# Quantum quenches in the thermodynamic limit

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*Quantum dynamics in systems with many coupled degrees of freedom: challenges for theory*

Center for Free-Electron Laser Science, Hamburg
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# Outline

1. Introduction
   - Computational techniques for quantum many-body problems
   - Numerical Linked Cluster Expansions
   - Quantum quenches
2. Quantum quenches in the thermodynamic limit
   - Diagonal ensemble and NLCEs
   - Quantum quenches in one-dimension
3. Conclusions

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# Finite temperature properties of lattice models

## Computational techniques for arbitrary dimensions

- Quantum Monte Carlo simulations
  Polynomial time $\Rightarrow$ Large systems $\Rightarrow$ Finite size scaling
  Sign problem $\Rightarrow$ Limited classes of models

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  Exponential problem ⇒ Small systems ⇒ Finite size effects
  No systematic extrapolation to larger system sizes
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  Thermodynamic limit ⇒ Extrapolations to low $T$
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- DMFT, DCA, DMRG, ...

# Linked-Cluster Expansions

Extensive observables $\hat{\mathcal{O}}$ per lattice site ($\mathcal{O}$) in the thermodynamic limit

$$\mathcal{O} = \sum_c L(c) \times W_{\mathcal{O}}(c)$$

where $L(c)$ is the number of embeddings of cluster $c$

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where $L(c)$ is the number of embeddings of cluster $c$ and $W_{\mathcal{O}}(c)$ is the weight of observable $\mathcal{O}$ in cluster $c$

$$W_{\mathcal{O}}(c) = \mathcal{O}(c) - \sum_{s \subset c} W_{\mathcal{O}}(s).$$

$\mathcal{O}(c)$ is the result for $\mathcal{O}$ in cluster $c$

$$\begin{aligned} \mathcal{O}(c) &= \mathrm{Tr}\left\{\hat{\mathcal{O}}\,\hat{\rho}_c^{\mathsf{GC}}\right\}, \\ \hat{\rho}_c^{\mathsf{GC}} &= \frac{1}{Z_c^{\mathsf{GC}}} \exp^{-\left(\hat{H}_c - \mu \hat{N}_c\right)/k_B T} \\ Z_c^{\mathsf{GC}} &= \mathrm{Tr}\left\{\exp^{-\left(\hat{H}_c - \mu \hat{N}_c\right)/k_B T}\right\} \end{aligned}$$

and the $s$ sum runs over all subclusters of $c$.

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  MR, T. Bryant, and R. R. P. Singh, PRL **97**, 187202 (2006).
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- 2D Hubbard-like models (square and honeycomb), spin models (kagome, checkerboard, pyroclore – experiments)

  MR and R. R. P. Singh, PRL **98**, 207204 (2007).
  MR and R. R. P. Singh, PRB **76**, 184403 (2007).
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  E. Khatami and MR, PRA **84**, 053611 (2011).
  E. Khatami, R. R. P. Singh, and MR, PRB **84**, 224411 (2011).
  E. Khatami, J. S. Helton, and MR, PRB **85**, 064401 (2012).
  E. Khatami and MR, PRA **86**, 023633 (2012).
  B. Tang, T. Paiva, E. Khatami, and MR, PRL **109**, 205301 (2012).
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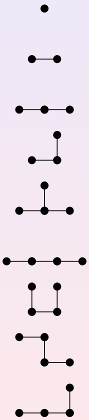
# Numerical Linked Cluster Expansions

