Quantum quenches and many-body localization

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Many-body Localization
KITP, Santa Barbara
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Outline

1. Introduction
   - Eigenstate thermalization hypothesis (ETH)
2. Non-equilibrium dynamics in the presence of disorder (ED)
   - Spinless fermions with random hopping
   - Hubbard model: quasi-periodic lattice vs disorder
3. Non-equilibrium dynamics in the presence of disorder (NLCEs)
   - Numerical linked cluster expansions
   - Numerical linked cluster expansions for quantum quenches
   - Hard-core bosons with binary disorder
4. Summary

Eigenstate thermalization

Eigenstate thermalization hypothesis

[J. Deutsch, PRA **43** 2046 (1991); M. Srednicki, PRE **50**, 888 (1994) & JPA **32** 1163 (1999); MR, V. Dunjko, and M. Olshanii, Nature **452**, 854 (2008).]

- Matrix elements of observables in the basis of the Hamiltonian eigenstates

$$O_{mn} = O\left(\bar{E}\right)\delta_{mn} + e^{-S\left(\bar{E}\right)/2} f_O\left(\bar{E},\omega\right) R_{mn},$$

where $\bar{E} \equiv (E_m + E_n)/2$, $\omega \equiv E_n - E_m$, and $S(E)$ is the thermodynamic entropy at energy E. $O\left(\bar{E}\right)$ and $f_O\left(\bar{E},\omega\right)$ are smooth functions of their arguments, and R_{mn} is a random variable with zero mean and unit variance.

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- L. D'Alessio, Y. Kafri, A. Polkovnikov, and M. Rigol, arXiv:1509.06411.
  From Quantum Chaos and Eigenstate Thermalization to Statistical Mechanics and Thermodynamics.

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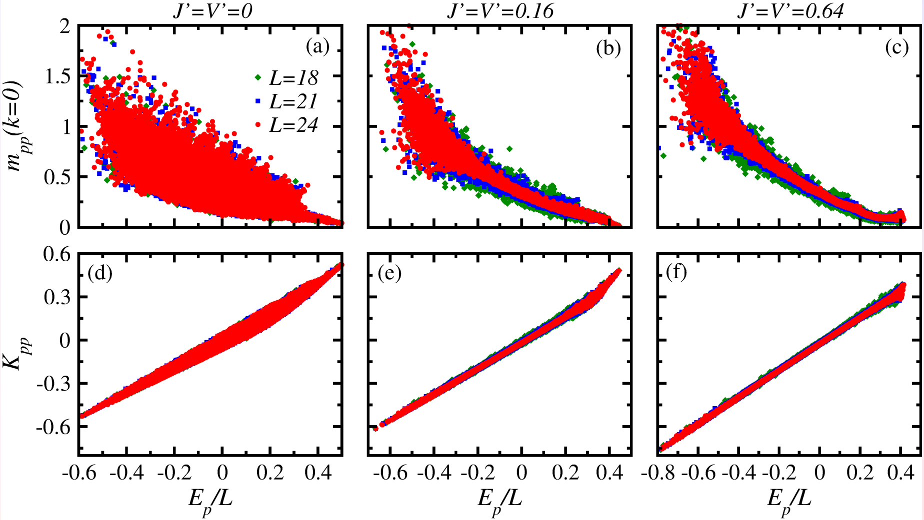
- Various aspects of eigenstate thermalization have been studied for:
  (i) Hard-core bosons (in 1D and 2D) and interacting spin chains (finite number of nearest neighbors, $1/r^3$ interactions, disordered spin chains)
  (ii) Spinless and spinful fermions (finite number of nearest neighbors, Fermi Hubbard, diagonal and off-diagonal disorder)
  (iii) Soft-core bosons (1D Bose-Hubbard model)

