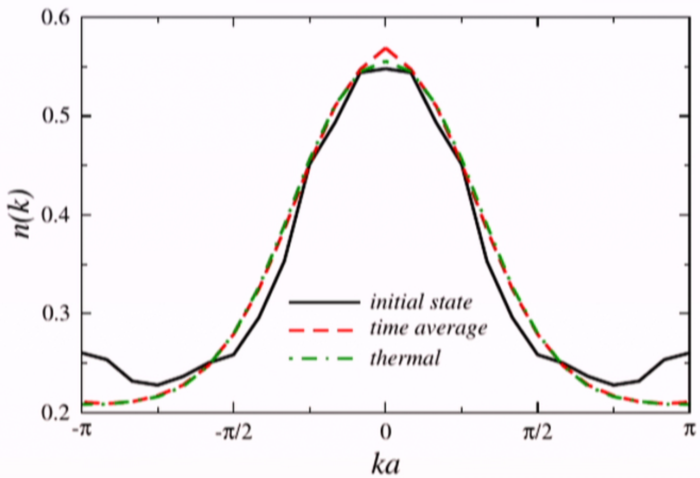

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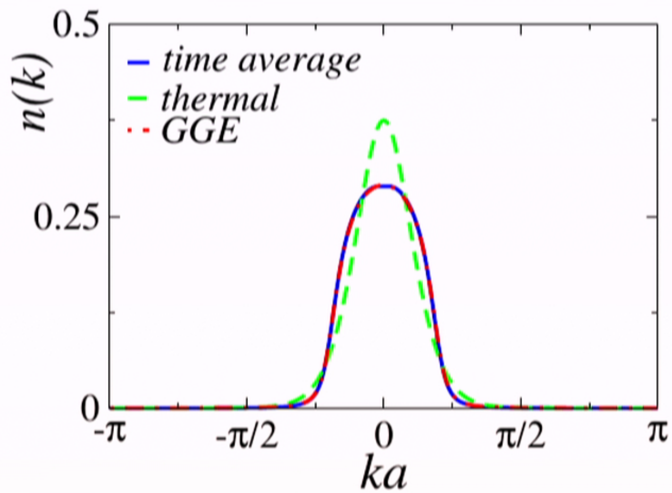

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Eigenstate thermalization

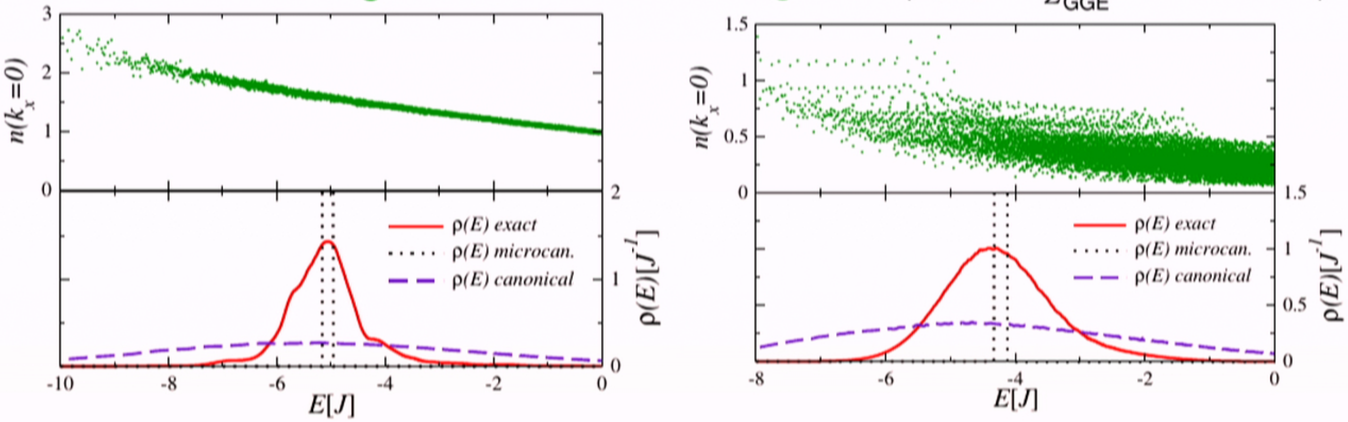
Eigenstate thermalization hypothesis

[Deutsch, PRA **43** 2046 (1991); Srednicki, PRE **50**, 888 (1994).]

- The expectation value $\langle\alpha|\widehat{O}|\alpha\rangle$ of a few-body observable $\widehat{O}$ in an eigenstate of the Hamiltonian $|\alpha\rangle$, with energy E_α, of a many-body system is equal to the thermal average of $\widehat{O}$ at the mean energy E_α:

$$\langle\alpha|\widehat{O}|\alpha\rangle = \langle\widehat{O}\rangle_{\rm ME}(E_\alpha).$$

Nonintegrable — Integrable ($\hat{\rho}_{\rm GGE} = \frac{1}{Z_{\rm GGE}} e^{-\sum_m \lambda_m \hat{I}_m}$)



