Quantum quenches in the thermodynamic limit

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Correlations, criticality, and coherence in quantum systems

Evora, Portugal

October 9, 2014

Outline

Quenches in one-dimensional superlattices

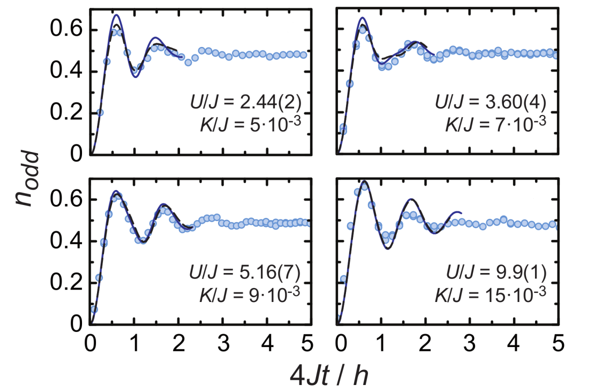
Quantum dynamics in a 1D superlattice

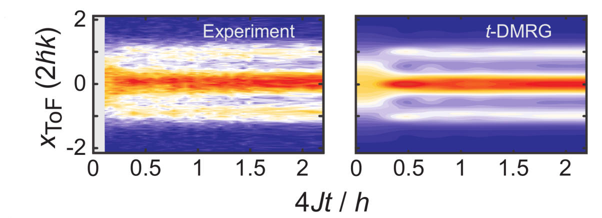
Trotzky *et al.* (Bloch's group), Nature Phys. **8**, 325 (2012).

Initial state $|01010\ldots1010\rangle$

Unitary dynamics under the "Bose-Hubbard" Hamiltonian

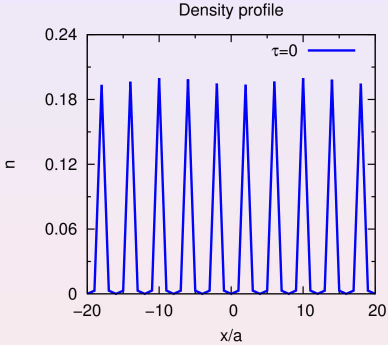
Experimental results ($\circ$) vs exact t-DMRG calculations (lines) without free parameters

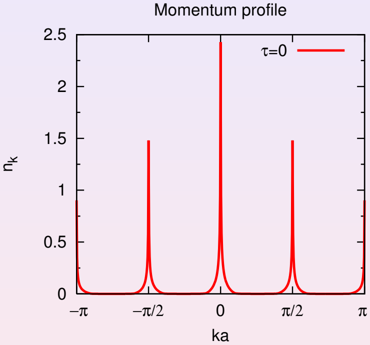




local observables (top)
vs
nonlocal observables (bottom)

Relaxation dynamics after turning off a superlattice





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

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

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?

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

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What is it that we call thermalization?

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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 $\hat{\rho}_{\text{DE}} \equiv \sum_\alpha |C_\alpha|^2|\alpha\rangle\langle\alpha|$)

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

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

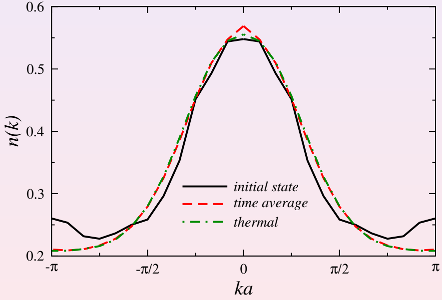
Description after relaxation (lattice models)

