Dynamics and thermalization in isolated quantum systems

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Outline

1. Introduction
   - Quantum dynamics, quenches, and thermalization
   - Many-body quantum systems in thermal equilibrium
   - Numerical linked cluster expansions
2. Quantum quenches in the thermodynamic limit
   - Diagonal ensemble and NLCEs
   - Quenches in the t-V-t'-V' chain
   - Many-body localization
3. Conclusions

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Foundations of quantum statistical mechanics

Quantum ergodicity: John von Neumann ‘29
(Proof of the ergodic theorem and the
H-theorem in quantum mechanics)

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Recent works:

Tasaki ‘98
(From Quantum Dynamics to the Canonical Distribution. . .)

Goldstein, Lebowitz, Tumulka, and Zanghi ‘06
(Canonical Typicality)

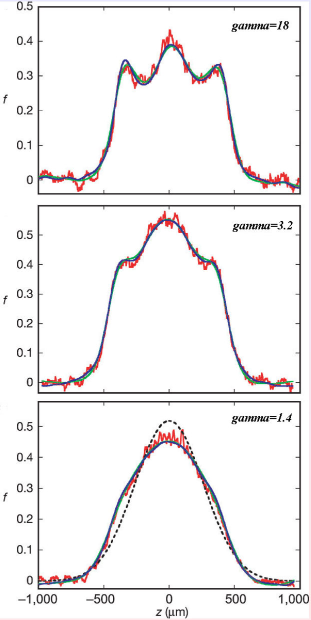
Popescu, Short, and A. Winter ‘06
(Entanglement and the foundation of statistical mechanics)

Goldstein, Lebowitz, Mastrodonato, Tumulka, and Zanghi ‘10
(Normal typicality and von Neumann’s quantum ergodic theorem)

MR and Srednicki ‘12
(Alternatives to Eigenstate Thermalization)

P. Reimann ‘15
(Generalization of von Neumann’s Approach to Thermalization)

Absence of thermalization in 1D



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

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

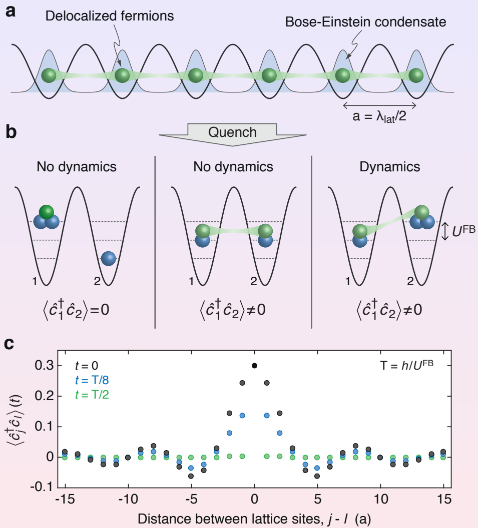
g_{1D}: Interaction strength
ρ: One-dimensional density

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

Gring *et al.*, Science **337**, 1318 (2012).

Coherence after quenches in Bose-Fermi mixtures



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

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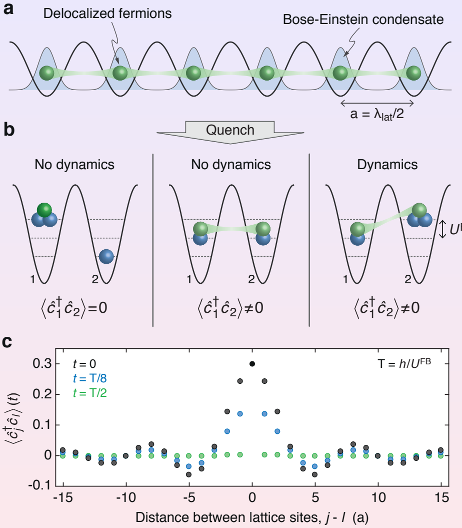

