Quantum quenches and many-body localization

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Entanglement and non-equilibrium physics of pure and disordered systems
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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 (ETH)

[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 $S(\bar{E})$ is the thermodynamic entropy at energy $\bar{E}$. $O\left(\bar{E}\right)$ 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.

L. D'Alessio, Y. Kafri, A. Polkovnikov, and MR, *From Quantum Chaos and Eigenstate Thermalization to Statistical Mechanics and Thermodynamics*, arXiv:1509.06411 (Advances in Physics, in press).

Integrability to quantum chaos transition in 1D

Spinless fermions with nearest and next nearest neighbors in 1D

$$\hat{H} = \sum_{i=1}^{L} \left\{ -J \left(\hat{f}_i^\dagger \hat{f}_{i+1} + \text{H.c.} \right) + V \hat{n}_i \hat{n}_{i+1} - J' \left(\hat{f}_i^\dagger \hat{f}_{i+2} + \text{H.c.} \right) + V' \hat{n}_i \hat{n}_{i+2} \right\}$$

L. Santos and MR, PRE **81**, 036206 (2010).

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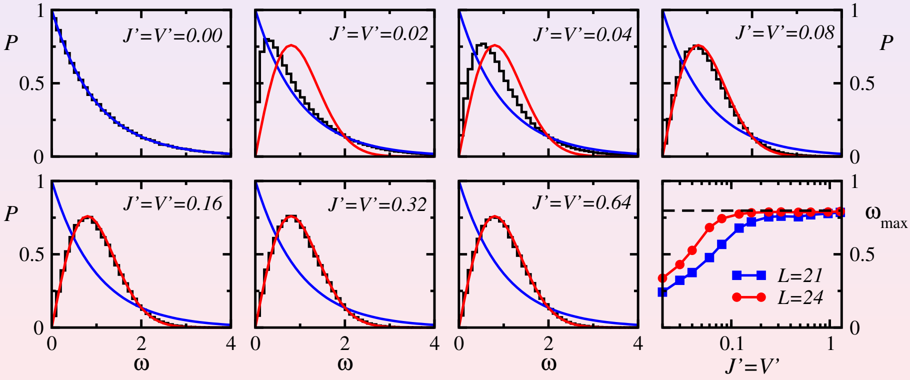
Level spacing distribution $(J = V = 1)$



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Matrix elements of Hermitian operators within RMT

Let $\hat{O} = \sum_i O_i |i\rangle\langle i|$, where $\hat{O}|i\rangle = O_i|i\rangle$,

$$O_{\alpha\beta} \equiv \langle\alpha|\hat{O}|\beta\rangle = \sum_i O_i \langle\alpha|i\rangle\langle i|\beta\rangle = \sum_i O_i (\psi_i^\alpha)^* \psi_i^\beta$$

$|\alpha\rangle$ and $|\beta\rangle$ are eigenstates of a random matrix. Averaging over $|\alpha\rangle$ and $|\beta\rangle$ (random orthogonal unit vectors in arbitrary bases): $\overline{(\psi_i^\alpha)^*(\psi_i^\beta)} = \frac{1}{\mathcal{D}}\delta_{\alpha\beta}$.

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This means that:

$$\overline{O_{\alpha\alpha}} = \frac{1}{\mathcal{D}} \sum_i O_i \equiv \bar{O}, \quad \text{while} \quad \overline{O_{\alpha\beta}} = 0 \quad \text{for} \quad \alpha \neq \beta.$$

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With more work one can show that ($\eta = 2$ for GOE and $\eta = 1$ for GUE):

$$\overline{O_{\alpha\alpha}^2} - \overline{O_{\alpha\alpha}}^2 = \eta\overline{|O_{\alpha\beta}|^2} = \frac{\eta}{\mathcal{D}^2}\sum_i O_i^2 \equiv \frac{\eta}{\mathcal{D}}\overline{O^2}.$$