Hard-core boson (spinless fermion) Hamiltonian

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

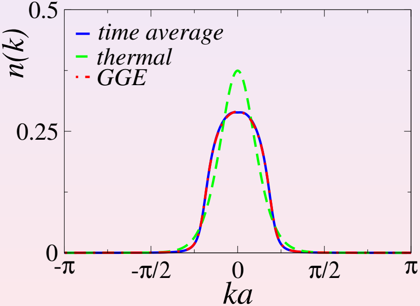
Dynamics vs statistical ensembles

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

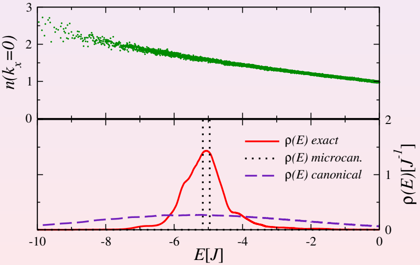
Eigenstate thermalization hypothesis

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

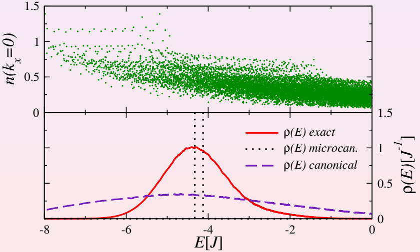
- The expectation value $\langle\alpha|\widehat{O}|\alpha\rangle$ of a few-body observable $\widehat{O}$ in an eigenstate of the Hamiltonian $|\alpha\rangle$, with energy E_α, of a many-body system is equal to the thermal average of $\widehat{O}$ at the mean energy E_α:

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

Nonintegrable

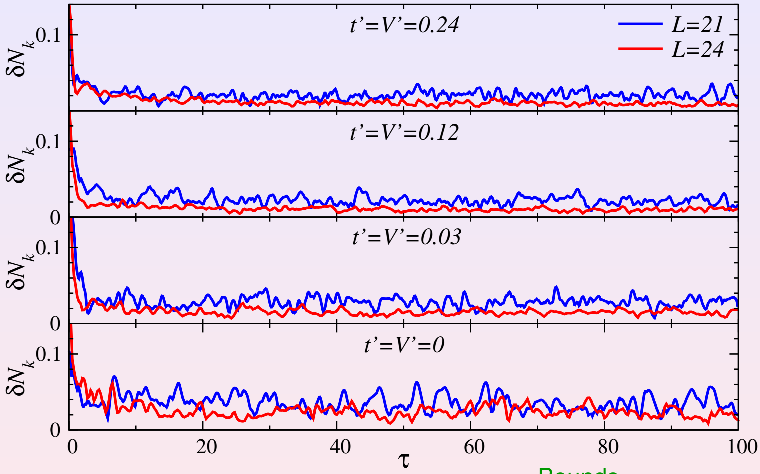


Integrable $\left(\hat{\rho}_{\mathrm{GGE}} = \frac{1}{Z_{\mathrm{GGE}}} e^{-\sum_m \lambda_m \hat{I}_m}\right)$



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

Time fluctuations and their scaling with system size



Relative differences (struct. factor)

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

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?

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

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

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

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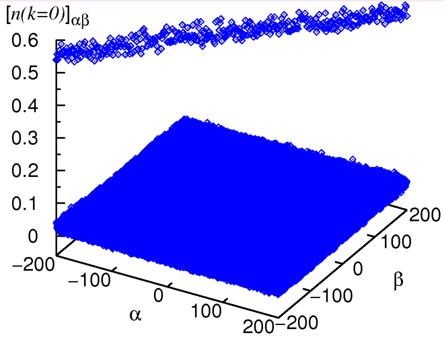

MR, PRA **80**, 053607 (2009)

Outline

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

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  Thermodynamic limit $\Rightarrow$ 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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- In numerical linked cluster expansions (NLCEs) an exact diagonalization of the cluster is used to calculate $\mathcal{O}(c)$ at any temperature.

  (Spins models in the square, triangular, and kagome lattices)
  MR, T. Bryant, and R. R. P. Singh, PRL **97**, 187202 (2006).
  MR, T. Bryant, and R. R. P. Singh, PRE **75**, 061118 (2007).

  (t-J model in the square lattice)
  MR, T. Bryant, and R. R. P. Singh, PRE **75**, 061119 (2007).

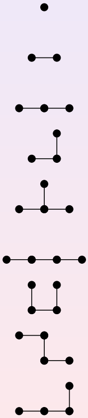
PRL **98**, 207204 (2007), PRB **76**, 184403 (2007), PRB **83**, 134431 (2011), PRA **84**, 053611 (2011), PRB **84**, 224411 (2011), PRB **85**, 064401 (2012), PRA **86**, 023633 (2012), PRL **109**, 205301 (2012), CPC **184**, 557 (2013), PRB **88**, 125127 (2013), . . .