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)

| No. of bonds | topological clusters |
|---:|---:|
| 0 | 1 |
| 1 | 1 |
| 2 | 1 |
| 3 | 2 |
| 4 | 4 |
| 5 | 6 |
| 6 | 14 |
| 7 | 28 |
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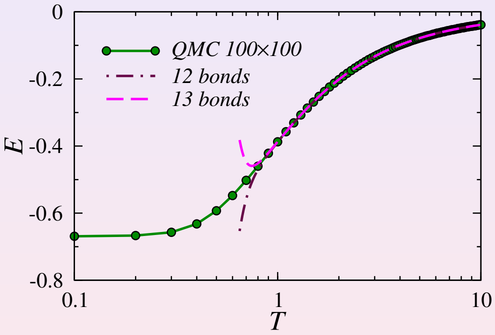
v) Perform the subgraph substraction to compute the weight of each cluster

Heisenberg Model

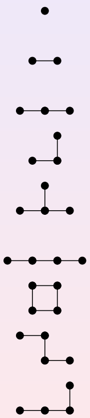



MR *et al.*, PRE **75**, 061118 (2007).

B. Tang *et al.*, CPC **184**, 557 (2013).

# Numerical Linked-Cluster Expansions

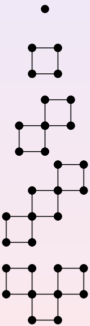
## Site clusters



| $c$ | $L(c)$ |
|---|---|
| 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 |

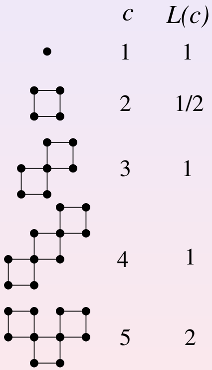
## Square clusters



| $c$ | $L(c)$ |
|---|---|
| 1 | 1 |
| 2 | 1/2 |
| 3 | 1 |
| 4 | 1 |
| 5 | 2 |

| No. of squares | topological clusters |
|---|---|
| 0 | 1 |
| 1 | 1 |
| 2 | 1 |
| 3 | 2 |
| 4 | 5 |
| 5 | 11 |

## Square clusters

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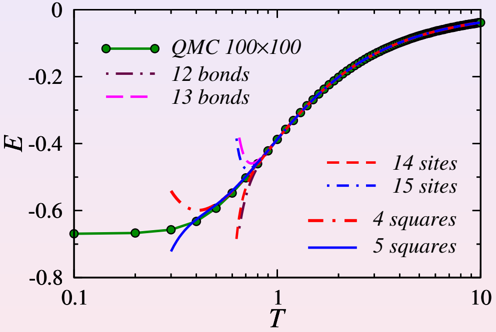


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# Resummation algorithms

We can define partial sums

$$\mathcal{O}_n = \sum_{i=1}^{n} S_i, \quad \text{with} \quad S_i = \sum_{c_i} L(c_i) \times W_{\mathcal{O}}(c_i)$$

where all clusters $c_i$ share a given characteristic (no. of bonds, sites, etc).

Goal: Estimate $\mathcal{O} = \lim_{n\to\infty} \mathcal{O}_n$ from a sequence $\{\mathcal{O}_n\}$, with $n = 1, \ldots, N$.

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Wynn's algorithm:

$$\varepsilon_n^{(-1)} = 0, \qquad \varepsilon_n^{(0)} = \mathcal{O}_n, \qquad \varepsilon_n^{(k)} = \varepsilon_{n+1}^{(k-2)} + \frac{1}{\Delta\varepsilon_n^{(k-1)}}$$

where $\Delta\varepsilon_n^{(k-1)} = \varepsilon_{n+1}^{(k-1)} - \varepsilon_n^{(k-1)}$.