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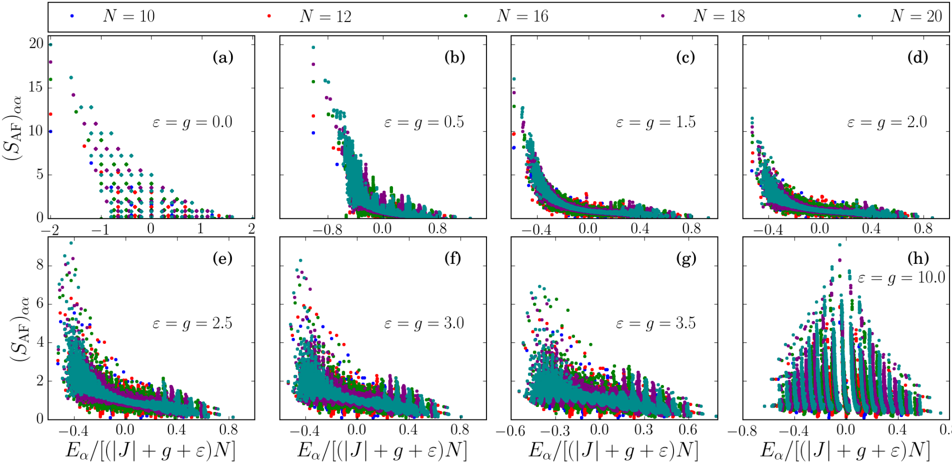
Combining these results one can write

$$O_{\alpha\beta} \approx \bar{O}\delta_{\alpha\beta} + \sqrt{\frac{\overline{O^2}}{\mathcal{D}}} R_{\alpha\beta},$$

where $R_{\alpha\beta}$ is a random variable (real for GOE and complex for GUE).

Diagonal part of ETH (2D AF-TFIM)

Hamiltonian: $\hat{H} = J \sum_{\langle \mathbf{i},\mathbf{j} \rangle} \hat{\sigma}^z_{\mathbf{i}} \hat{\sigma}^z_{\mathbf{j}} + g \sum_{\mathbf{i}} \hat{\sigma}^x_{\mathbf{i}} + \varepsilon \sum_{\mathbf{i}} \hat{\sigma}^z_{\mathbf{i}},$



R. Mondaini, K. R. Fratus, M. Srednicki, and MR, Phys. Rev. E. **93**, 032104 (2016).

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

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

where N is the total number of lattice sites.

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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

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

E. Khatami, MR, A. Relaño, and A. García-García, PRE **85**, 050102(R) (2012); arXiv:1103.0787.

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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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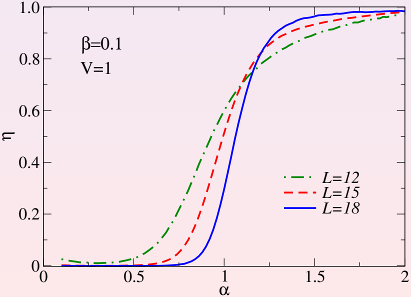
Ergodic-MBL transition

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

var: variance of level spacing distribution



Breakdown of ETH

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:

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

Constant effective temperature:

$(T = 10)$

$$E_{\text{ME}} = \frac{1}{Z}\text{Tr}[\hat{H} e^{-H/(k_B T)}]$$

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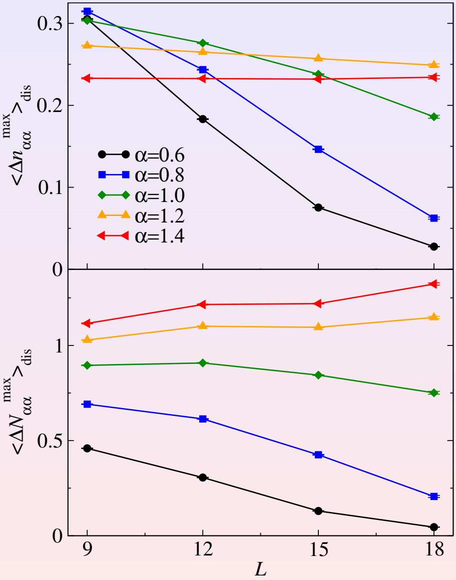

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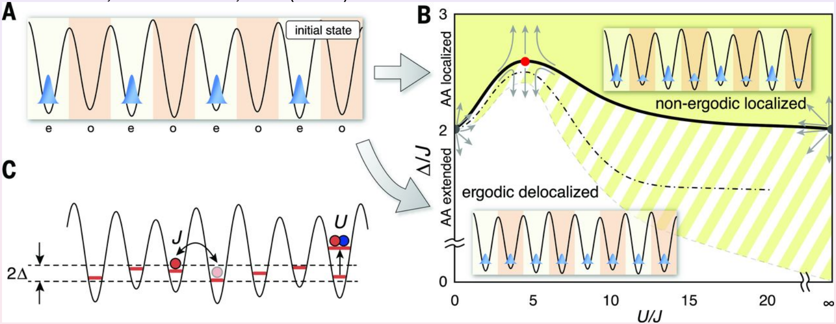
Experimental results