Outline

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
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3	2
4	4
5	6
6	14
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10	399
11	1012
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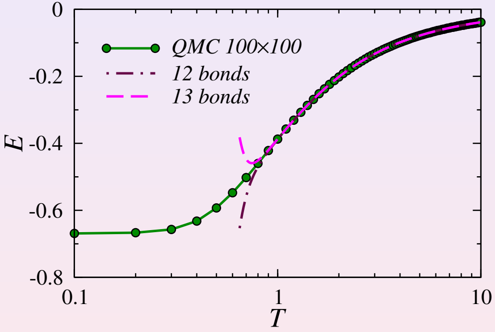
v) Compute the weight of each cluster and compute the direct sum of the weights

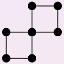
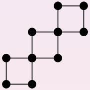
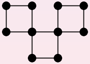
Heisenberg Model



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

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

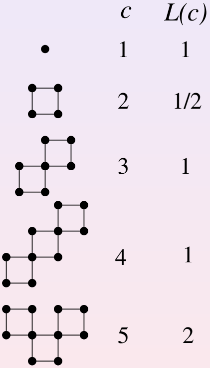
Square clusters

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

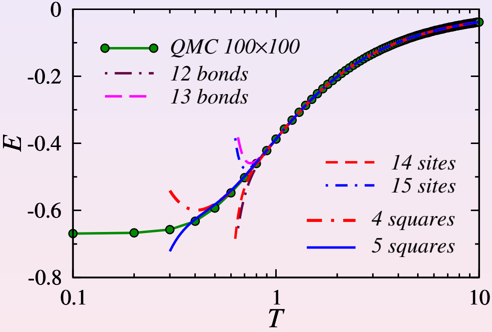
No. of squares	topological clusters
0	1
1	1
2	1
3	2
4	5
5	11

Numerical Linked-Cluster Expansions

Square clusters



Heisenberg Model



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

Outline

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

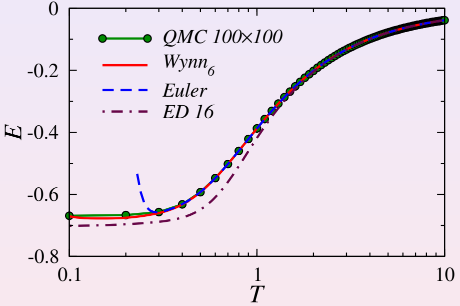
Brezinski's algorithm [$\theta_n^{(-1)} = 0, \; \theta_n^{(0)} = \mathcal{O}_n$]:

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

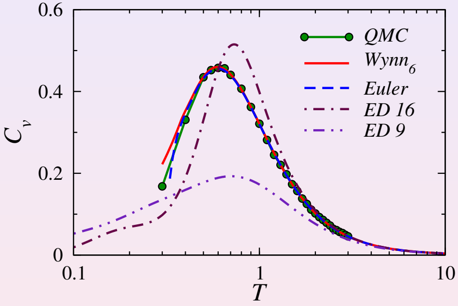
where $\Delta^2\theta_n^{(k)} = \theta_{n+2}^{(k)} - 2\theta_{n+1}^{(k)} + \theta_n^{(k)}$.

Resummation results (Heisenberg model)

Energy (square lattice)



C_v (square lattice)



MR, T. Bryant, and R. R. P. Singh, PRE **75**, 061118 (2007).

B. Tang, E. Khatami, and MR, Comput. Phys. Commun. **184**, 557 (2013).

Outline

1. Introduction
   - Quantum quenches
   - Many-body quantum systems in thermal equilibrium
2. Numerical Linked Cluster Expansions
   - Direct sums
   - Resummations
3. Quantum quenches in the thermodynamic limit
   - Diagonal ensemble and NLCEs
   - Quenches in the t-V-t'-V' chain (thermalization)
   - Quenches in XXZ chain from a Neel state (QA vs GGE)
4. Conclusions

Diagonal ensemble and NLCEs

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

$$\hat{\rho}^I_c = \frac{\sum_a e^{-(E^c_a - \mu_I N^c_a)/T_I} |a_c\rangle\langle a_c|}{Z^I_c}, \quad \text{where} \quad Z^I_c = \sum_a e^{-(E^c_a - \mu^I N^c_a)/T_I},$$

$|a_c\rangle$ (E^c_a) are the eigenstates (eigenvalues) of the initial Hamiltonian $\hat{H}^I_c$ in c.

MR, PRL **112**, 170601 (2014).

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

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 $\hat{H}_c$

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

where

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

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

MR, PRL **112**, 170601 (2014).