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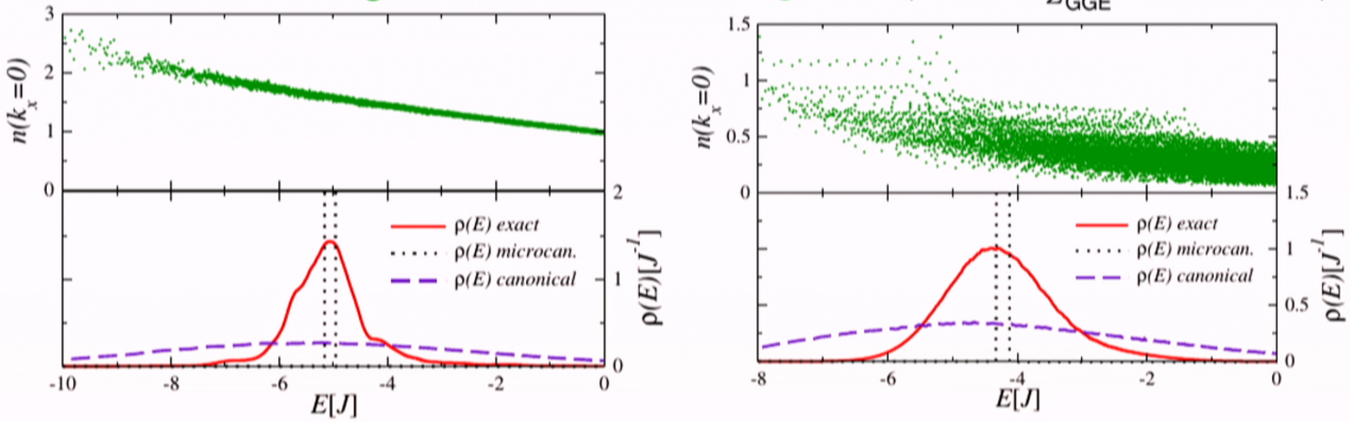

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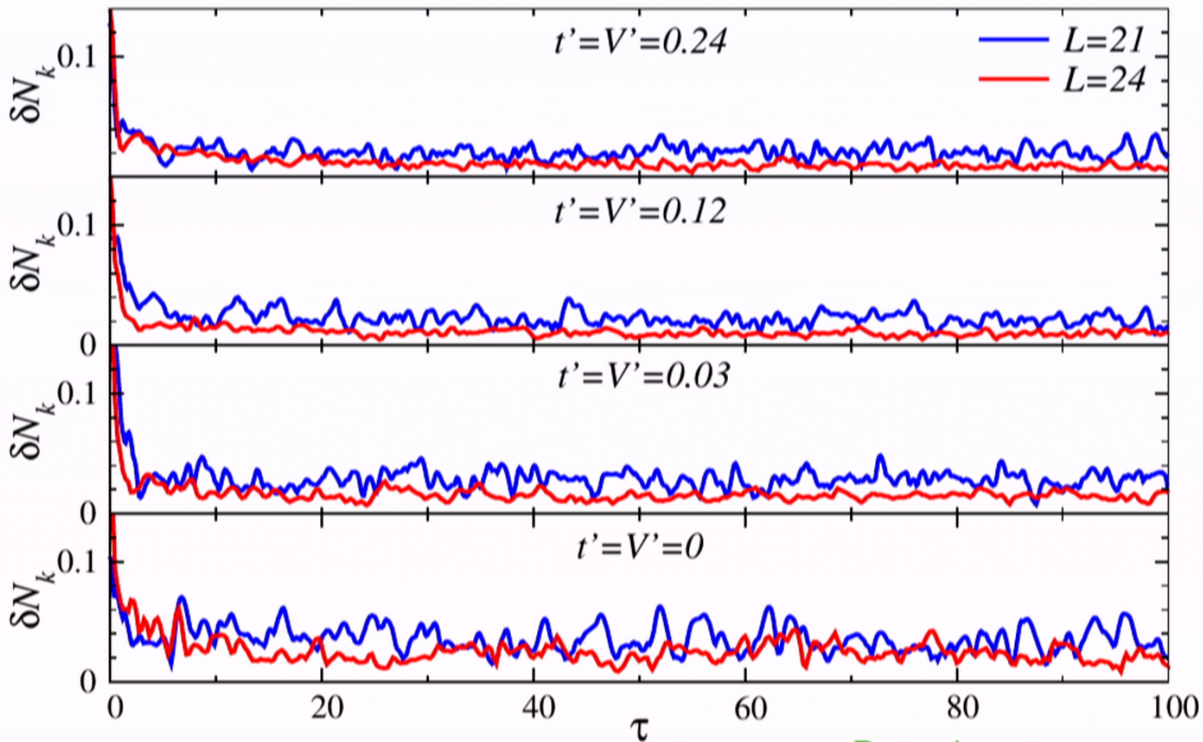
Time fluctuations and their scaling with system size



Relative differences (struct. factor)

$$\delta N(\tau) = \frac{\sum_k |N(k,\tau) - N_{\rm diag}(k)|}{\sum_k N_{\rm diag}(k)}$$

Bounds

(G) P. Reimann, PRL **101**, 190403 (2008).
(G) Linden *et al.*, PRE **79**, 061103 (2009).
(N) Cramer *et al.*, PRL **100**, 030602 (2008).
(N) Venuti&Zanardi, PRE **87**, 012106 (2013).

