Dynamics and thermalization in isolated quantum systems

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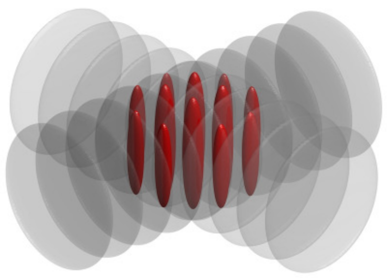
QCD Hadronization and the Statistical Model
ECT* Trento, Italy
October 6, 2014

With comments by H.G. Evertz v2021

Outline

1. Introduction
   - Experiments with ultracold gases
   - Unitary evolution and thermalization
2. Generic (nonintegrable) systems
   - Time evolution vs exact time average
   - Statistical description after relaxation
   - Eigenstate thermalization hypothesis
   - Time fluctuations
3. Integrable systems
   - Time evolution
   - Generalized Gibbs ensemble
4. Summary

Experiments with ultracold gases in 1D



Effective one-dimensional δ potential

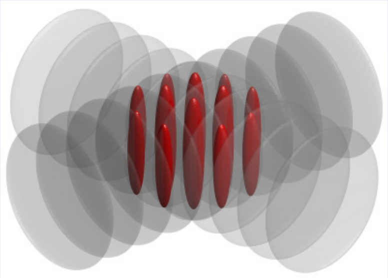
M. Olshanii, PRL **81**, 938 (1998).

$$U_{1D}(x) = g_{1D}\delta(x)$$

where

$$g_{1D} = \frac{2\hbar a_s \omega_\perp}{1 - C a_s \sqrt{\frac{m\omega_\perp}{2\hbar}}}$$

Experiments with ultracold gases in 1D



Girardeau '60, Lieb and Liniger '63

T. Kinoshita, T. Wenger, and D. S. Weiss, Science **305**, 1125 (2004).

T. Kinoshita, T. Wenger, and D. S. Weiss, Phys. Rev. Lett. **95**, 190406 (2005).

$$\gamma_{\text{eff}} = \frac{m g_{1D}}{\hbar^2 \rho}$$

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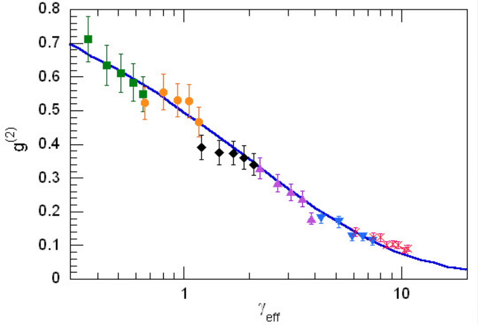
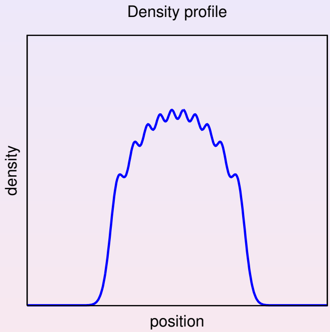
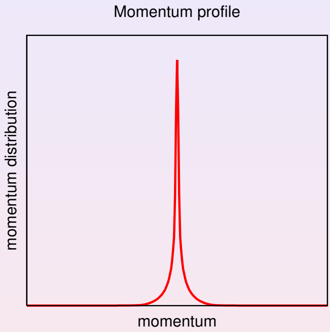


Absence of thermalization in 1D?





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

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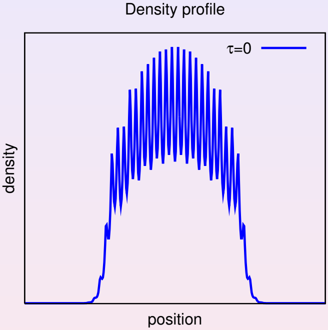