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

where

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

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

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, PRL **112**, 170601 (2014).

Outline

1. Introduction
   - Quantum quenches
   - Many-body quantum systems in thermal equilibrium
2. Numerical Linked Cluster Expansions
   - Direct sums
   - Resummations
3. Quantum quenches in the thermodynamic limit
   - Diagonal ensemble and NLCEs
   - Quenches in the t-V-t'-V' chain (thermalization)
   - Quenches in XXZ chain from a Neel state (QA vs GGE)
4. 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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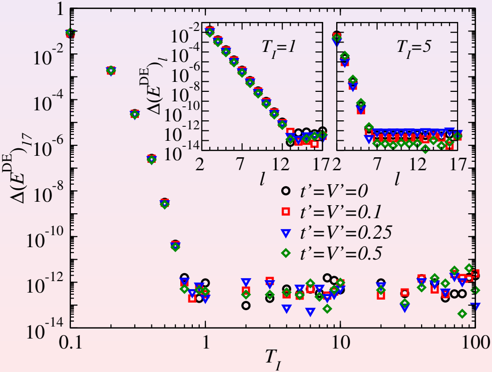
NLCE with maximally connected clusters ($l = 18$ sites)

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

Convergence:

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

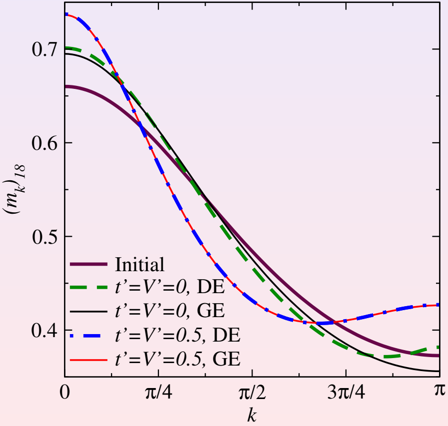
Convergence of E^{DE} with l



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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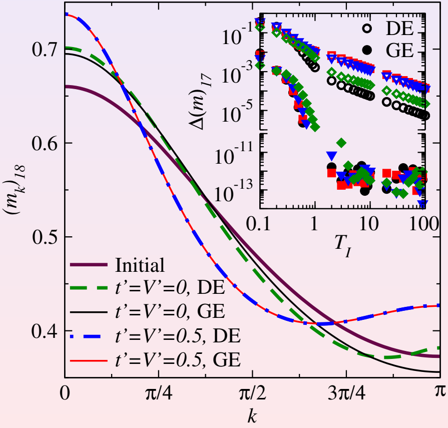
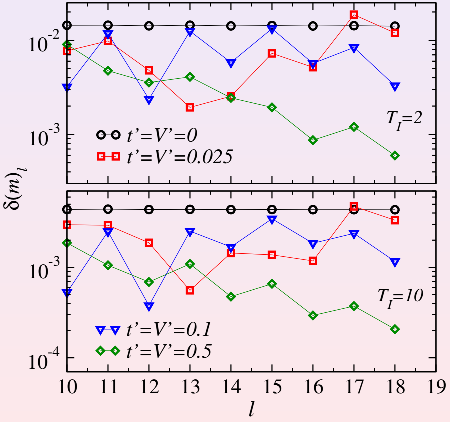


Differences between DE and GE

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



Outline

Failure of the GGE based on local quantities

XXZ (integrable) Hamiltonian

$$\hat{H} = J\left(\sum_i \sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y + \Delta\sigma_i^z\sigma_{i+1}^z\right)$$

Quench starting from the Neel state to different values of $\Delta \geq 1$

Quench action solution differs from GGE based on local quantities:

B. Wouters, J. De Nardis, M. Brockmann, D. Fioretto, MR, and J.-S. Caux,
PRL **113**, 117202 (2014).

B. Pozsgay, M. Mestyán, M. A. Werner, M. Kormos, G. Zaránd, and G. Takács,
PRL **113**, 117203 (2014).

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Can we use NLCEs for ground states (pure states)?