Time fluctuations

Are they small because of dephasing?

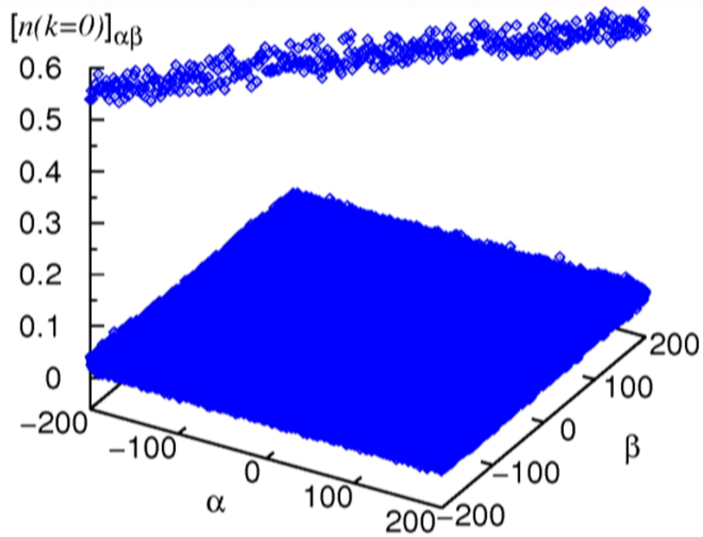
$$\langle\hat{O}(t)\rangle - \overline{\langle\hat{O}(t)\rangle} = \sum_{\substack{\alpha',\alpha\\ \alpha'\neq\alpha}} C^\star_{\alpha'} C_\alpha e^{i(E_{\alpha'}-E_\alpha)t} O_{\alpha'\alpha} \sim \sum_{\substack{\alpha',\alpha\\ \alpha'\neq\alpha}} \frac{e^{i(E_{\alpha'}-E_\alpha)t}}{N_{\text{states}}} O_{\alpha'\alpha}$$

$$\sim \frac{\sqrt{N^2_{\text{states}}}}{N_{\text{states}}} O^{\text{typical}}_{\alpha'\alpha} \sim O^{\text{typical}}_{\alpha'\alpha}$$

Time average of $\langle\hat{O}\rangle$

$$\overline{\langle\hat{O}\rangle} = \sum_\alpha |C_\alpha|^2 O_{\alpha\alpha}$$

$$\sim \sum_\alpha \frac{1}{N_{\text{states}}} O_{\alpha\alpha} \sim O^{\text{typical}}_{\alpha\alpha}$$



One needs: $O^{\text{typical}}_{\alpha'\alpha} \ll O^{\text{typical}}_{\alpha\alpha}$

MR, PRA **80**, 053607 (2009)

Finite temperature properties of lattice models

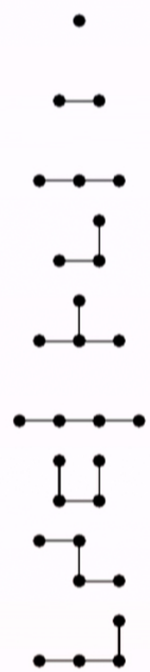
Computational techniques for arbitrary dimensions

- Quantum Monte Carlo simulations
  Polynomial time ⇒ Large systems ⇒ Finite size scaling
  Sign problem ⇒ Limited classes of models
- Exact diagonalization
  Exponential problem ⇒ Small systems ⇒ Finite size effects
  No systematic extrapolation to larger system sizes
  Can be used for any model!

Numerical Linked Cluster Expansions

i) Find all clusters that can be embedded on the lattice

Bond clusters



c	$L(c)$
1	1
2	2
3	2
4	4
5	4
6	2
7	4
8	4
9	8

Numerical Linked Cluster Expansions

i) Find all clusters that can be embedded on the lattice

ii) Group the ones with the same Hamiltonian (Topological cluster)

iii) Find all subclusters of a given topological cluster

No. of bonds	topological clusters
0	1
1	1
2	1
3	2
4	4
5	6
6	14
7	28
8	68
9	156
10	399
11	1012
12	2732
13	7385
14	20665

Numerical Linked Cluster Expansions

i) Find all clusters that can be embedded on the lattice

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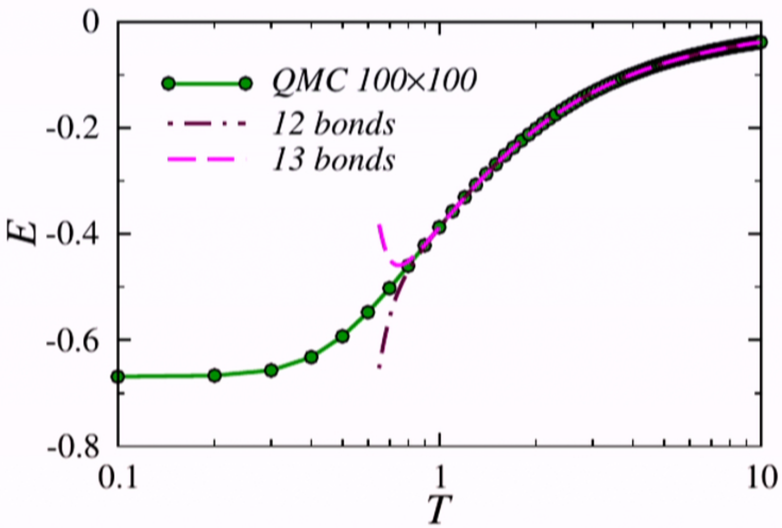
iv) Diagonalize the topological clusters and compute the observables