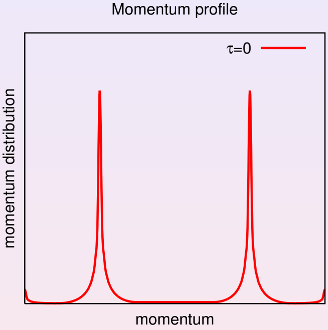

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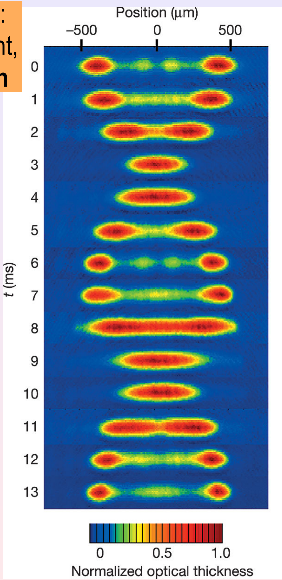
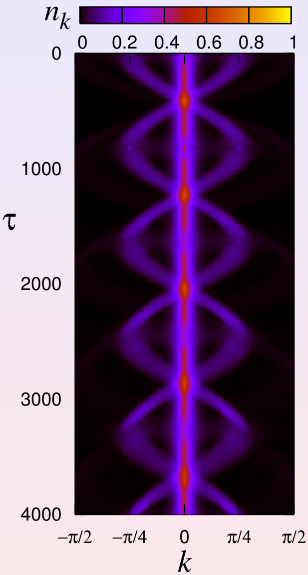
Absence of thermalization in 1D?

In this experiment:
periodic movement,
no thermalization

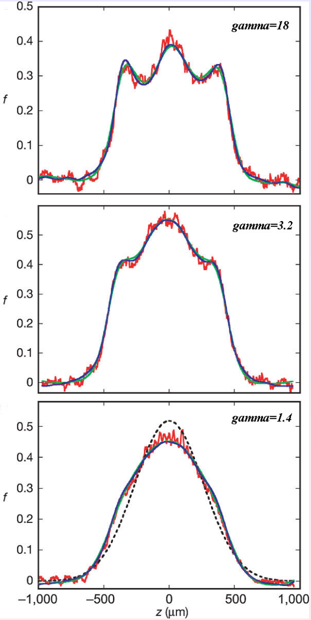
Experiment





Theory

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).

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Classical physics:

Chaotic evolution --> ergodicity (uniform)
--> thermal description
(Exception: integrable systems:
many conserved quantities
--> orbits in phase space,
not ergodic)

Quantum physics:

NOT ergodic ! (only a tiny part of Hilbert
space is relevant)
Is there thermalization of an isolated system?
In what sense ?

Need to consider states, observables,
matrix elements

(Integrable systems again do not thermalize)

Exact results from quantum mechanics

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 generic observable O will evolve in time following

$$O(\tau) \equiv \langle\psi(\tau)|\widehat{O}|\psi(\tau)\rangle \quad \text{where} \quad |\psi(\tau)\rangle = e^{-i\widehat{H}\tau}|\psi_0\rangle.$$

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What is it that we call thermalization?

Thermal expectation value expected to depend only on **a few parameters** !

average: $$\overline{O(\tau)} \stackrel{?}{=} O(E_0) \stackrel{?}{=} O(T) \stackrel{?}{=} O(T,\mu).$$

(Definitions follow) "diagonal ensemble" =? microcan. =? canonical =? grand canonical ensemble (in therm.dyn. limit)

Exact results from quantum mechanics

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What is it that we call thermalization?

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

"diagonal ensemble" =? microcan. =? canonical =? grand canonical ensemble (in therm.dyn. limit)

One can rewrite

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

(Assume: no degeneracies)

and taking the infinite time average (diagonal ensemble) (=definition(!) of "diag. ensemble")

(could also integrate from some later time)

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

(since all oscillating terms vanish after integral)

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

t

Many parameters !

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 $\tau = 0$ (Example, not important)

"Global quench" $\widehat{H}_0 \rightarrow \widehat{H} = \widehat{H}_0 + \widehat{W}$ with $\widehat{W} = \sum_j \hat{w}(j)$ and $\widehat{H}|\alpha\rangle = E_\alpha|\alpha\rangle$.

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

Width of the energy density after a sudden quench

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

The width of the weighted energy density ΔE is then Delta E = sqrt(<H^2> - <H>^2) =

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

or

expect ?:

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

(unless terms in the sum are highly correlated!)

where N is the total number of lattice sites.

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

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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).

Outline

Example: relaxation of hardcore bosons in 2D

Relaxation dynamics of hard-core bosons in 2D

Hard-core boson Hamiltonian

(Equivalent to spin 1/2 Quantum Heisenberg model)

$$\widehat{H} = -J \sum_{\langle i,j \rangle} \left(\hat{b}_i^\dagger \hat{b}_j + \text{H.c.} \right) + U \sum_{\langle i,j \rangle} \hat{n}_i \hat{n}_j, \qquad \hat{b}_i^{\dagger 2} = \hat{b}_i^2 = 0$$

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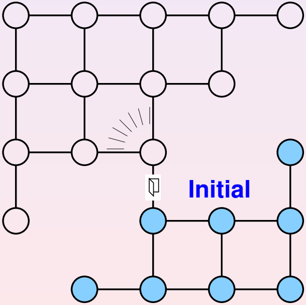
Nonequilibrium dynamics in 2D



Weak n.n. $U = 0.1J$

$N_b = 5$ bosons

$N = 21$ lattice sites

Hilbert space: $D = 20349$

All states are used!