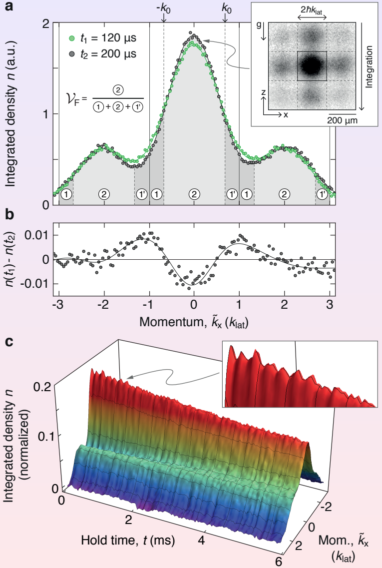

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Dynamics and thermalization in quantum systems

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

Width of the energy density after a sudden quench

Initial state $|\psi_0\rangle = \sum_\alpha C_\alpha |\alpha\rangle$ is an eigenstate of $\widehat{H}_0$. At $\tau = 0$

$$\widehat{H}_0 \to \widehat{H} = \widehat{H}_0 + \widehat{W} \qquad \text{with} \quad \widehat{W} = \sum_j \hat{w}(j) \quad \text{and} \quad \widehat{H}|\alpha\rangle = E_\alpha|\alpha\rangle.$$

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The width of the weighted energy density $\Delta E = \sqrt{\langle\psi_0|\widehat{H}^2|\psi_0\rangle - \langle\psi_0|\widehat{H}|\psi_0\rangle^2}$ is

$$\Delta E = \sqrt{\sum_\alpha E_\alpha^2 |C_\alpha|^2 - (\sum_\alpha E_\alpha |C_\alpha|^2)^2} = \sqrt{\langle\psi_0|\widehat{W}^2|\psi_0\rangle - \langle\psi_0|\widehat{W}|\psi_0\rangle^2},$$

or

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

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 W of the full energy spectrum is $\propto N$

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

so, as in any thermal ensemble, $\Delta\epsilon$ vanishes in the thermodynamic limit.

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

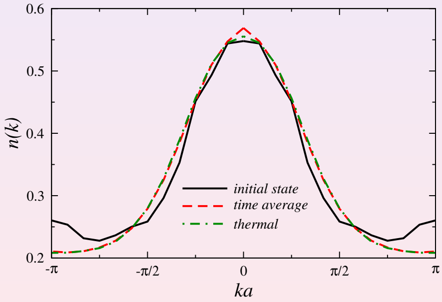
Description after relaxation (lattice models)

Hard-core boson (spinless fermion) Hamiltonian

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

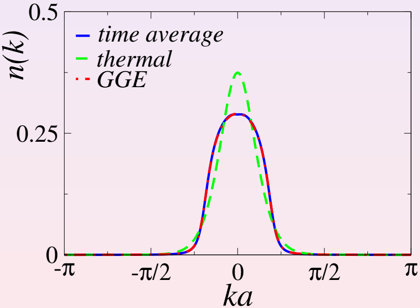
Dynamics vs statistical ensembles

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



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

Integrable: $V = t' = V' = 0$



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

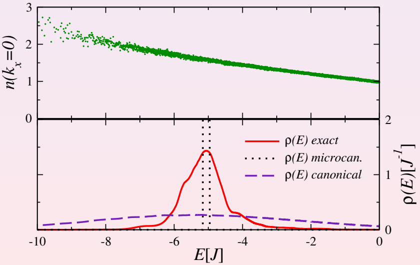
Eigenstate thermalization hypothesis

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

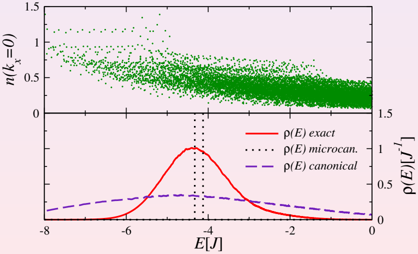
- The expectation value $\langle\alpha|\widehat{O}|\alpha\rangle$ of a few-body observable $\widehat{O}$ in an eigenstate of the Hamiltonian $|\alpha\rangle$, with energy E_α, of a many-body system is equal to the thermal average of $\widehat{O}$ at the mean energy E_α:

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

Nonintegrable

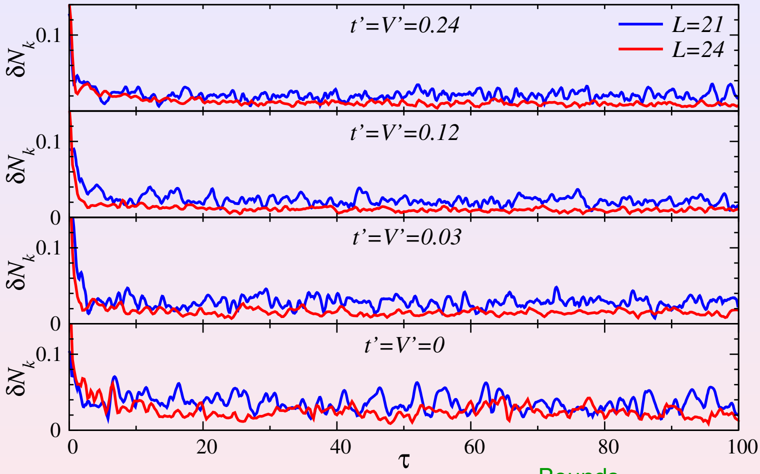


Integrable ($\hat{\rho}_{\text{GGE}} = \frac{1}{Z_{\text{GGE}}} e^{-\sum_m \lambda_m \hat{I}_m}$)



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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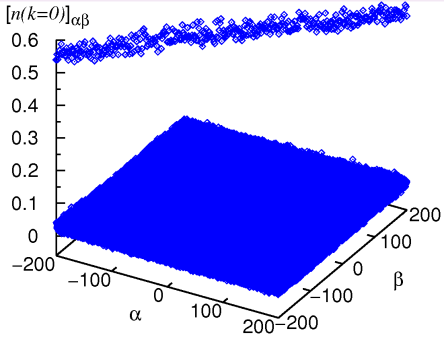

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Finite temperature properties of lattice models

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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- DMFT, DCA, DMRG, ...

Linked-Cluster Expansions

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

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

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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

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

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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).

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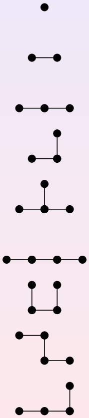
Numerical linked cluster expansions (square lattice)

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 (square lattice)

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
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6	14
7	28
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10	399
11	1012
12	2732
13	7385
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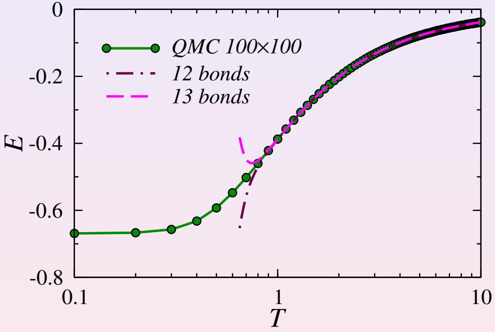
v) Compute the weight of each cluster and compute the direct sum of the weights

Heisenberg Model in 2D

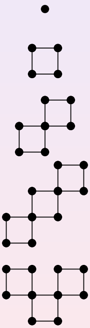


MR *et al.*, PRE **75**, 061118 (2007).