v) Compute the weight of each cluster and compute the direct sum of the weights

Heisenberg Model



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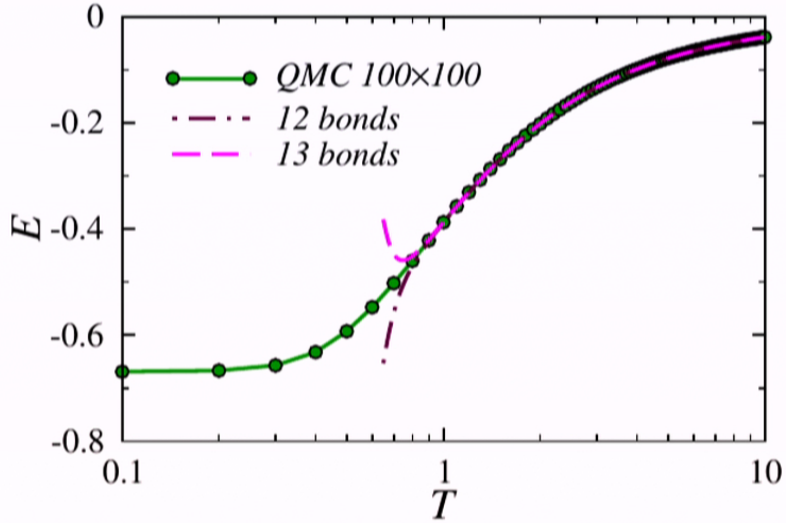

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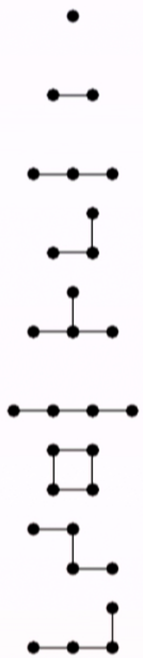
Numerical Linked-Cluster Expansions

Site clusters

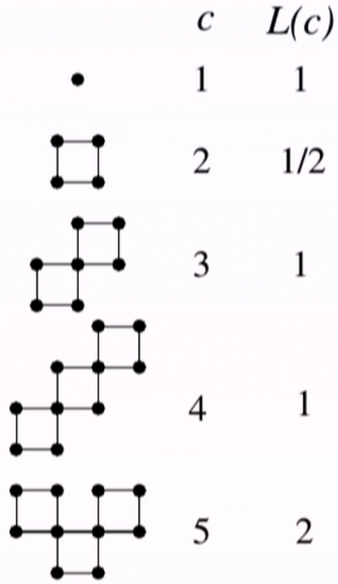


c	$L(c)$
1	1
2	2
3	2
4	4
5	4
6	2
7	1
8	4
9	8

No. of sites	topological clusters
1	1
2	1
3	1
4	3
5	4
6	10
7	19
8	51
9	112
10	300
11	746
12	2042
13	5450
14	15197
15	42192

Numerical Linked-Cluster Expansions

Square clusters



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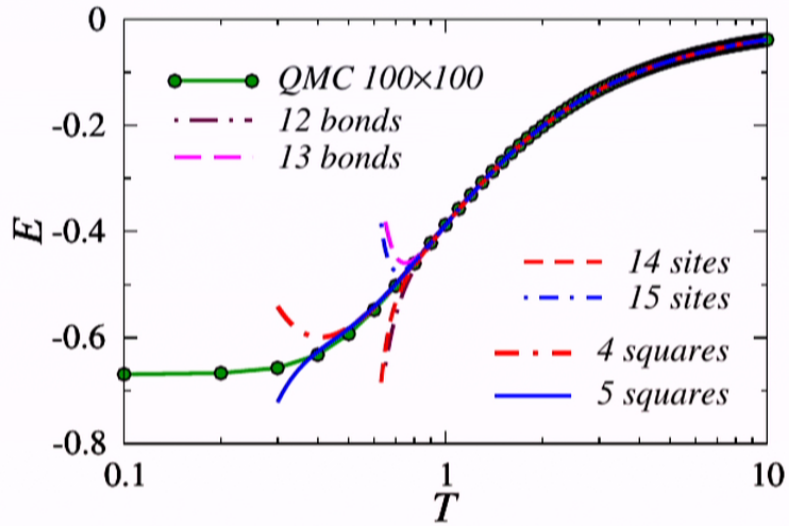

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Resummation results (Heisenberg model)
Energy (square lattice)

Models and quenches

Hard-core bosons in 1D lattices at half filling $(\mu_I = 0)$

$$\hat{H} = \sum_{i=1}^{L} -t\left(\hat{b}_i^\dagger \hat{b}_{i+1} + \text{H.c.}\right) + V\hat{n}_i\hat{n}_{i+1} - t'\left(\hat{b}_i^\dagger \hat{b}_{i+2} + \text{H.c.}\right) + V'\hat{n}_i\hat{n}_{i+2}$$