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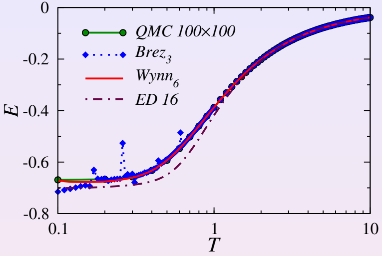
Brezinski's algorithm [$\theta_n^{(-1)} = 0, \ \ \theta_n^{(0)} = \mathcal{O}_n$]:

$$\theta_n^{(2k+1)} = \theta_n^{(2k-1)} + \frac{1}{\Delta\theta_n^{(2k)}}, \qquad \theta_n^{(2k+2)} = \theta_{n+1}^{(2k)} + \frac{\Delta\theta_{n+1}^{(2k)}\Delta\theta_{n+1}^{(2k+1)}}{\Delta^2\theta_n^{(2k+1)}}$$

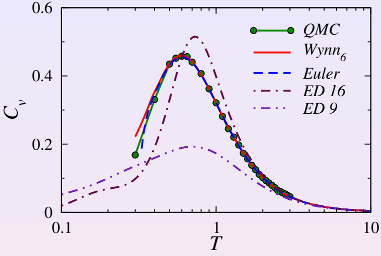
where $\Delta^2\theta_n^{(k)} = \theta_{n+2}^{(k)} - 2\theta_{n+1}^{(k)} + \theta_n^{(k)}$.

# Resummation results (Heisenberg model)

Energy (square lattice)




$C_v$ (square lattice)



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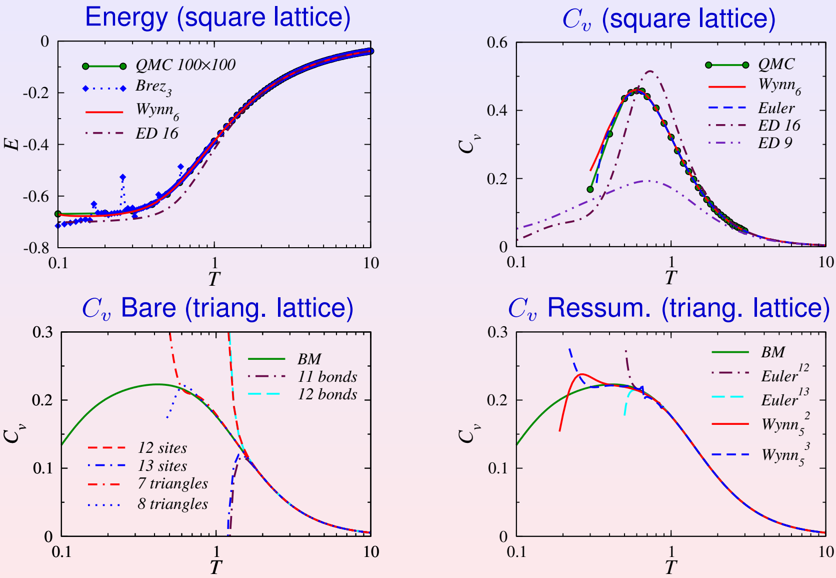


(BM) B. Bernu and G. Misguich, PRB **63**, 134409 (2001).

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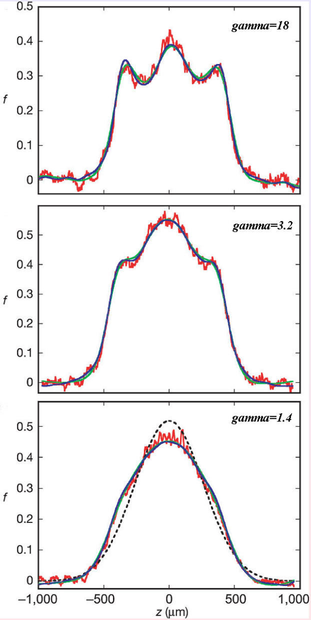
# Quantum Newton's Cradle




T. Kinoshita, T. Wenger, and D. S. Weiss, Nature **440**, 900 (2006).

$$\gamma = \frac{mg_{1D}}{\hbar^2 \rho}$$

$g_{1D}$: Interaction strength
$\rho$: One-dimensional density

If $\gamma \gg 1$ the system is in the strongly correlated Tonks-Girardeau regime

If $\gamma \ll 1$ the system is in the weakly interacting regime

Also in: M. Gring *et al.* (Schmiedmayer's group), Science **337**, 1318 (2012).