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

Numerical linked cluster expansions

Square clusters

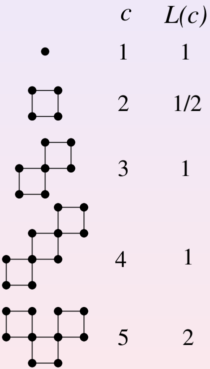


c	$L(c)$
1	1
2	1/2
3	1
4	1
5	2

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

Numerical linked cluster expansions

Square clusters



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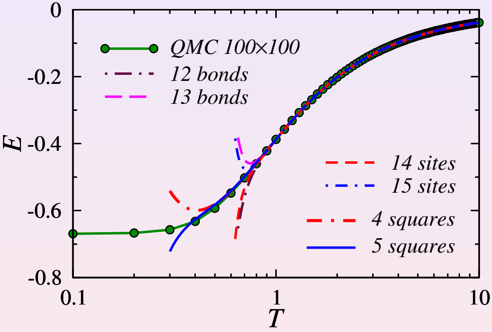

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Resummation algorithms

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:

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

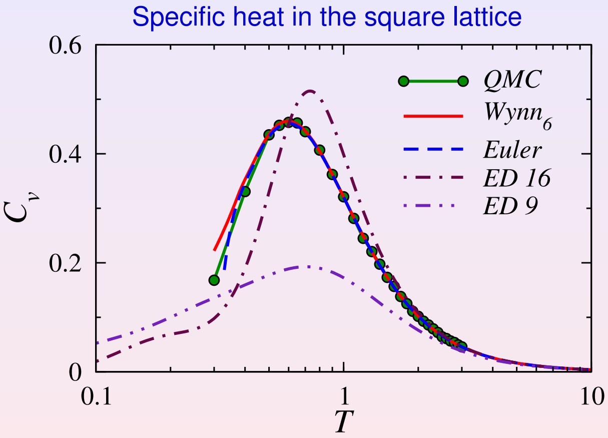
where $\Delta\varepsilon_n^{(k-1)} = \varepsilon_{n+1}^{(k-1)} - \varepsilon_n^{(k-1)}$.

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)



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

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

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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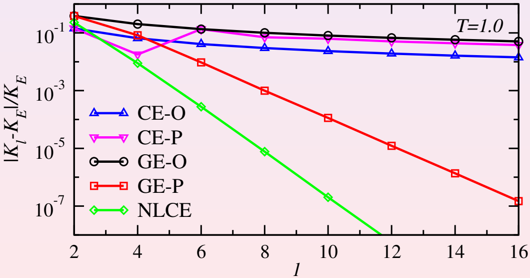
Kinetic energy in the t-V model



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

Outline

1. Introduction
   - Quantum dynamics, quenches, and thermalization
   - Many-body quantum systems in thermal equilibrium
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2. Quantum quenches in the thermodynamic limit
   - Diagonal ensemble and NLCEs
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3. 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); PRE **90**, 031301(R) (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 $\hat{H}_c$

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

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.

MR, PRL **112**, 170601 (2014); PRE **90**, 031301(R) (2014).

Diagonal ensemble and NLCEs

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

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

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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); PRE **90**, 031301(R) (2014).

Outline

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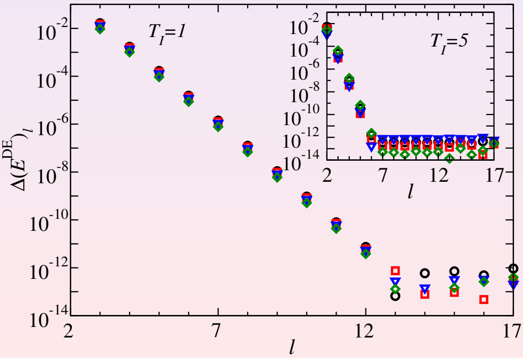
NLCE with maximally connected clusters ($l = 18$ sites)

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

Convergence:

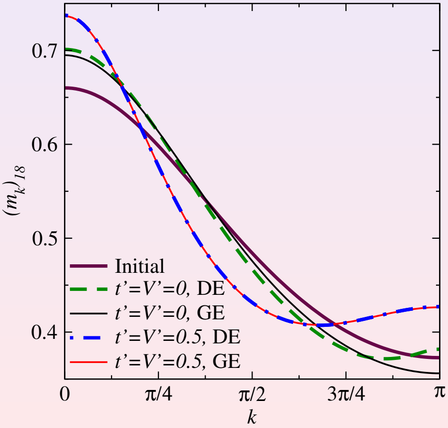
$$\Delta(\mathcal{O}^{\text{DE}})_l = \frac{|\mathcal{O}_l^{\text{DE}} - \mathcal{O}_{18}^{\text{DE}}|}{|\mathcal{O}_{18}^{\text{DE}}|}$$

Convergence of E^{DE} with l



Momentum distribution

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



Few-body experimental observables in the DE

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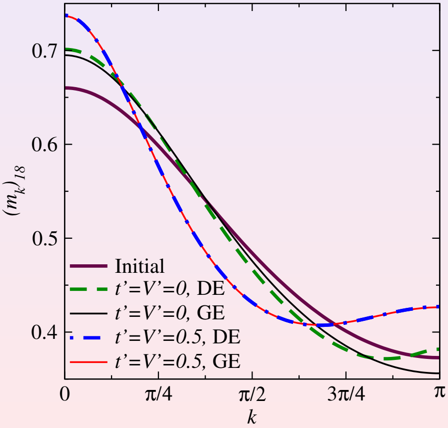
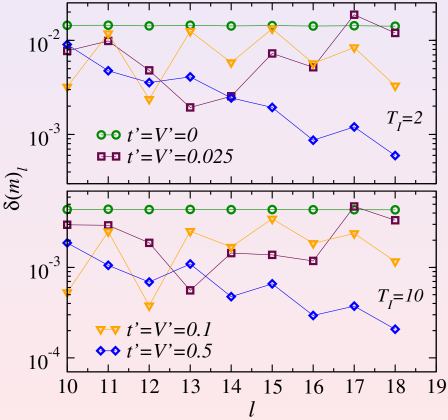


Differences between DE and GE

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



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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, PRB **91**, 161109(R) (2015).

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Disorder average restores translational invariance (exactly!)

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

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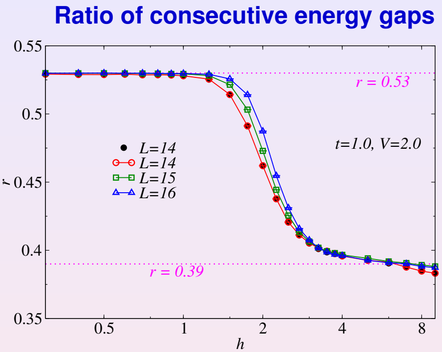
where $\langle \cdot \rangle_{\mathrm{dis}}$ represents the disorder average.

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, PRB **91**, 161109(R) (2015).

Disordered systems and many-body localization



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

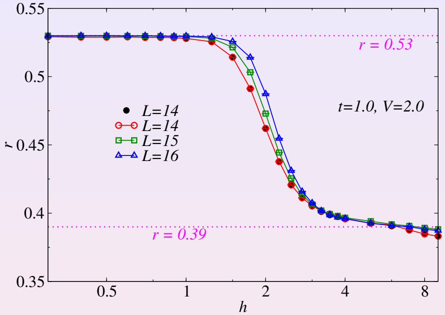
$$r_n = \min[\delta^E_{n-1}, \delta^E_n]/\max[\delta^E_{n-1}, \delta^E_n], \qquad \text{where} \quad \delta^E_n \equiv E_{n+1} - E_n$$

we compute $r = \langle\langle r^{\text{dis}}_n \rangle_n \rangle_{\text{dis}}$.

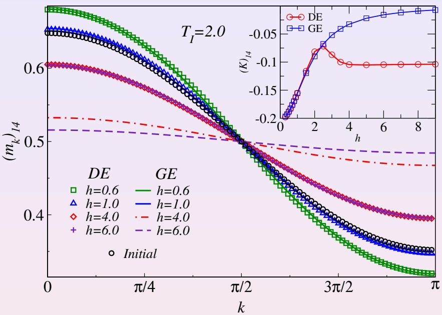
Continuous disorder: $h_c \approx 7$ [A. Pal and D. A. Huse, PRB **82**, 174411 (2010).]