Quench: $T_I,\, t_I = 0.5,\, V_I = 1.5,\, t'_I = V'_I = 0 \rightarrow t = V = 1.0,\, t' = V'$

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Quench: T_I, $t_I = 0.5$, $V_I = 1.5$, $t'_I = V'_I = 0 \rightarrow t = V = 1.0$, $t' = V'$

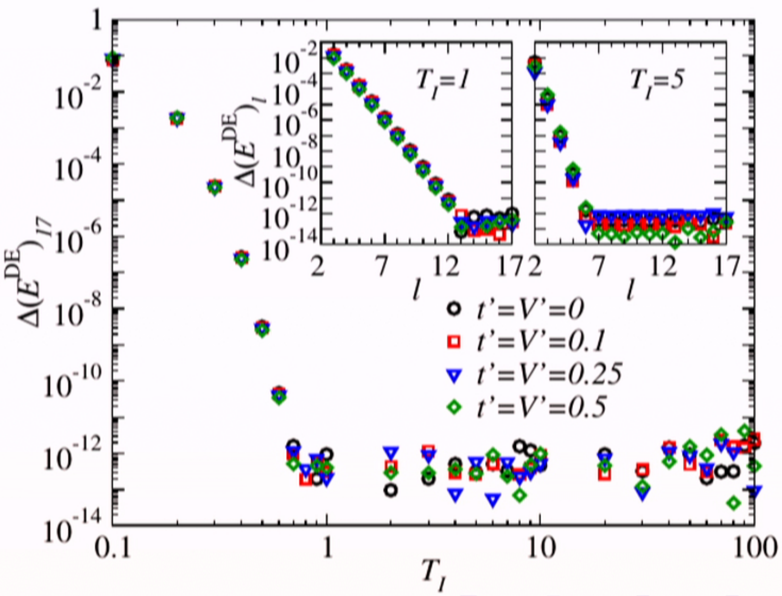
NLCE with maximally connected clusters ($l = 18$ sites)

Energy: $E^{\text{DE}} = \text{Tr}[\hat{H}\hat{\rho}^{\text{DE}}]$

Convergence:

$$\Delta(\mathcal{O}^{\text{ens}})_l = \frac{|\mathcal{O}_l^{\text{ens}} - \mathcal{O}_{18}^{\text{ens}}|}{|\mathcal{O}_{18}^{\text{ens}}|}$$

Convergence of E^{DE} with l



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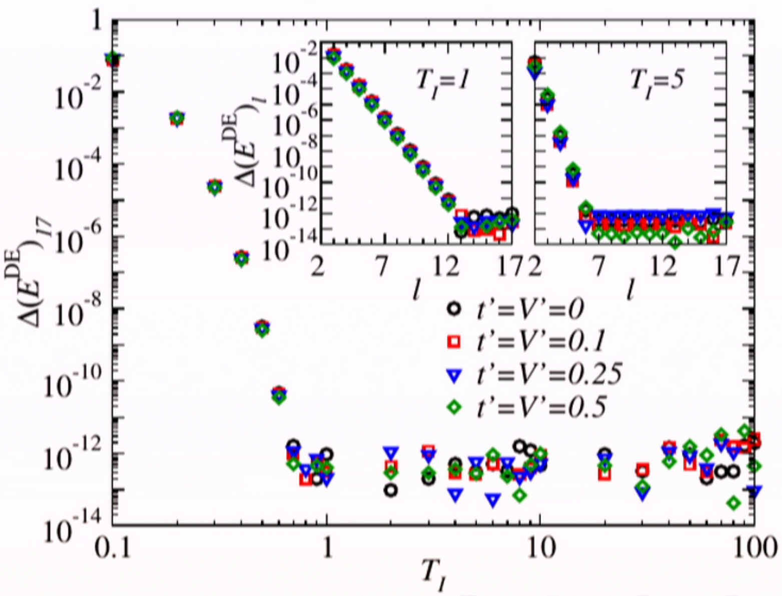


