Numerical Linked Cluster Expansions for Quantum Quenches in the Thermodynamic Limit

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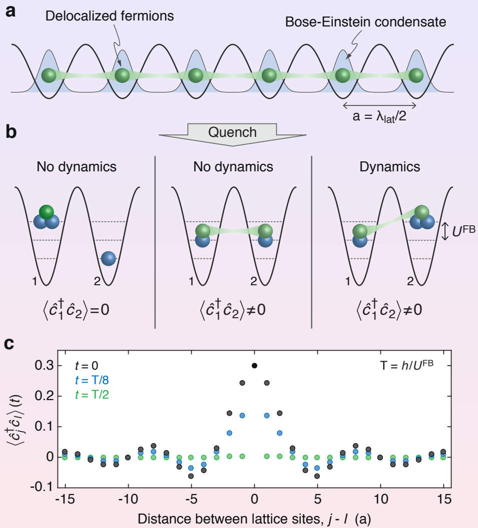
Outline

1. Introduction
   - Quantum quench
   - Linked-cluster expansions, HTEs, and NLCEs

2. 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)
   - Many-body localization

3. Conclusions

Quenches in Bose-Fermi mixtures



S. Will, D. Iyer, and MR
Nat. Commun. **6**, 6009 (2015).

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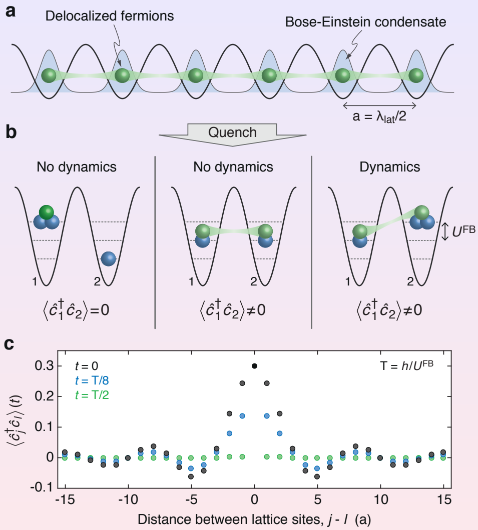

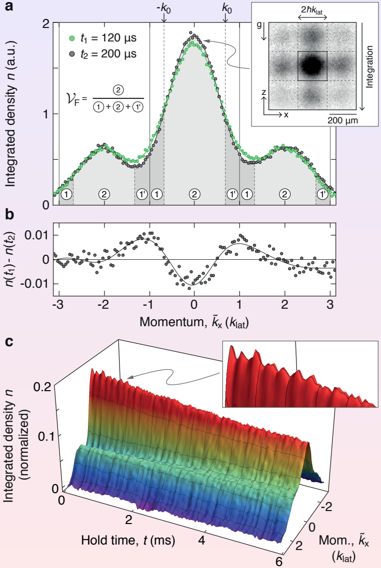

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Quantum quench

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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One can write

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

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 $C_\alpha = \langle\alpha|\psi_0\rangle$.

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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)
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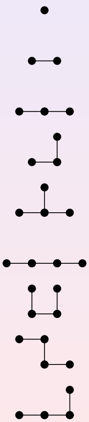
  A. B. Kallin, K. Hyatt, R. R. P. Singh, and R. G. Melko, PRL **110**, 135702 (2013).
- Disordered systems
  (spin-1/2 models with binary disorder in 2D)
  B. Tang, D. Iyer and MR, arXiv:1501.00990.

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
8	68
9	156
10	399
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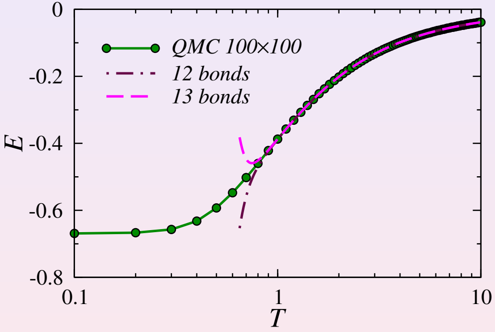
v) Compute the weight of each cluster and compute the direct sum of the weights

Heisenberg Model in 2D

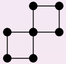
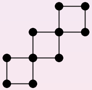
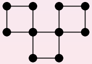


MR *et al.*, PRE **75**, 061118 (2007).