Diagonal part of eigenstate thermalization

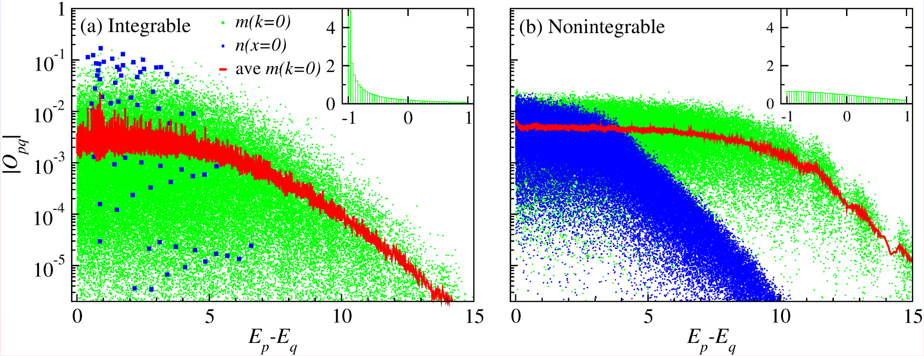
$$\hat{H} = \sum_{j=1}^{L} -J\left(\hat{b}_j^\dagger \hat{b}_{j+1} + \text{H.c.}\right) + V\left(\hat{n}_j - \frac{1}{2}\right)\left(\hat{n}_{j+1} - \frac{1}{2}\right) - J'\left(\hat{b}_j^\dagger \hat{b}_{j+2} + \text{H.c.}\right) + V'\left(\hat{n}_j - \frac{1}{2}\right)\left(\hat{n}_{j+2} - \frac{1}{2}\right)$$



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

Off-diagonal part of eigenstate thermalization

$$\hat{H} = -J \sum_{j=1}^{L-1} \left(\hat{b}_j^\dagger \hat{b}_{j+1} + \text{H.c.} \right) + V \sum_{j<l} \frac{\hat{n}_j \hat{n}_l}{|j-l|^3} + g \sum_j x_j^2 \, \hat{n}_j .$$



(Inset) Histogram of:

$$\frac{|O_{pq}| - |O_{pq}|_{\text{avg}}}{|O_{pq}|_{\text{avg}}}$$

E. Khatami, G. Pupillo, M. Srednicki, and MR, PRL **111**, 050403 (2013).

Width of the energy density after a sudden quench

Initial state $|\psi_I\rangle = \sum_m C_m |m\rangle$ is an eigenstate of $\widehat{H}_0$. At $\tau = 0$

$$\widehat{H}_0 \to \widehat{H} = \widehat{H}_0 + \widehat{H}_1 \qquad \text{with} \quad \widehat{H}_1 = \sum_j \hat{h}(j) \quad \text{and} \quad \widehat{H}|m\rangle = E_m |m\rangle.$$

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The width of the weighted energy density ΔE is then

$$\Delta E = \sqrt{\sum_m E_m^2|C_m|^2 - (\sum_m E_m|C_m|^2)^2} = \sqrt{\langle\psi_0|\widehat{H}_1^2|\psi_0\rangle - \langle\psi_0|\widehat{H}_1|\psi_0\rangle^2},$$

or

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

where N is the total number of lattice sites.

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where N is the total number of lattice sites.
Since the width of the spectrum $W \propto N$, then the ratio

$$\frac{\Delta E}{W} \overset{N\to\infty}{\propto} \frac{1}{\sqrt{N}},$$

so, as in any thermal ensemble, it vanishes in the thermodynamic limit.

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Model Hamiltonian and the MBL transition

Spinless fermion Hamiltonian in 1D

$$\hat{H} = \sum_{ij} J_{ij} \left(\hat{f}_i^\dagger \hat{f}_j + \text{H.c.} \right) + V \sum_i \left(\hat{n}_i - \frac{1}{2} \right) \left(\hat{n}_{i+1} - \frac{1}{2} \right)$$

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Hopping amplitudes

Gaussian random distribution $\langle J_{ij}\rangle = 0$

$$\langle (J_{ij})^2\rangle = \left[1 + \left(\frac{|i-j|}{\beta}\right)^{2\alpha}\right]^{-1}$$

$$V = 0$$

- Properties depend on α but not on $\beta > 0$
- $\alpha < 1$, eigenstates are delocalized
- $\alpha > 1$, eigenstates are localized
- $\alpha = 1$, eigenstates are multifractal

Mirlin *et al.*, PRE **54**, 3221 (1996).