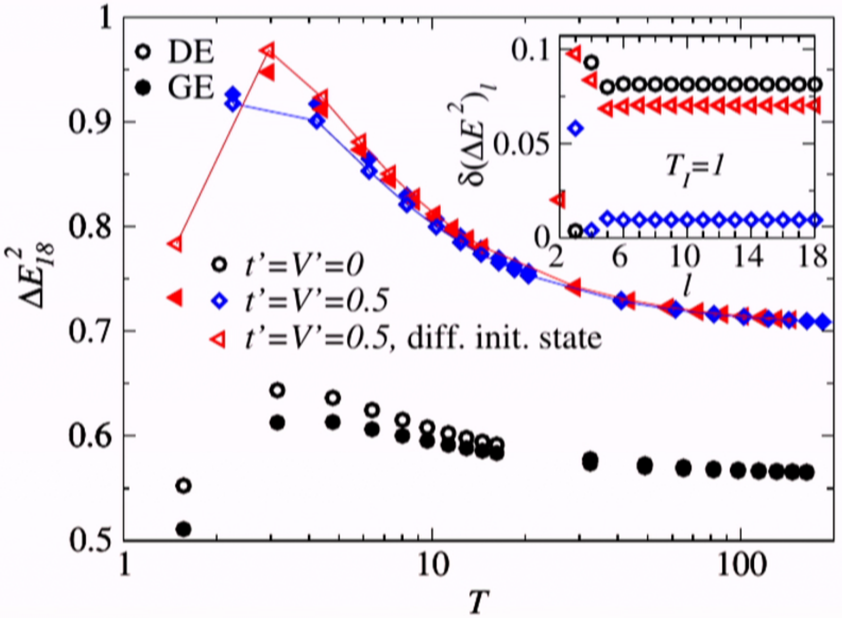
Dispersion of the energy in the DE

Dispersion of the energy

$$\Delta E^2 = \frac{1}{L}(\langle \hat{H}^2 \rangle - \langle \hat{H} \rangle^2)$$

Deviations from the GE

$$\delta(\mathcal{O})_l = \frac{|\mathcal{O}_l^{\mathrm{DE}} - \mathcal{O}_{18}^{\mathrm{GE}}|}{|\mathcal{O}_{18}^{\mathrm{GE}}|}$$

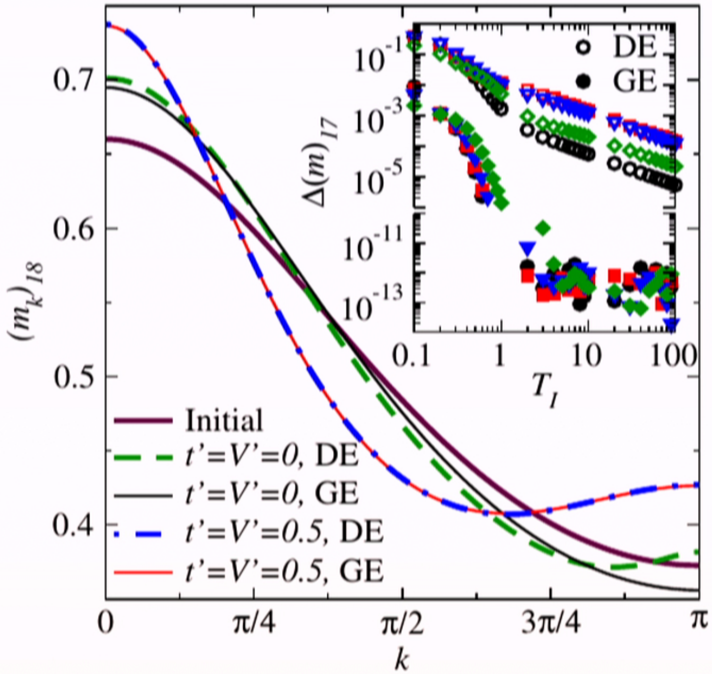


The dispersion of the energy (and of the particle number) in the DE depends on the initial state independently of whether the system is integrable or not.

Few-body experimental observables in the DE

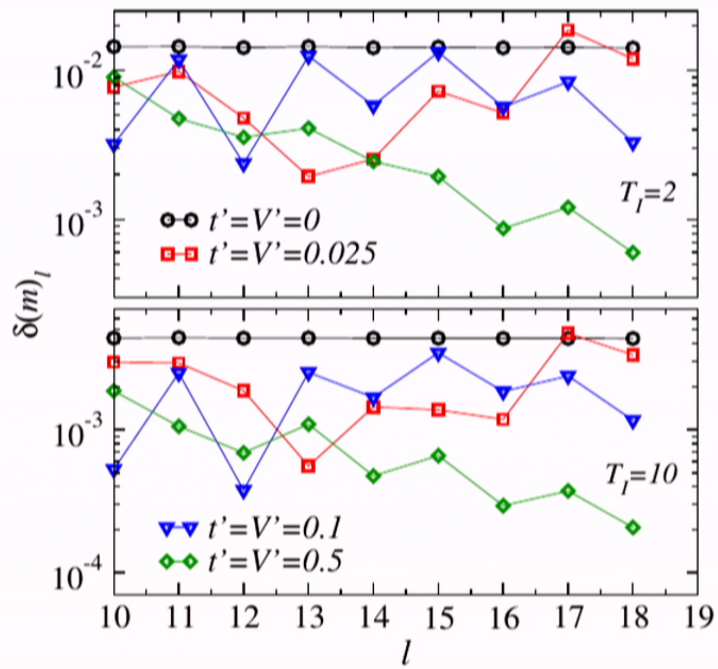
Momentum distribution

$$\hat{m}_k = \frac{1}{L}\sum_{jj'} e^{ik(j-j')}\hat{\rho}_{jj'}$$



Differences between DE and GE

$$\delta(m)_l = \frac{\sum_k |(m_k)_l^{\text{DE}} - (m_k)_{18}^{\text{GE}}|}{\sum_k (m_k)_{18}^{\text{GE}}}$$