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

Numerical Linked-Cluster Expansions

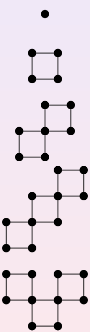
Square clusters

	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

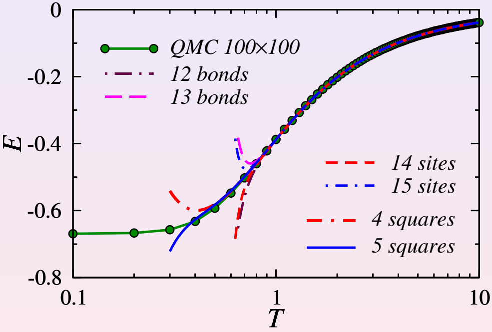
Numerical Linked-Cluster Expansions

Square clusters



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

Heisenberg Model in 2D



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

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

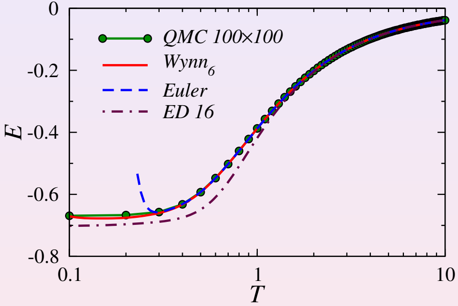
Brezinski's algorithm [$\theta_n^{(-1)} = 0, \ \ \theta_n^{(0)} = \mathcal{O}_n$]:

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

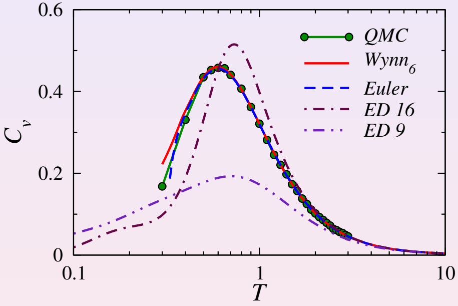
where $\Delta^2\theta_n^{(k)} = \theta_{n+2}^{(k)} - 2\theta_{n+1}^{(k)} + \theta_n^{(k)}$.

Resummation results (Heisenberg model)

Energy (square lattice)



C_v (square lattice)



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

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

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

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

where

$$W^c_\alpha = \frac{\sum_a e^{-(E^c_a - \mu_I N^c_a)/T_I} |\langle \alpha_c | a_c\rangle|^2}{Z^I_c},$$

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

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Using $\hat{\rho}_c^{\mathrm{DE}}$ 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).

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

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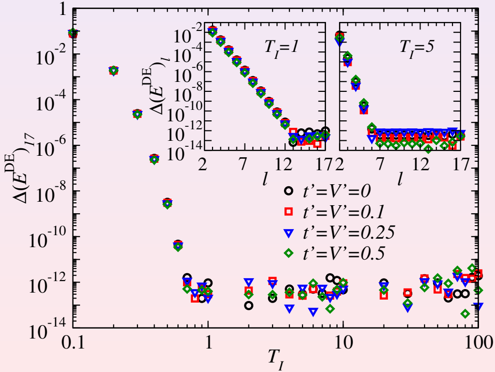
NLCE with maximally connected clusters ($l = 18$ sites)

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

Convergence:

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

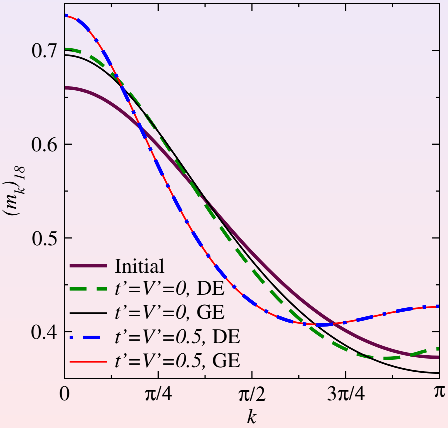
Convergence of E^{DE} with l



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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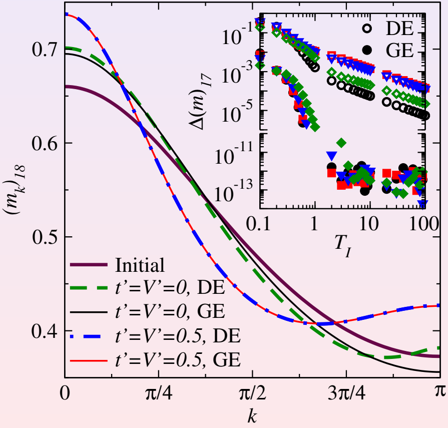
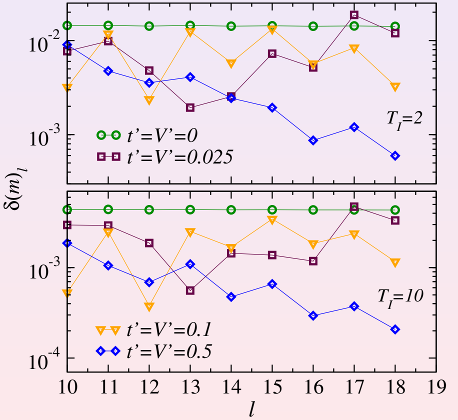


Differences between DE and GE

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



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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)?

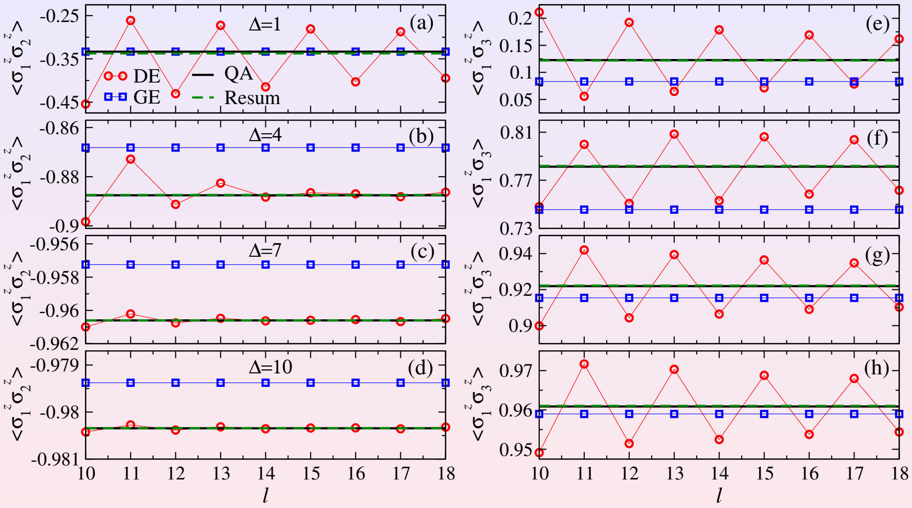
Using the parity symmetry of the clusters:

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

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

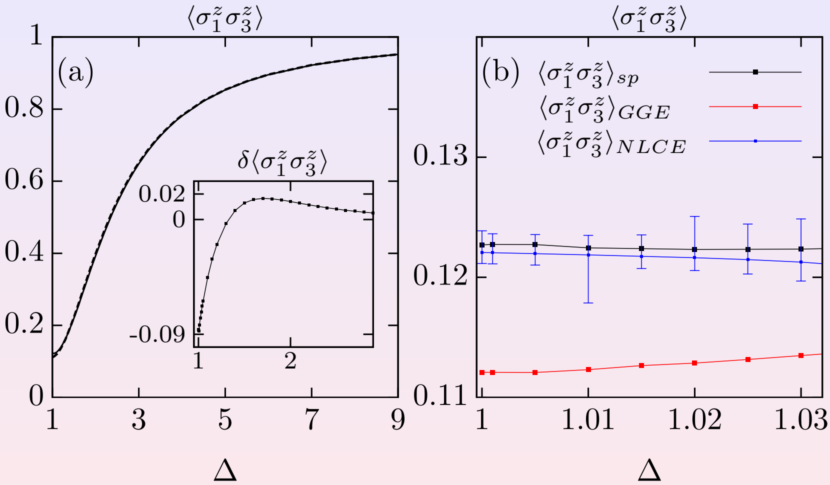
$$W_\alpha^{c,e/o} = |\langle\alpha_c^{e/o}|a_c^{e/o}\rangle|^2$$

Results for spin-spin correlations



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

Quench action, GGE, and NLCE



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

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

Outline

NLCEs for disordered systems

Hamiltonian with diagonal disorder

$$\hat{H} = \sum_i \left[-t(\hat{b}_i^\dagger \hat{b}_{i+1} + \text{H.c.}) + V\left(\hat{n}_i - \frac{1}{2}\right)\left(\hat{n}_{i+1} - \frac{1}{2}\right) + h_i\left(\hat{n}_i - \frac{1}{2}\right)\right]$$

binary disorder (equal probabilities for $h_i = \pm h$).