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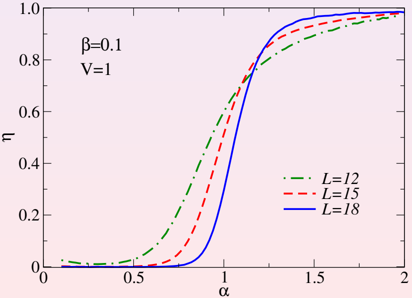
Ergodic-MBL transition

$$\eta = [\text{var} - \text{var}_{\text{WD}}]/[\text{var}_{\text{P}} - \text{var}_{\text{WD}}]$$

var: variance of level spacing distribution



Dynamics after a quench

Quench protocol

- Start from an eigenstate of $\hat{H}$ ($|\psi_I\rangle$) in a certain disorder realization.
- Evolve under another disorder realization with the same α.
- $E = \langle\psi_I|\hat{H}_{\text{fin}}|\psi_I\rangle$ is the energy of a thermal state with temperature $T = 10$.

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Eigenstate thermalization

Observables:

$$\hat{n}(k) = \frac{1}{L}\sum_{l,m} e^{ik(l-m)}\hat{f}_l^\dagger \hat{f}_m$$

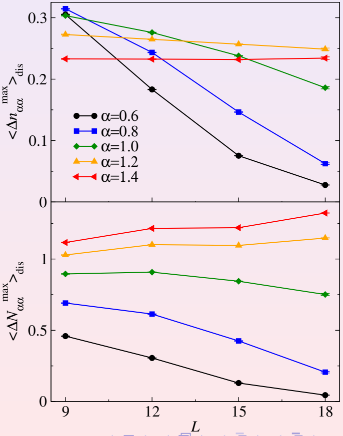
$$\hat{N}(k) = \frac{1}{L}\sum_{l,m} e^{ik(l-m)}\hat{n}_l\hat{n}_m$$

Maximal normalized difference:

$$\Delta O_{\alpha\alpha}^{\text{max}} = \frac{\sum_k |O_{\alpha\alpha}^{\text{max}}(k) - O_{\text{ME}}(k)|}{\sum_k O_{\text{ME}}(k)}$$

Disorder average:

$$\langle \Delta O_{\alpha\alpha}^{\text{max}}\rangle_{\text{dis}}$$



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Microcanonical vs diagonal

Observables:

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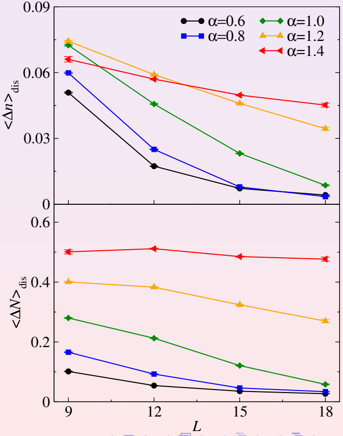
$$\hat{N}(k) = \frac{1}{L}\sum_{l,m} e^{ik(l-m)}\hat{n}_l\hat{n}_m$$

Normalized difference:

$$\Delta O = \frac{\sum_k |O_{\text{ME}}(k) - O_{\text{DE}}(k)|}{\sum_k O_{\text{DE}}(k)}$$

Disorder average:

$$\langle\Delta O\rangle_{\text{dis}}$$



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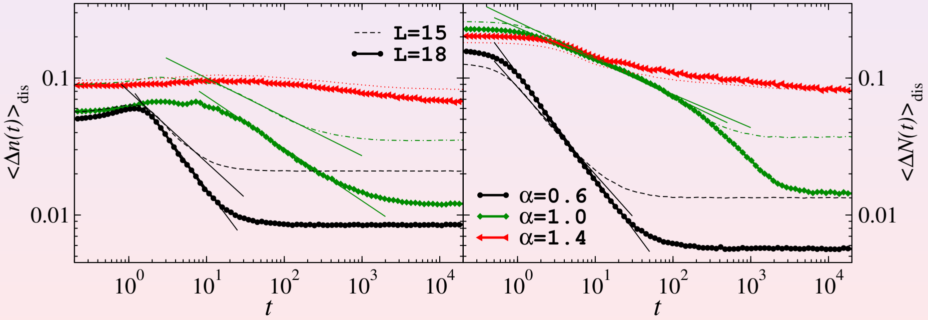
Time evolution $\left[\Delta O(t) = \frac{\sum_k |O(k,t) - O_{\text{DE}}(k)|}{\sum_k O_{\text{DE}}(k)}\right]$