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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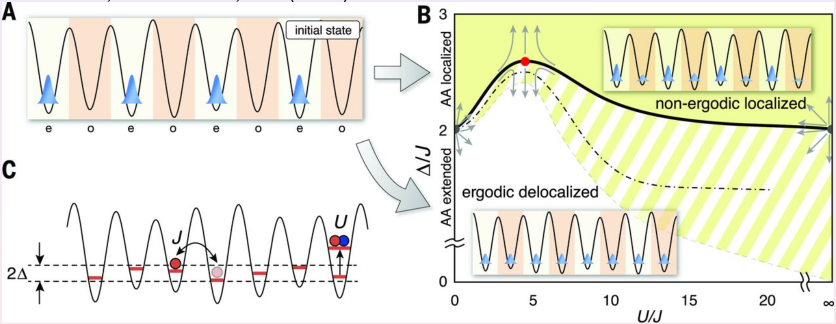
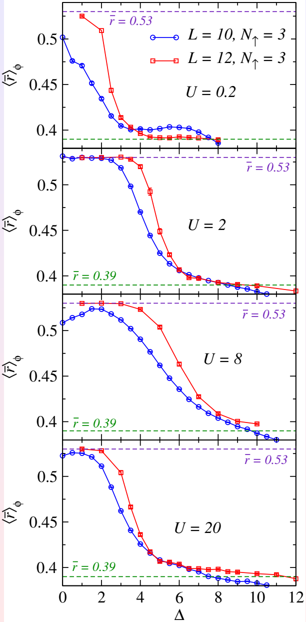


We add: ($J' = J/2$, and also consider $\varepsilon_i \in [-W/2, W/2]$, at quarter filling)

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

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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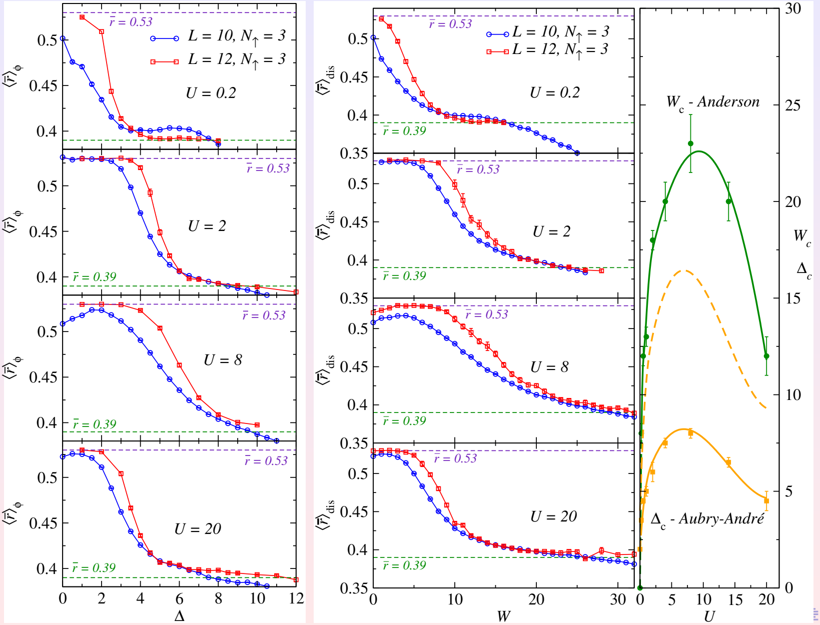
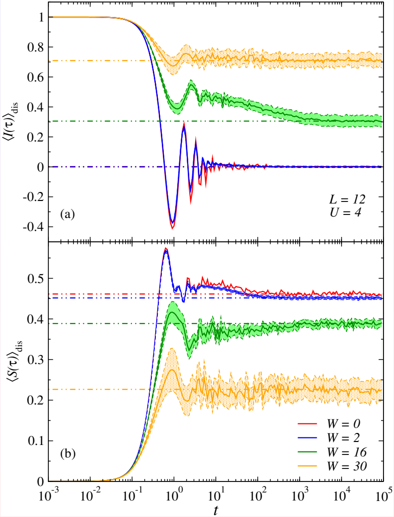