B. Tang, D. Iyer, and MR, arXiv:1411.0699.

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Disorder average restores translational invariance (exactly!)

$$\mathcal{O}(c) = \left\langle \mathrm{Tr}[\hat{\mathcal{O}}\hat{\rho}_c] \right\rangle_{\mathrm{dis}},$$

where $\langle \cdot \rangle_{\mathrm{dis}}$ represents the disorder average.

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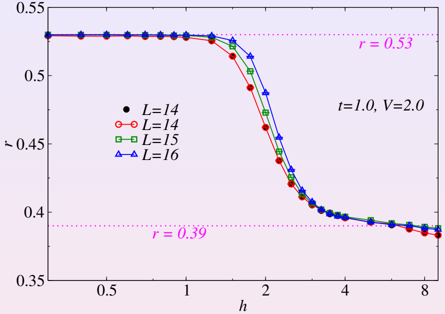
Initial state: $t_I = 0.5$, $V_I = 2.5$, $h_j = 0$, and T_I (no disorder)
Final Hamiltonian: $t = 1$, $V = 2.0$, and different values of $h \neq 0$

B. Tang, D. Iyer, and MR, arXiv:1411.0699.

Disordered systems and many-body localization

Ratio of consecutive energy gaps



Ratio of the smaller and the larger of two consecutive energy gaps

$$r_n = \min[\delta^E_{n-1}, \delta^E_n]/\max[\delta^E_{n-1}, \delta^E_n], \qquad \text{where} \quad \delta^E_n \equiv E_{n+1} - E_n$$

we compute $r = \langle\langle r_n^{\mathrm{dis}} \rangle_n \rangle_{\mathrm{dis}}$.

Continuous disorder: $h_c \approx 3.5$ [A. Pal and D. A. Huse, PRB **82**, 174411 (2010).]

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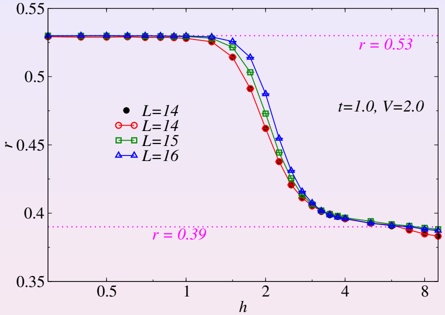
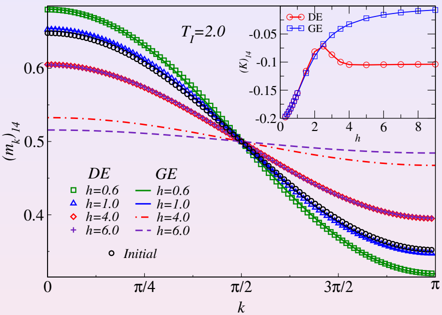


Diagonal vs Thermal



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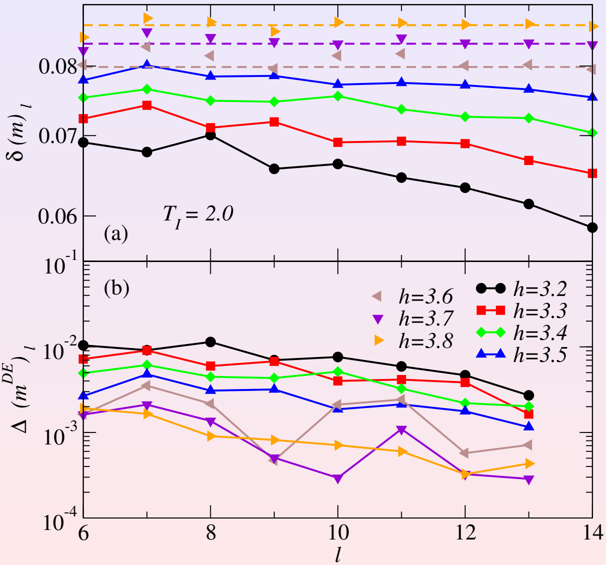
Scaling of the differences and errors



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. Time scale for thermalization as one approaches the integrable point.
- 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.
- Quantum quenches and NLCEs can be used to study the transition between delocalization and many-body localization. Arbitrary dimensions.

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