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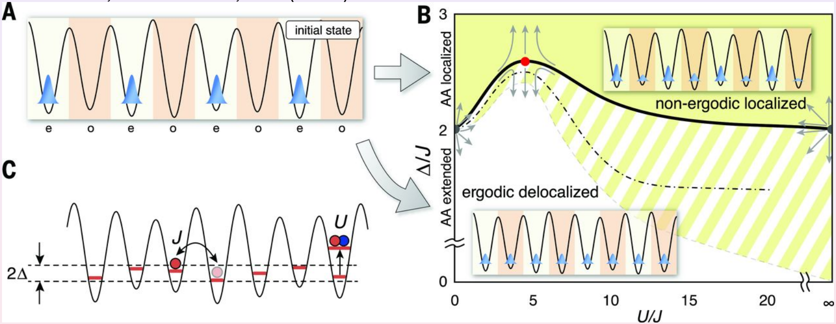
Experimental results

Hubbard Hamiltonian in 1D: [$\varepsilon_i = \Delta \cos(2\pi\beta i + \phi)$, and $\beta \approx 0.721$]

$$\hat{H} = -J \sum_{i,\sigma} (\hat{c}^\dagger_{i\sigma} \hat{c}_{i+1,\sigma} + \text{H.c.}) + U \sum_{i}^{L} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + \sum_{i\sigma} \varepsilon_i \hat{n}_{i\sigma}$$

Schreiber *et al.*, Science **349**, 842 (2015).



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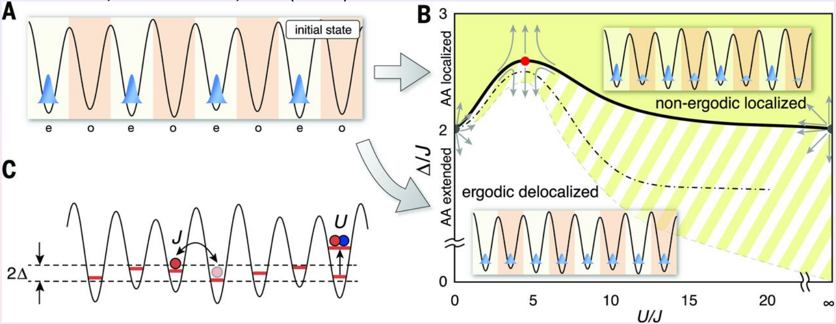
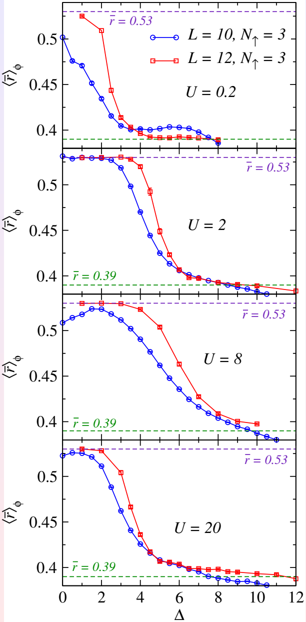


We add: $(J' = J/2$, and also consider $\varepsilon_i \in [-W/2, W/2]$, at quarter filling)

$$\hat{H}' = -J'\sum_{i,\sigma}^{L-2}(\hat{c}^\dagger_{i\sigma}\hat{c}_{i+2,\sigma} + \text{H.c.}) + \mu_b(\hat{n}_{L,\uparrow} + \hat{n}_{L,\downarrow}) + h_b(\hat{n}_{1,\uparrow} - \hat{n}_{1,\downarrow})$$

R. Mondaini and MR, Phys. Rev. A **92**, 041601(R) (2015).

Results for $r_n = \min[\delta^E_{n-1}, \delta^E_n]/\max[\delta^E_{n-1}, \delta^E_n]$