Disordered systems and many-body localization

Ratio of consecutive energy gaps



Diagonal vs Thermal



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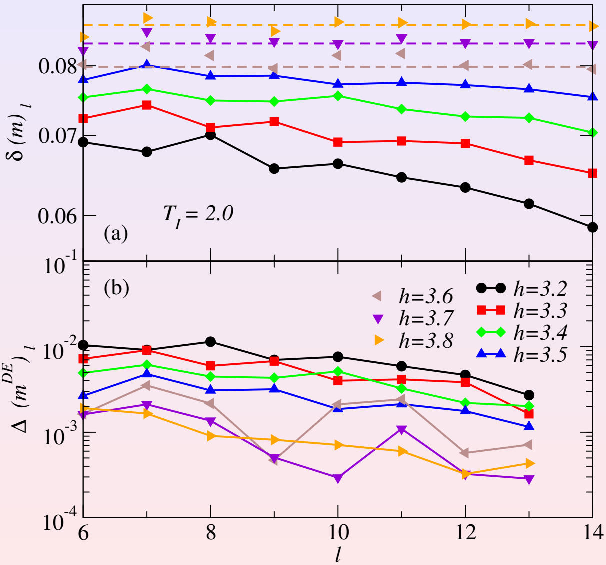
Scaling of the differences and errors



Conclusions

- NLCEs provide a general framework to study the diagonal ensemble in lattice systems after a quantum quench in the thermodynamic limit.
- The grand canonical ensemble in translationally invariant systems *is special* (exponentially small finite size effects vs power law for other cases). NLCEs also converge exponentially, but even faster!
- NLCE results indicate 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.
- Quantum quenches within NLCEs can be used to study the transition between ergodicity and many-body localization (arbitrary dimensions). In one dimension, the NLCE results support the existence of many-body localization in the thermodynamics limit.

Collaborators

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PRB **91**, 161109(R) (2015).

Deepak Iyer (Penn State)
Mark Srednicki (UCSB)

PRE **91**, 062142 (2015).

Supported by:

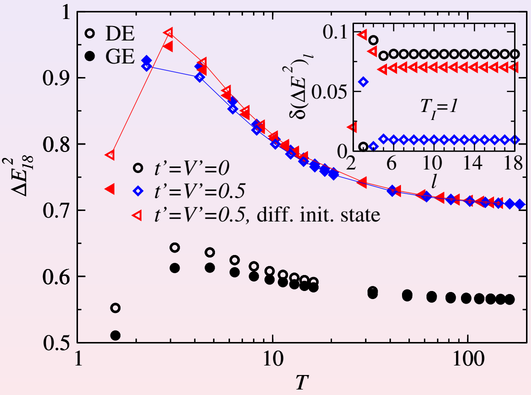
Dispersion of the energy in the DE

Dispersion of the energy

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

Deviations from the GE

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

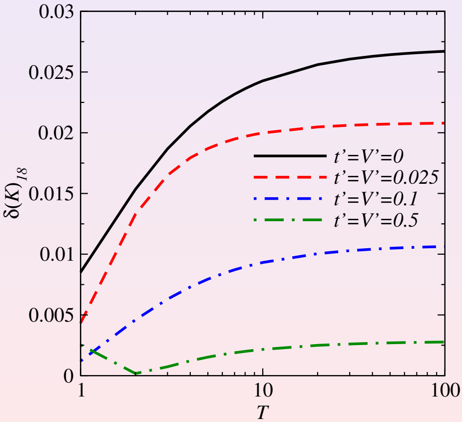


The dispersion of the energy (and of the particle number) in the DE depends on the initial state independently of whether the system is integrable or not.

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

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