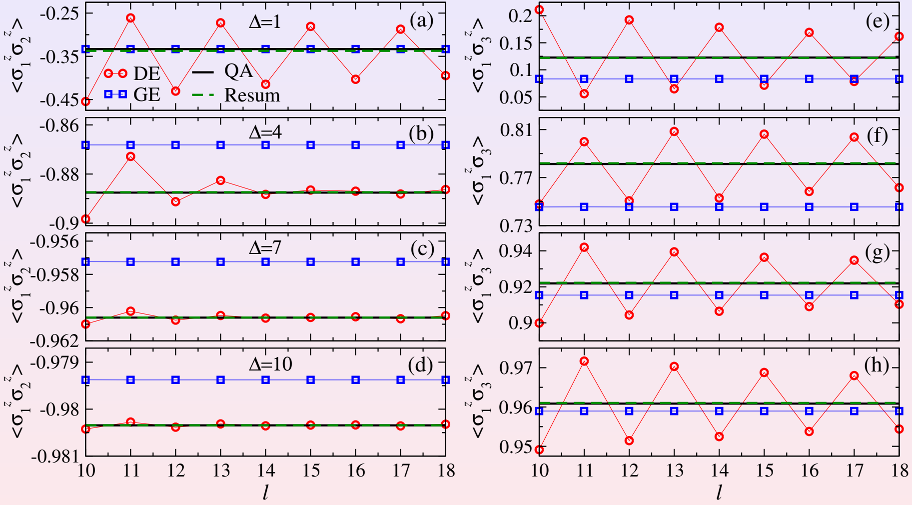
Using the parity symmetry of the clusters:

$$|a_c^e\rangle = \frac{1}{\sqrt{2}}(|\ldots\uparrow\downarrow\uparrow\downarrow\ldots\rangle + |\ldots\downarrow\uparrow\downarrow\uparrow\ldots\rangle)$$

$$|a_c^o\rangle = \frac{1}{\sqrt{2}}(|\ldots\uparrow\downarrow\uparrow\downarrow\ldots\rangle - |\ldots\downarrow\uparrow\downarrow\uparrow\ldots\rangle)$$

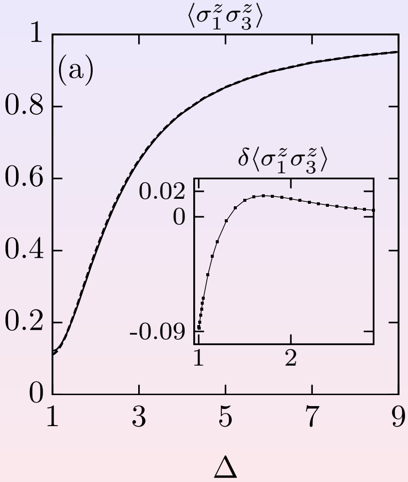
$$W_\alpha^{c,e/o} = |\langle\alpha_c^{e/o}|a_c^{e/o}\rangle|^2$$

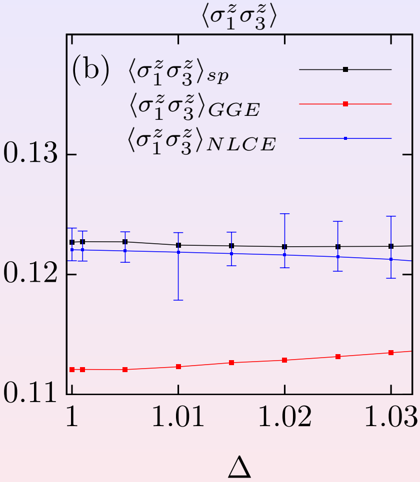
Results for spin-spin correlations



MR, PRE **90**, 031301(R) (2014)

Quench action, GGE, and NLCE





$$\delta\langle\sigma_1^z\sigma_3^z\rangle = \langle\sigma_1^z\sigma_3^z\rangle_{\mathsf{GGE}}/\langle\sigma_1^z\sigma_3^z\rangle_{\mathsf{QA}} - 1$$

B. Wouters *et al.*, PRL **113**, 117202 (2014).

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.
- The GGE based on known local conserved quantities does not describe observables after relaxation, while the QA does, as suggested by the NLCE results. New things to be learned about integrable systems!