# Quenches in one-dimensional superlattices

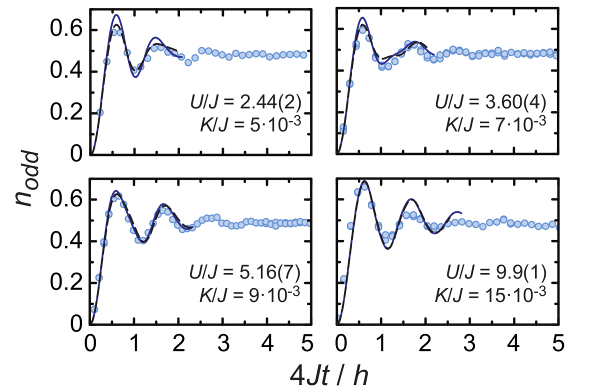
Quantum dynamics in a 1D superlattice

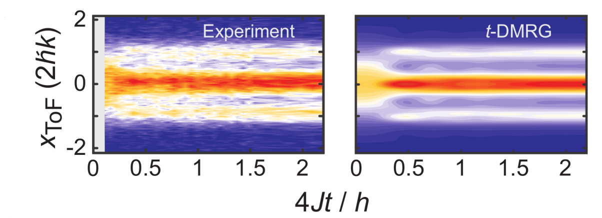
Trotzky *et al.* (Bloch's group), Nature Phys. **8**, 325 (2012).

Initial state $|01010\ldots1010\rangle$

Unitary dynamics under the "Bose-Hubbard" Hamiltonian

Experimental results ($\circ$) vs exact $t$-DMRG calculations (lines) without free parameters




local observables (top)
vs
nonlocal observables (bottom)

# 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

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

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What is it that we call thermalization?

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What is it that we call thermalization?

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

One can rewrite

$$O(\tau) = \sum_{\alpha',\alpha} C^\star_{\alpha'} C_\alpha e^{i(E_{\alpha'}-E_\alpha)\tau/\hbar} O_{\alpha'\alpha} \quad \text{where} \quad |\psi_0\rangle = \sum_\alpha C_\alpha|\alpha\rangle.$$

Taking the infinite time average (diagonal ensemble $\hat{\rho}_{\mathsf{DE}} \equiv \sum_\alpha |C_\alpha|^2|\alpha\rangle\langle\alpha|$)

$$\overline{O(\tau)} = \lim_{\tau\to\infty}\frac{1}{\tau}\int_0^\tau d\tau'\langle\Psi(\tau')|\hat{O}|\Psi(\tau')\rangle = \sum_\alpha |C_\alpha|^2 O_{\alpha\alpha} \equiv \langle\hat{O}\rangle_{\mathrm{DE}},$$

which depends on the initial conditions through $C_\alpha = \langle\alpha|\psi_0\rangle$.

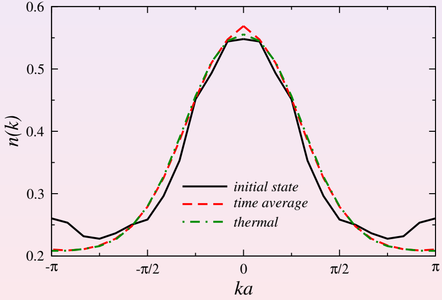
# Description after relaxation (lattice models)

Hard-core boson (spinless fermion) Hamiltonian

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

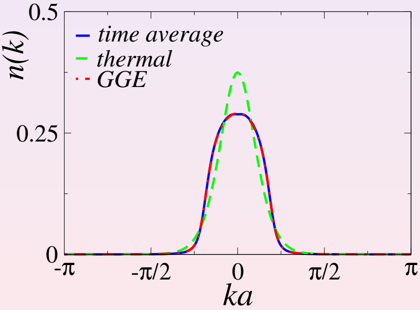
Dynamics vs statistical ensembles

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




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

Integrable: $t' = V' = 0$




MR, Dunjko, Yurovsky, and Olshanii, PRL **98**, 050405 (2007), . . .