Initial state: a single occupation number state.
Time zero: become connected at one bond.
During the time evolution, ALL occupation number states occur.

Relaxation dynamics of hard-core bosons in 2D

Hard-core boson Hamiltonian

$$\widehat{H} = -J \sum_{\langle i,j \rangle} \left(\hat{b}_i^\dagger \hat{b}_j + \text{H.c.} \right) + U \sum_{\langle i,j \rangle} \hat{n}_i \hat{n}_j, \qquad \hat{b}_i^{\dagger 2} = \hat{b}_i^2 = 0$$

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

"One can rewrite

(quote from page 8)

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

and taking the infinite time average (diagonal ensemble)

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

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

Relaxation dynamics of hard-core bosons in 2D

Hard-core boson Hamiltonian

$$\widehat{H} = -J \sum_{\langle i,j \rangle} \left(\hat{b}_i^\dagger \hat{b}_j + \text{H.c.} \right) + U \sum_{\langle i,j \rangle} \hat{n}_i \hat{n}_j, \qquad \hat{b}_i^{\dagger 2} = \hat{b}_i^2 = 0$$

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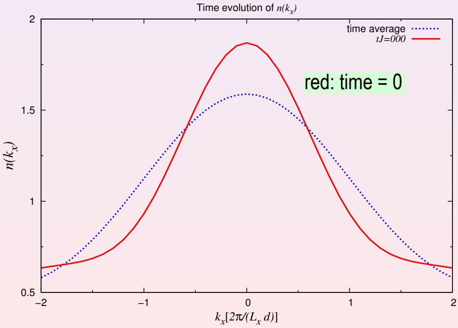
Nonequilibrium dynamics in 2D

n_k = < b^dagger_k b_k >



Weak n.n. $U = 0.1J$

$N_b = 5$ bosons

$N = 21$ lattice sites

Hilbert space: $D = 20349$

All states are used!

Distribution of momenta in time average is very different from initial state

Relaxation dynamics of hard-core bosons in 2D

Hard-core boson Hamiltonian

$$\widehat{H} = -J \sum_{\langle i,j \rangle} \left(\hat{b}_i^\dagger \hat{b}_j + \text{H.c.} \right) + U \sum_{\langle i,j \rangle} \hat{n}_i \hat{n}_j , \qquad \hat{b}_i^{\dagger 2} = \hat{b}_i^2 = 0$$

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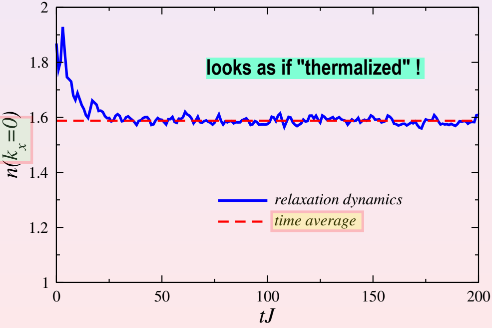

Weak n.n. $U = 0.1J$

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Hilbert space: $D = 20349$

All states are used!

Outline

Try to describe time averaged momentum distribution

Not good: Canonical calculation

$$O = \mathrm{Tr}\left\{\hat{O}\hat{\rho}\right\}$$

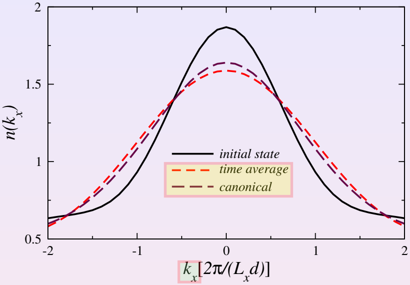
$$\hat{\rho} = Z^{-1}\exp\left(-\hat{H}/k_B T\right)$$

$$Z = \mathrm{Tr}\left\{\exp\left(-\hat{H}/k_B T\right)\right\}$$

$$E_0 = \mathrm{Tr}\left\{\hat{H}\hat{\rho}\right\} \qquad T = 1.9J$$

(T: best match)