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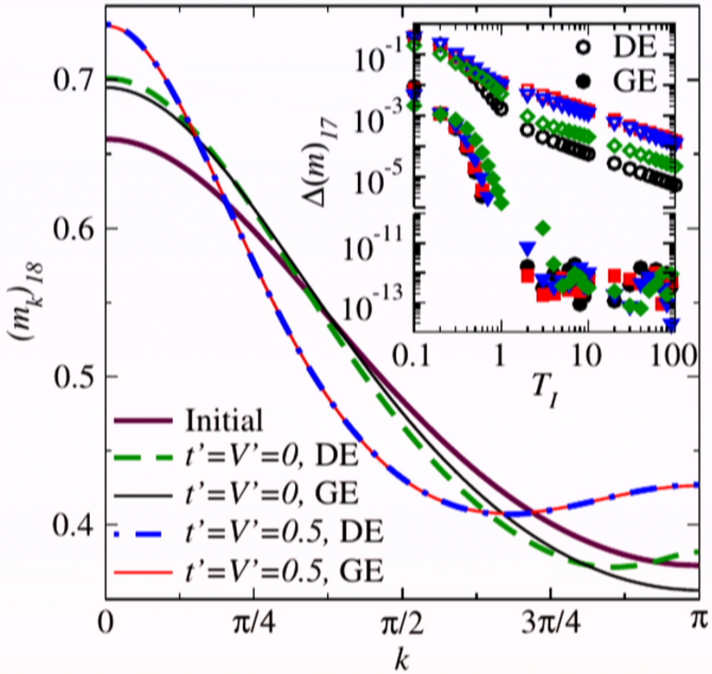

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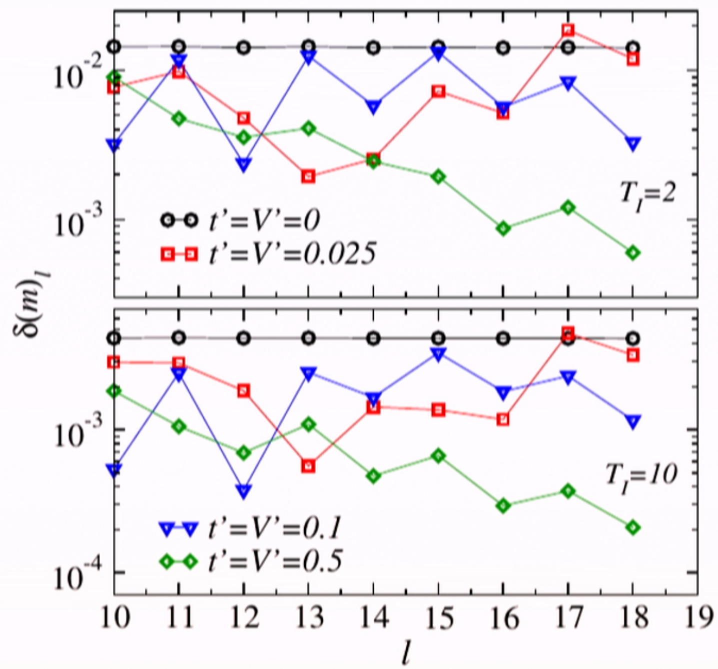