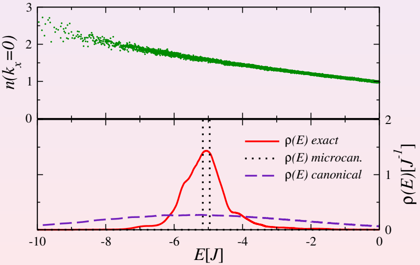
## Eigenstate thermalization hypothesis

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

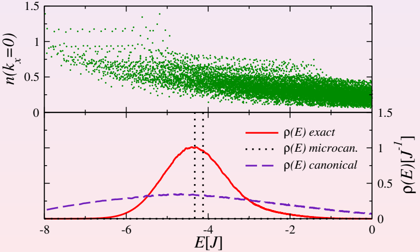
- The expectation value $\langle\alpha|\widehat{O}|\alpha\rangle$ of a few-body observable $\widehat{O}$ in an eigenstate of the Hamiltonian $|\alpha\rangle$, with energy $E_\alpha$, of a many-body system is equal to the thermal average of $\widehat{O}$ at the mean energy $E_\alpha$:

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

Nonintegrable

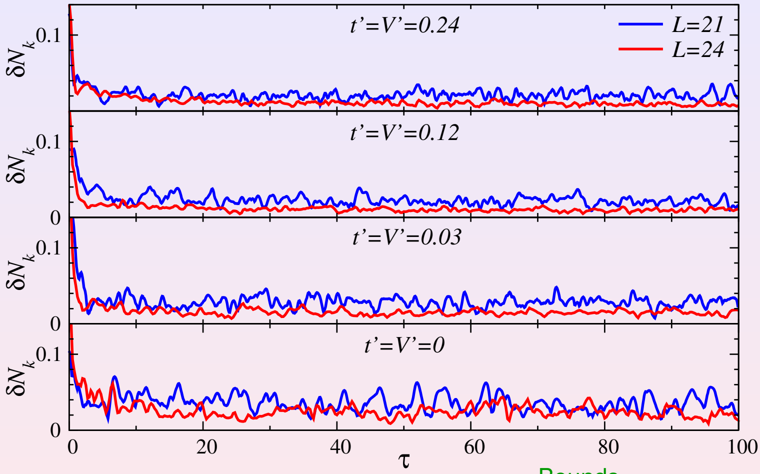



Integrable ($\hat{\rho}_{\text{GGE}} = \frac{1}{Z_{\text{GGE}}} e^{-\sum_m \lambda_m \hat{I}_m}$)




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

# Time fluctuations and their scaling with system size




Relative differences (struct. factor)

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

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?

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

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

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

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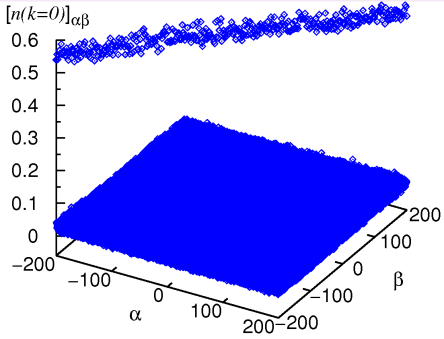
$$\sim \sum_\alpha \frac{1}{N_{\text{states}}} O_{\alpha\alpha} \sim O^{\text{typical}}_{\alpha\alpha}$$

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




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

# Outline

# Diagonal ensemble and NLCEs

The initial state is in thermal equilibrium in contact with a reservoir

$$\hat{\rho}_c^I = \frac{\sum_a e^{-(E_a^c - \mu_I N_a^c)/T_I} |a_c\rangle\langle a_c|}{Z_c^I}, \quad \text{where} \quad Z_c^I = \sum_a e^{-(E_a^c - \mu^I N_a^c)/T_I},$$

$|a_c\rangle$ ($E_a^c$) are the eigenstates (eigenvalues) of the initial Hamiltonian $\hat{H}_c^I$ in $c$.