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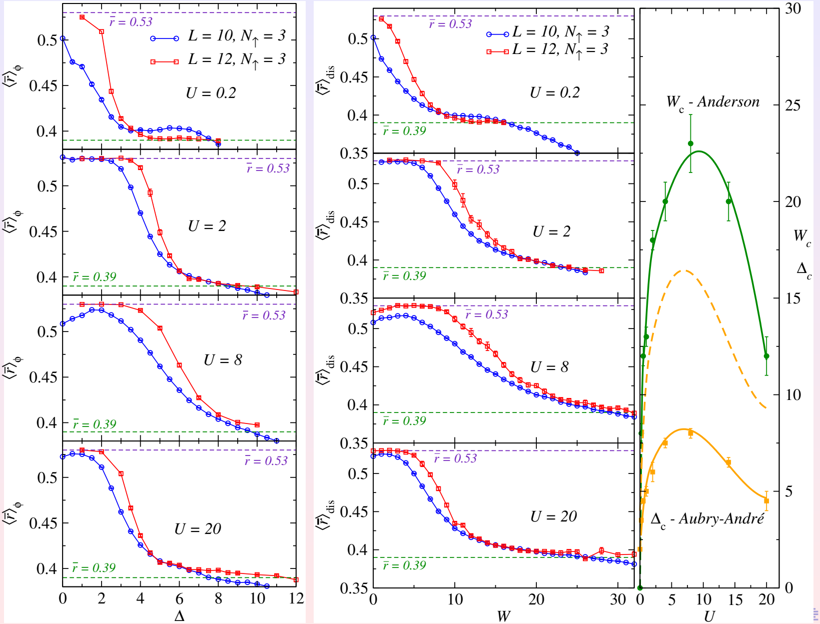
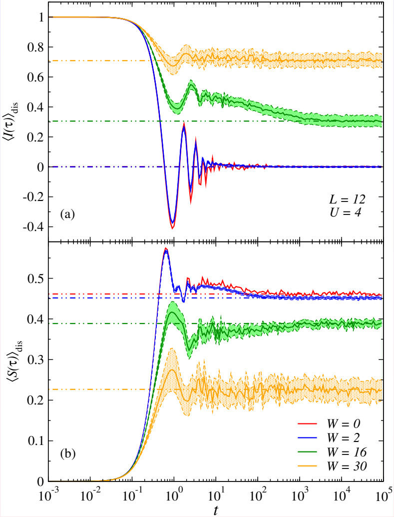


Dynamics and thermalization: $|\psi_I\rangle = |\uparrow 0 \downarrow 0 \uparrow 0 \downarrow \ldots\rangle$

Relaxation Dynamics



$$I = \frac{(\langle \hat{n}^e \rangle - \langle \hat{n}^o \rangle)}{(\langle \hat{n}^e \rangle + \langle \hat{n}^o \rangle)}$$

$$S = \frac{1}{L} \sum_{i,j} e^{i\pi(i-j)} \langle (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})(\hat{n}_{j\uparrow} - \hat{n}_{j\downarrow}) \rangle$$

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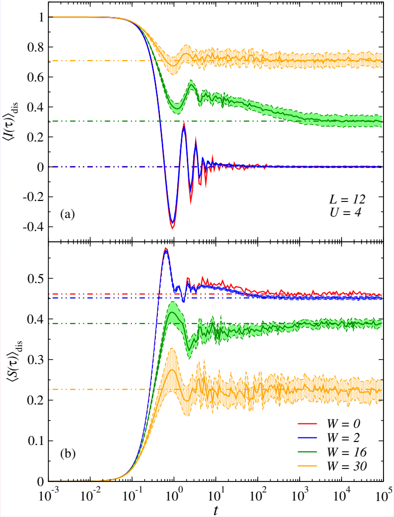
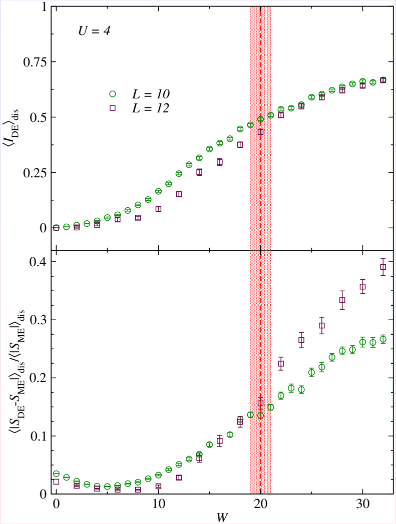


Thermalization



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

$\mathcal{O}(c)$ 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\}
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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.

MR, T. Bryant, and R. R. P. Singh, PRL **97**, 187202 (2006).

Finite size effects

- In unordered phases, not all ensemble calculations of finite systems approach the thermodynamic limit the same way

  There is a *preferred ensemble* (the grand canonical ensemble) and *preferred boundary conditions* (periodic boundary conditions, so that the system is translationally invariant) for which finite-size effects are exponentially small in the system size. All others exhibit power-law convergence with system size.