Dynamics and thermalization: $|\psi_I\rangle = |\uparrow 0 \downarrow 0 \uparrow 0 \downarrow \ldots\rangle$

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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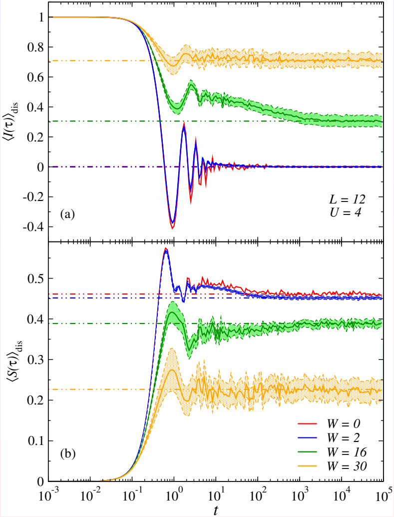
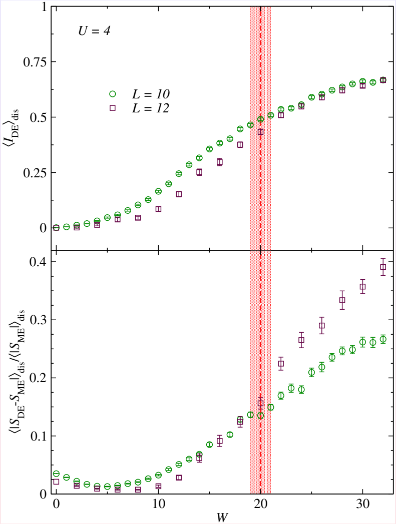


Thermalization



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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, & R. 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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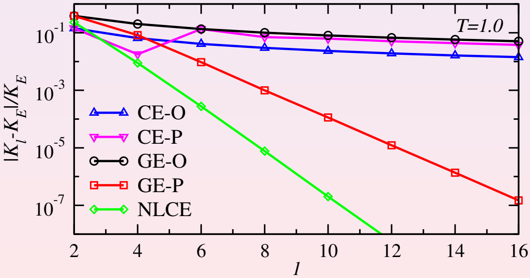
- NLCEs convergence is also exponential, but a faster one!

Kinetic energy in the J-V model



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

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4. Summary

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 $\hat{H}_c$

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

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.

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

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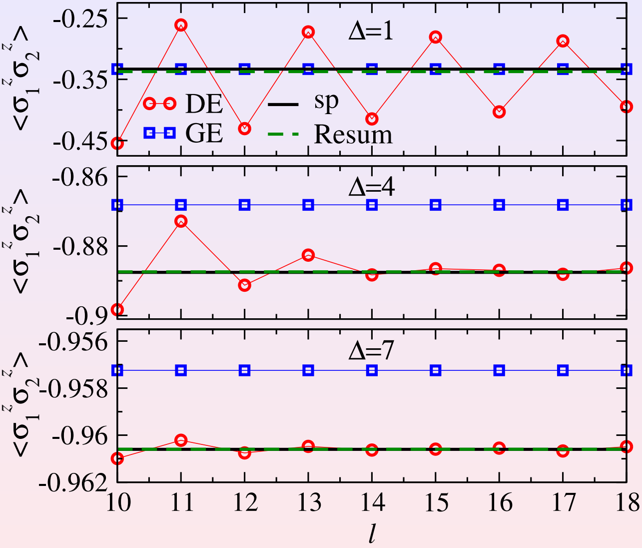
Using $\hat{\rho}_c^{\text{DE}}$ in the calculation of $\mathcal{O}(c)$, NLCEs allow one to compute observables in the DE in the thermodynamic limit.

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

Quenches in the XXZ model (Neel initial state)



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

Quantum quenches and many-body localization

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4. Summary

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).

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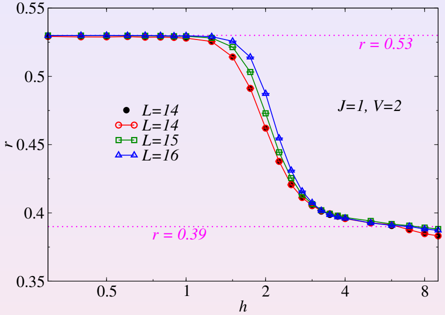
where $\langle\cdot\rangle_{\mathrm{dis}}$ represents the disorder average.