MR, arXiv:1401.2160.

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At the time of the quench $\hat{H}_c^I \to \hat{H}_c$ , the system is detached from the reservoir. Writing the eigenstates of $\hat{H}_c^I$ in terms of the eigenstates of $\hat{H}_c$

$$\hat{\rho}_c^{\mathrm{DE}} \equiv \lim_{\tau' \to \infty} \frac{1}{\tau'} \int_0^{\tau'} d\tau \, \hat{\rho}(\tau) = \sum_\alpha W_\alpha^c \, |\alpha_c\rangle\langle\alpha_c|$$

where

$$W_\alpha^c = \frac{\sum_a e^{-(E_a^c - \mu_I N_a^c)/T_I} |\langle \alpha_c | a_c \rangle|^2}{Z_c^I},$$

$|\alpha_c\rangle$ ($\varepsilon_\alpha^c$) are the eigenstates (eigenvalues) of the final Hamiltonian $\hat{H}_c$ in $c$.

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Using $\hat{\rho}_c^{\text{DE}}$ in the calculation of $\mathcal{O}(c)$, NLCEs allow one to compute observables in the DE in the thermodynamic limit.

MR, arXiv:1401.2160.

# Outline

1. Introduction
   - Computational techniques for quantum many-body problems
   - Numerical Linked Cluster Expansions
   - Quantum quenches
2. Quantum quenches in the thermodynamic limit
   - Diagonal ensemble and NLCEs
   - Quantum quenches in one-dimension
3. Conclusions

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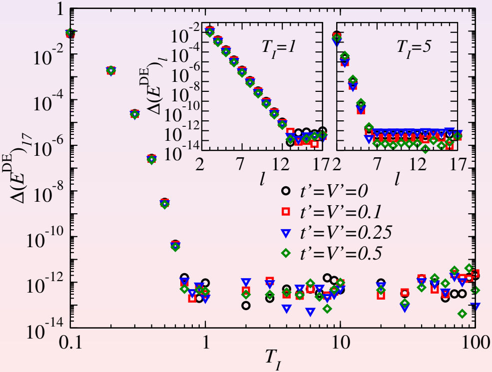
NLCE with maximally connected clusters ($l = 18$ sites)

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 $E^{\text{DE}}$ with $l$



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

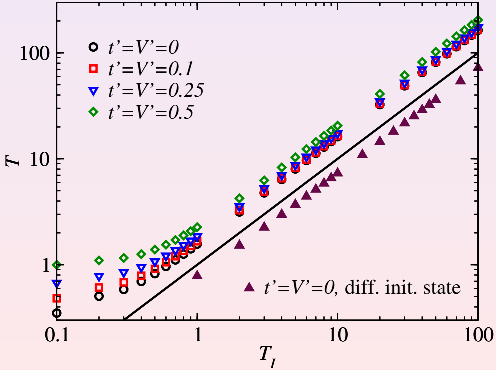
Temperature after the quench:
(if in thermal equilibrium)

$$E^{\text{DE}}_{l=18} = E^{\text{GE}}_{l=18}$$

$$E^{\text{GE}} = \frac{\text{Tr}[\hat{H}e^{-(\hat{H}-\mu\hat{N})/T}]}{\text{Tr}[e^{-(\hat{H}-\mu\hat{N})/T}]}$$

Relative energy difference between $E^{\text{DE}}_{18}$ and $E^{\text{GE}}_{18}$ is smaller than $10^{-11}$