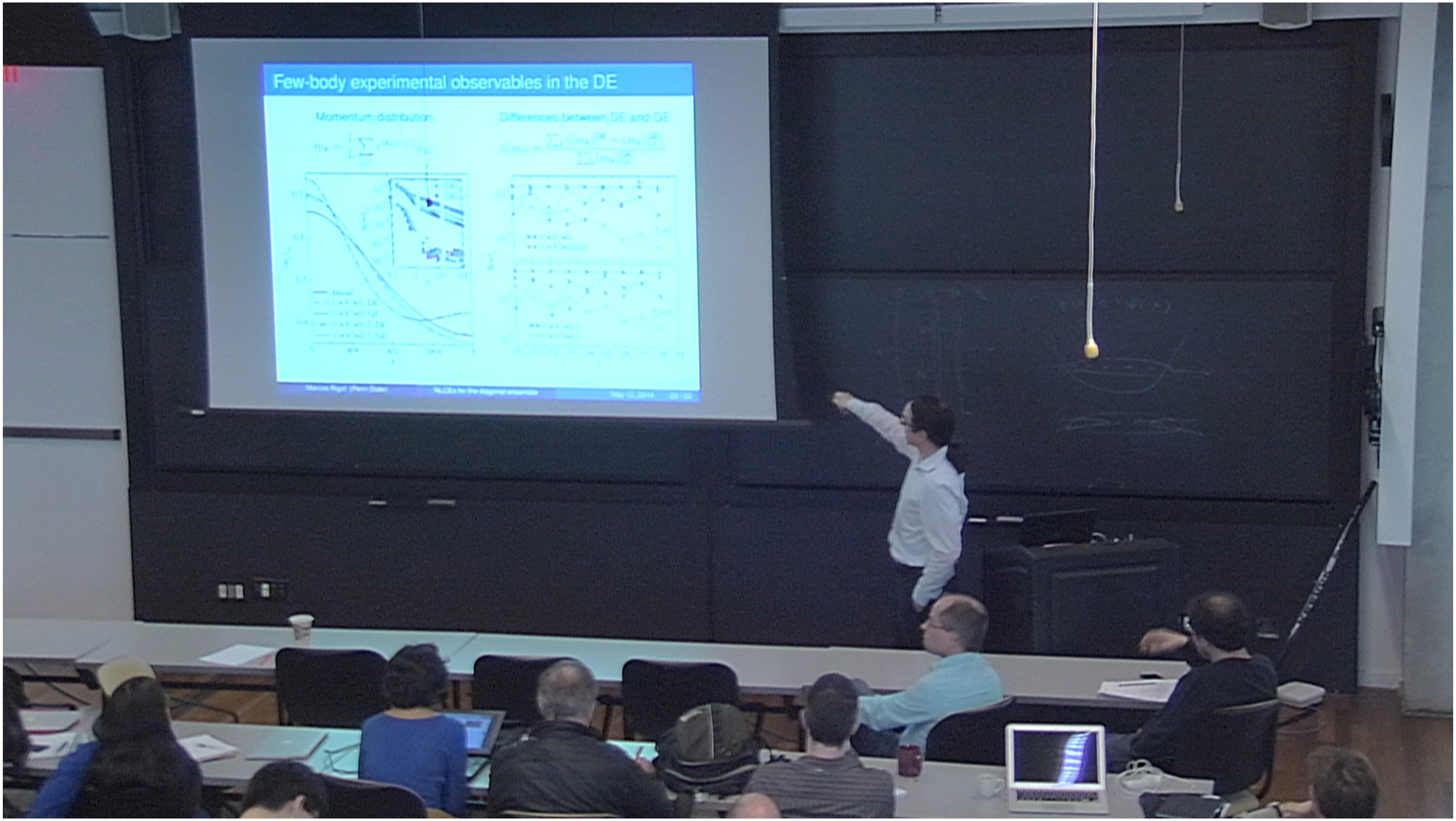
Few-body experimental observables in the DE
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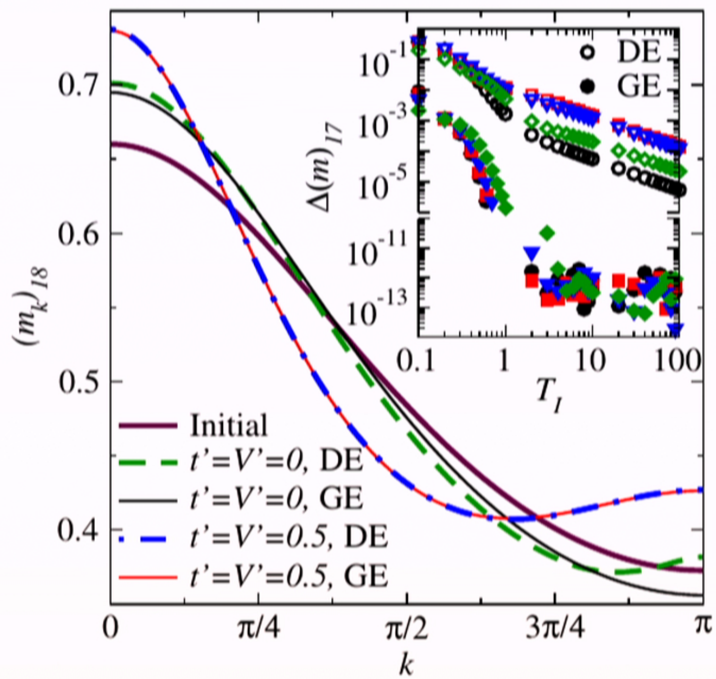

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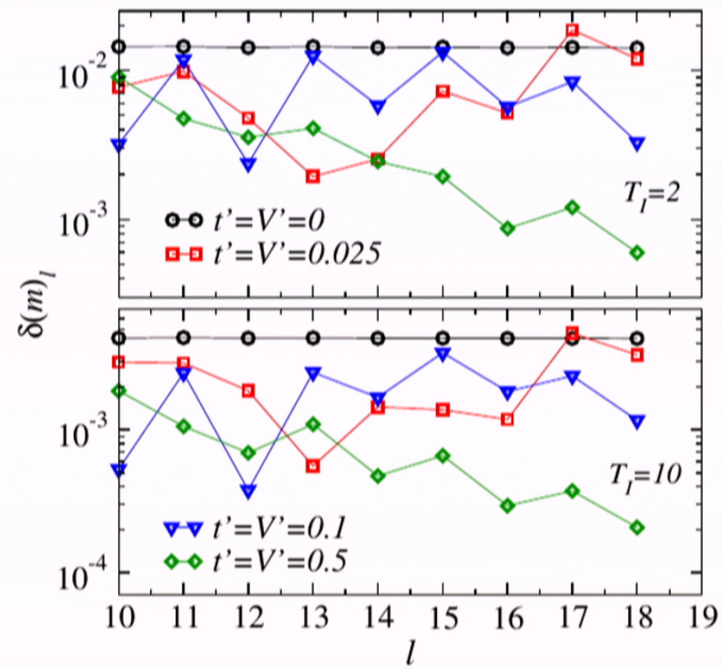

Conclusions

- NLCEs provide a general framework to study the diagonal ensemble in lattice systems after a quantum quench in the thermodynamic limit.
- NLCE results suggest that few-body observables thermalize in nonintegrable systems while they do not thermalize in integrable systems.
- As one approaches the integrable point DE-NLCEs behave as NLCEs for equilibrium systems approaching a phase transition. This suggests that a transition to thermalization may occur as soon as one breaks integrability.