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).

Ratio of consecutive energy gaps



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

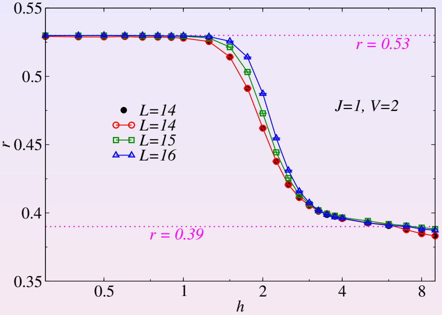
$$r_n = \min[\delta^E_{n-1}, \delta^E_n]/\max[\delta^E_{n-1}, \delta^E_n], \qquad \text{where} \quad \delta^E_n \equiv E_{n+1} - E_n$$

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

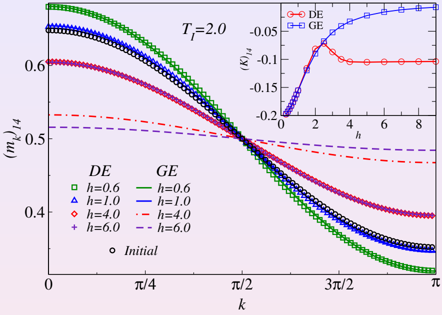
Continuous disorder: $h_c \approx 7.4$ [Luitz, Laflorencie & Alet, PRB **91**, 081103 (2015).]
$h_c \approx 9$ [T. Devakul & R.R.P. Singh, PRL **115**, 187201 (2015).]

Disordered systems and many-body localization

Ratio of consecutive energy gaps



Diagonal vs Thermal



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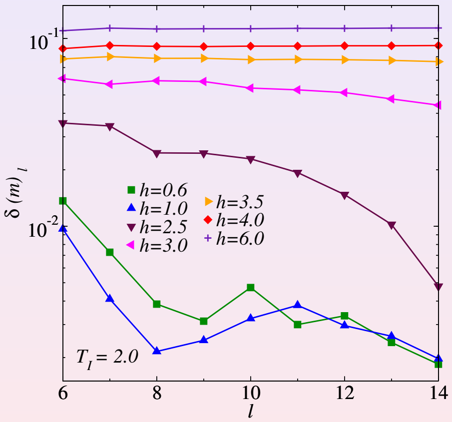
Scaling of the differences: $\delta(m)_l = \frac{\sum_k |(m_k)_l^{\mathrm{DE}} - (m_k)_{14}^{\mathrm{GE}}|}{\sum_k |(m_k)_{14}^{\mathrm{GE}}|}$



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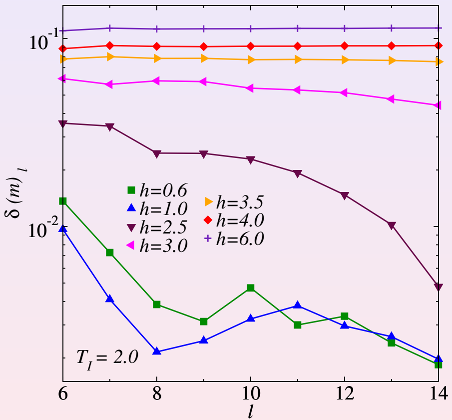

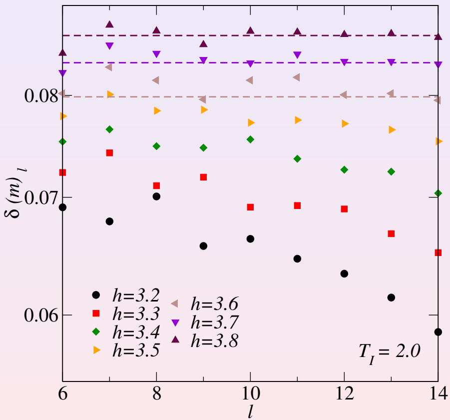

Summary

- 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-time and 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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PRB **91**, 161109(R) (2015)

Rubem Mondaini ($\longrightarrow$ Beijing CSRC)

PRA **92**, 041601(R) (2015)

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