D. Iyer, M. Srednicki, and MR, Phys. Rev. E **91**, 062142 (2015).

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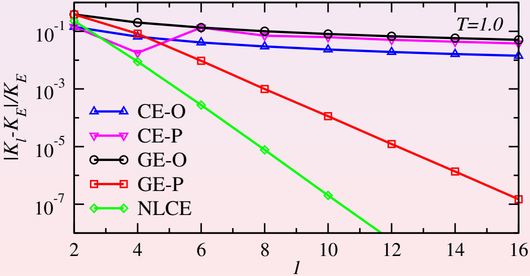
Kinetic energy in the J-V model



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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).

Diagonal ensemble and NLCEs

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

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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 $\hat{H}_c$

$$\hat{\rho}_c^{\mathrm{DE}} \equiv \lim_{t' \to \infty} \frac{1}{t'} \int_0^{t'} dt\, \hat{\rho}(t) = \sum_\alpha W_\alpha^c\, |\alpha_c\rangle\langle \alpha_c|$$

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

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

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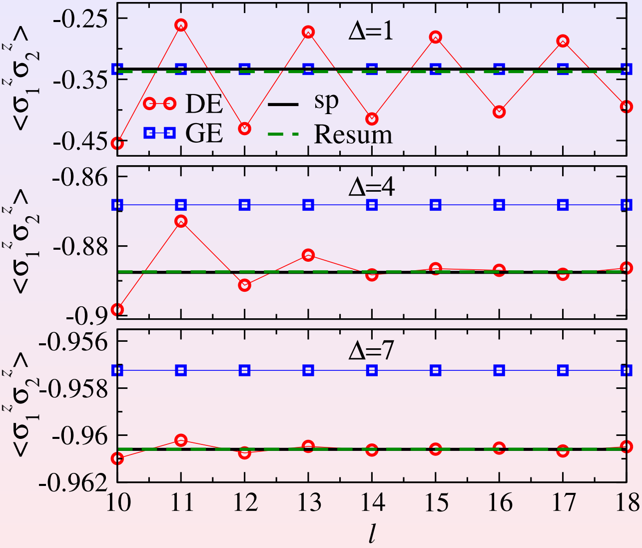
$|\alpha_c\rangle$ (ε_α^c) are the eigenstates (eigenvalues) of the final Hamiltonian $\hat{H}_c$ in c.

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).

Quenches in the XXZ model



MR, PRE **90**, 031301(R) (2014); B. Wouters *et al.*, PRL **113**, 117202 (2014).

Quantum quenches and many-body localization

Hard-core bosons with binary disorder

Hamiltonian with diagonal disorder

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

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

B. Tang, D. Iyer, and MR, Phys. Rev. B **91**, 161109(R) (2015).

Hard-core bosons with binary disorder

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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.

B. Tang, D. Iyer, and MR, Phys. Rev. B **91**, 161109(R) (2015).

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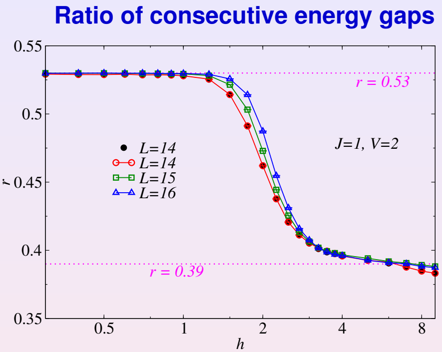
where $\langle\cdot\rangle_{\text{dis}}$ represents the disorder average.