Collaborators

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Bram Wouters (ITP Amsterdam)

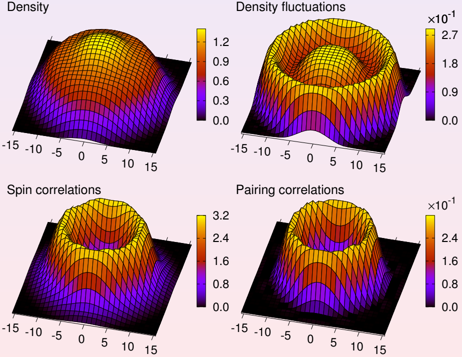
PRL **113**, 117202 (2014).

Supported by:

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).

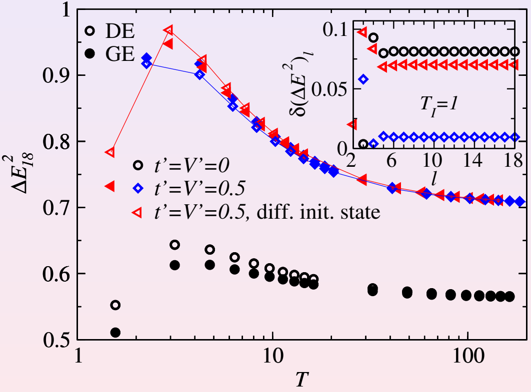
Dispersion of the energy in the DE

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.

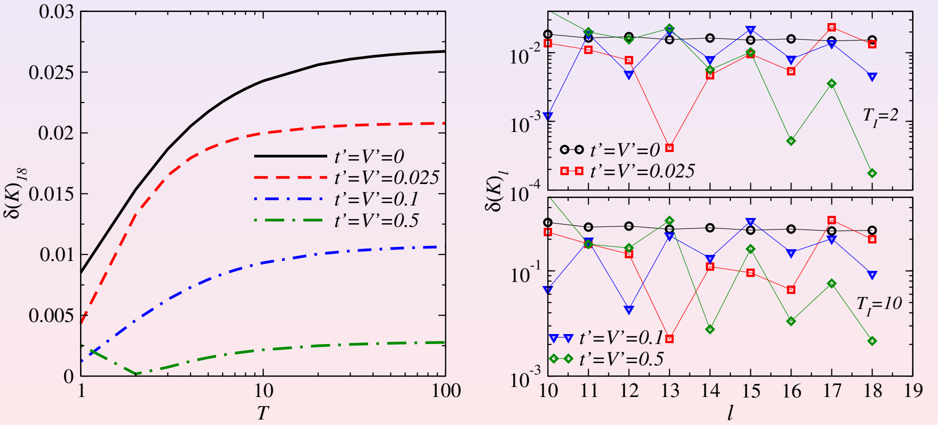
Few-body experimental observables in the DE

nn kinetic energy

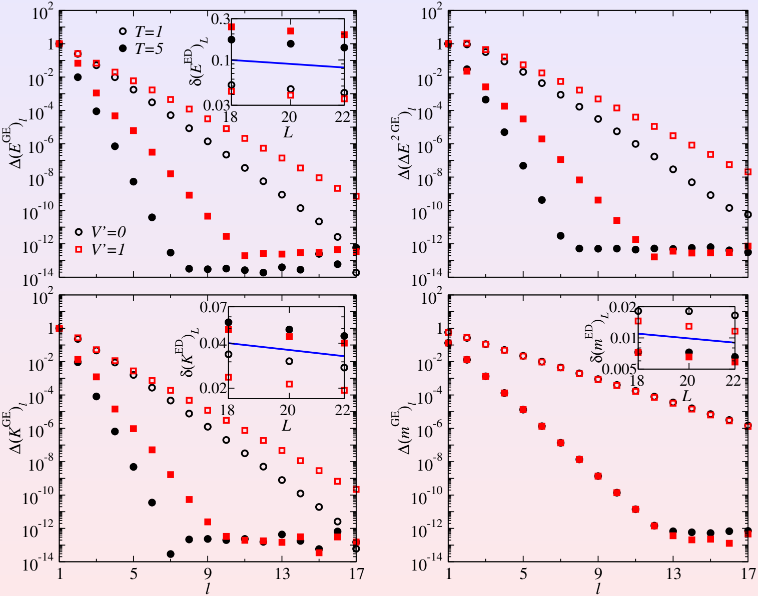
$$K = -t \sum_i \langle \hat{b}_i^\dagger \hat{b}_{i+1} \rangle$$

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 (equilibrium, $t' = 0$)



ED from L. Santos and MR, PRE **82**, 031130 (2010).