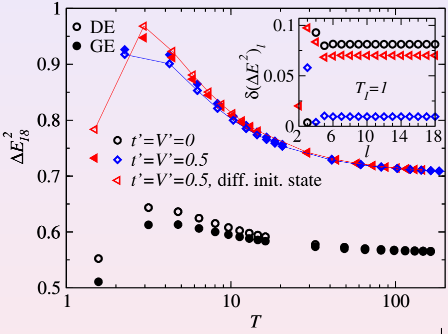
Temperature after the quench



# Energy and particle number dispersion in the DE

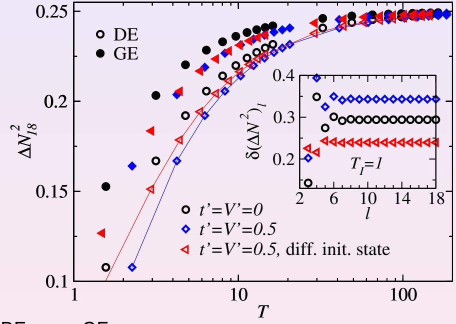
## Energy dispersion

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




## Particle number dispersion

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



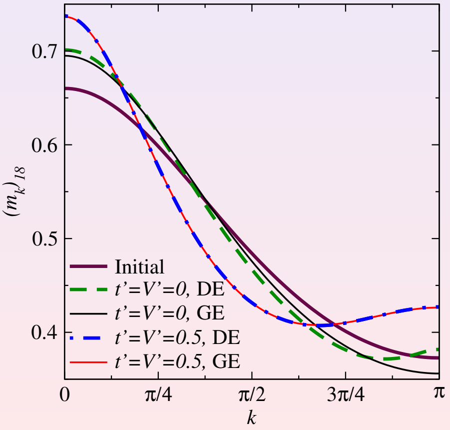

$$\delta(\mathcal{O})_l = \frac{|\mathcal{O}_l^{\text{DE}} - \mathcal{O}_{18}^{\text{GE}}|}{|\mathcal{O}_{18}^{\text{GE}}|}$$

The dispersion of the energy and 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

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



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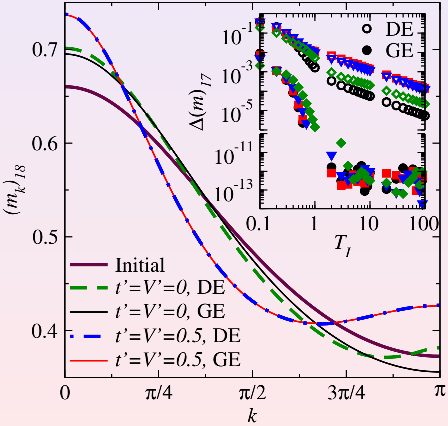
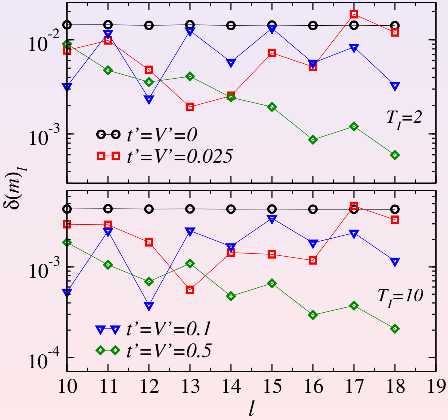



## Differences between DE and GE

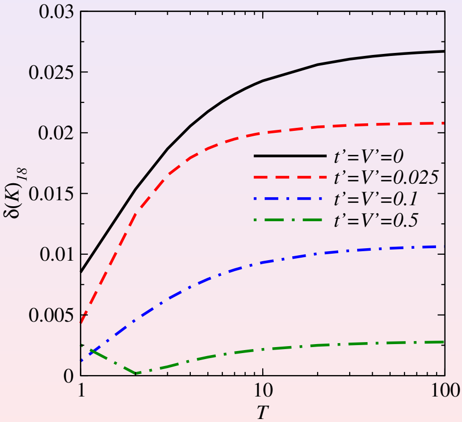
$$\delta(m)_l = \frac{\sum_k |(m_k)^{\text{DE}}_l - (m_k)^{\text{GE}}_{18}|}{\sum_k (m_k)^{\text{GE}}_{18}}$$