Initial state: $J_I = 0.5$, $V_I = 2.5$, $h_j = 0$, and T_I (no disorder)

Final Hamiltonian: $J = 1$, $V = 2$, and different values of $h \neq 0$

B. Tang, D. Iyer, and MR, Phys. Rev. B **91**, 161109(R) (2015).

Disordered systems and many-body localization



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

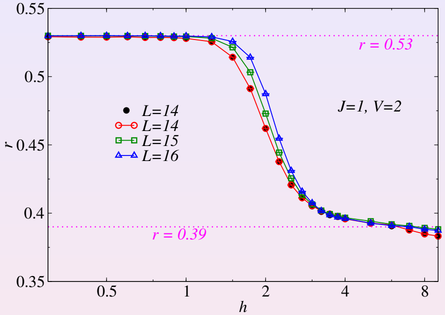
$$r_n = \min[\delta^E_{n-1}, \delta^E_n]/\max[\delta^E_{n-1}, \delta^E_n], \qquad \text{where} \quad \delta^E_n \equiv E_{n+1} - E_n$$

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

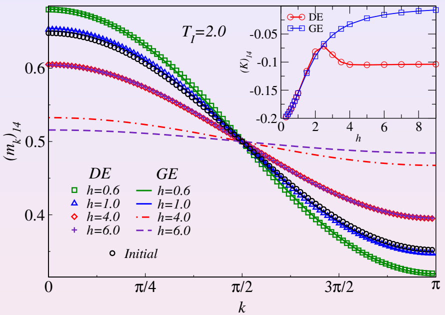
Continuous disorder: $h_c \approx 7.4$ [Luitz, Laflorencie, & Alet, PRB **91**, 081103 (2015).]

Disordered systems and many-body localization

Ratio of consecutive energy gaps



Diagonal vs Thermal



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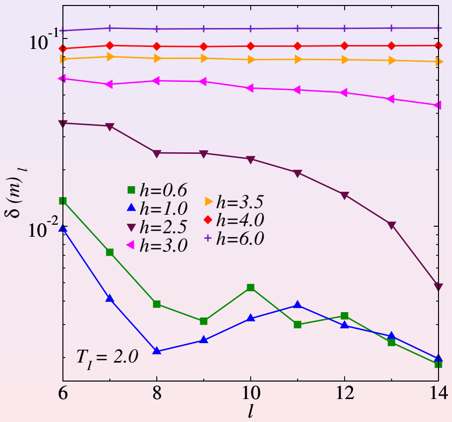
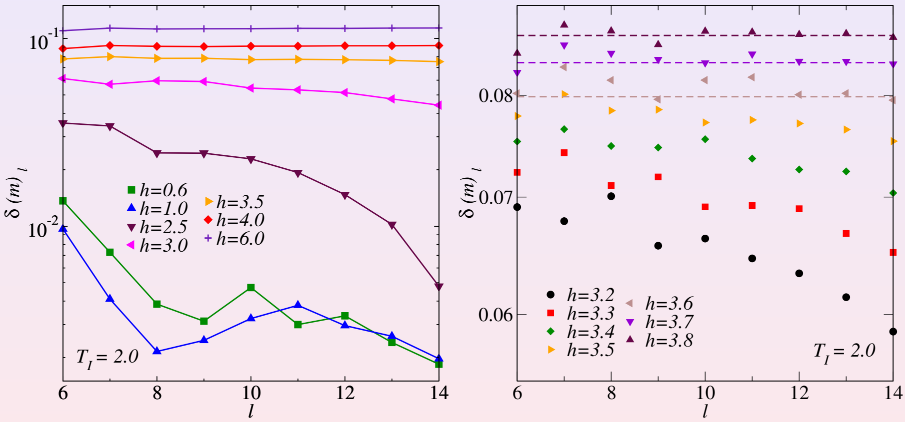
Scaling of the differences: $\delta(m)_l = \frac{\sum_k |(m_k)_l^{\mathrm{DE}} - (m_k)_{14}^{\mathrm{GE}}|}{\sum_k |(m_k)_{14}^{\mathrm{GE}}|}$



Scaling of the differences: $\delta(m)_l = \frac{\sum_k |(m_k)_l^{\text{DE}} - (m_k)_{14}^{\text{GE}}|}{\sum_k |(m_k)_{14}^{\text{GE}}|}$



Summary

- We have seen signatures of MBL, no eigenstate thermalization and/or failure of the system to thermalize after a quench, in three different models involving spinless and spinful fermions, and hard-core bosons.
- MBL for spinful fermions requires a disorder strength that is several times the single-particle bandwidth. This might be hidden by finite-size effects in the experiments.
- Numerical linked cluster expansions (NLCEs) provide an alternative way to look into these problems starting from a thermodynamic limit formulation.

Collaborators

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— PRE **85**, 050102(R) (2012)

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Deepak Iyer ($\longrightarrow$ Bucknell)
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