# Few-body experimental observables in the DE

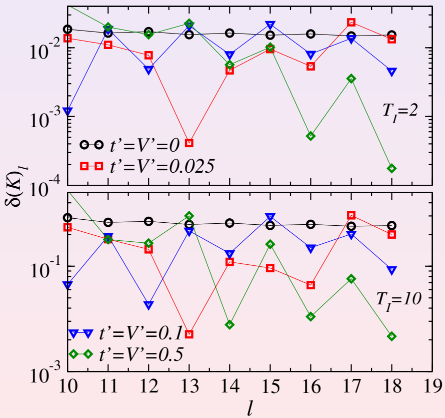
nn kinetic energy

$$K = -t \sum_i \langle \hat{b}_i^\dagger \hat{b}_{i+1} \rangle$$

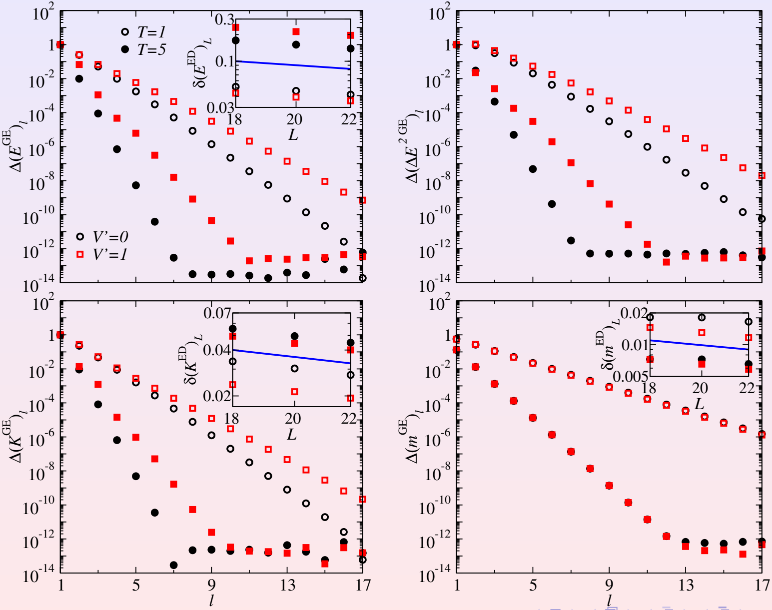



Differences between DE and GE

$$\delta(K)_l = \frac{|K_l^{\mathrm{DE}} - K_{18}^{\mathrm{GE}}|}{K_{18}^{\mathrm{GE}}}$$



# NLCEs vs exact diagonalization



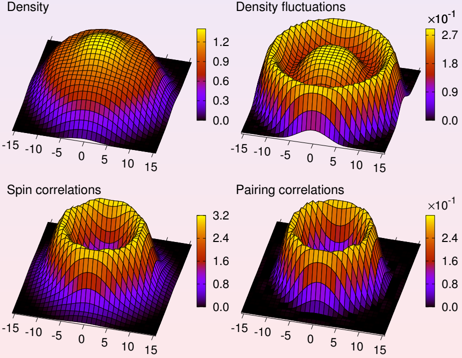
# Conclusions

- 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.

## Computational techniques for arbitrary dimensions

- Quantum Monte Carlo simulations
  Polynomial time ⇒ Large systems ⇒ Finite size scaling
  Sign problem ⇒ Limited classes of models

DQMC of a 2D system with: $U = 6t$, $V = 0.04t$, $T = 0.31t$ and 560 fermions




S. Chiesa, C. N. Varney, MR, and R. T. Scalettar, PRL **106**, 035301 (2011).