Momentum distribution



Statistical description after relaxation

Canonical calculation

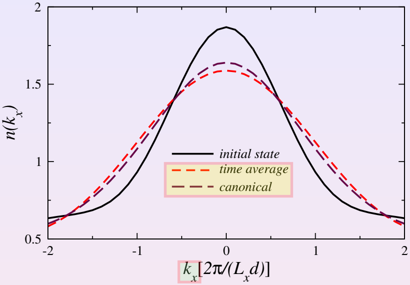
$$O = \mathrm{Tr}\left\{\hat{O}\hat{\rho}\right\}$$

$$\hat{\rho} = Z^{-1}\exp\left(-\hat{H}/k_B T\right)$$

$$Z = \mathrm{Tr}\left\{\exp\left(-\hat{H}/k_B T\right)\right\}$$

$$E_0 = \mathrm{Tr}\left\{\hat{H}\hat{\rho}\right\} \quad T = 1.9J$$

Momentum distribution



Very good: "Microcanonical" calculation with energy of initial state

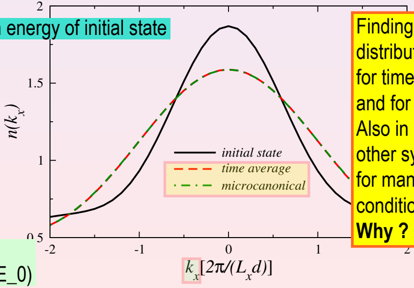
$$O = \frac{1}{N_{states}}\sum_{\alpha}\langle\Psi_\alpha|\hat{O}|\Psi_\alpha\rangle$$

= eigenstates

with $E_0 - \Delta E < E_\alpha < E_0 + \Delta E$

N_{states} : # of states in the window

E_0: energy of initial state !
Delta E: a small energy width (here approx. 2% of E_0)



Finding same distribution for time average and for "microcan."
Also in many other systems, for many initial conditions.
Why ?

Outline

Paradox?

$$\text{Time average} = \sum_{\alpha} |C_\alpha|^2 O_{\alpha\alpha} \stackrel{!?}{=} \langle O\rangle_{\text{microcan.}}(E_0) \equiv \frac{1}{N_{E_0,\Delta E}} \sum_{|E_0-E_\alpha|<\Delta E} \square \; O_{\alpha\alpha} \qquad (1)$$

Left hand side: Depends on the initial conditions through $C_\alpha = \langle \Psi_\alpha | \psi_I \rangle$
Right hand side: Depends only on the initial energy

Eigenstate thermalization hypothesis

Paradox?

Time average = $\sum_{\alpha} |C_\alpha|^2 O_{\alpha\alpha} = \langle O \rangle_{\text{microcan.}}(E_0) \equiv \frac{1}{N_{E_0,\Delta E}} \sum_{|E_0 - E_\alpha| < \Delta E} O_{\alpha\alpha}$

Left hand side: Depends on the initial conditions through $C_\alpha = \langle \Psi_\alpha | \psi_I \rangle$
Right hand side: Depends only on the initial energy

Potential explanations:
(cases in which (1) holds)

0) Usually required: C_alpha significant only in a small energy window around E_0
(or suitable cancellations, see e.g. page 16)

i) ~~For physically relevant initial conditions, $|C_\alpha|^2$ practically do not fluctuate. (in alpha, within the energy window)~~ (not typically true, see next page)

ii) Large (and uncorrelated) (with Oaa) fluctuations occur in ~~both $O_{\alpha\alpha}$ and~~ $|C_\alpha|^2$. ~~A physically relevant~~ Then the initial state performs an unbiased sampling of $O_{\alpha\alpha}$. i.e., then the equality (1) is true.

?

MR and M. Srednicki, PRL **108**, 110601 (2012).

or iiia) The matrix elements **O_aa** of the observable are almost **constant** in the relevant energy range, *and cancel for other energie*s.

Then equality (1) is true AND also equal to exp. value <O> in a SINGLE eigenstate within the energy window !!

Eigenstate thermalization hypothesis

Paradox?

$$\sum_{\alpha} |C_\alpha|^2 O_{\alpha\alpha} = \langle O\rangle_{\text{microcan.}}(E_0) \equiv \frac{1}{N_{E_0,\Delta E}} \sum_{|E_0-E_\alpha|<\Delta E} O_{\alpha\alpha}$$

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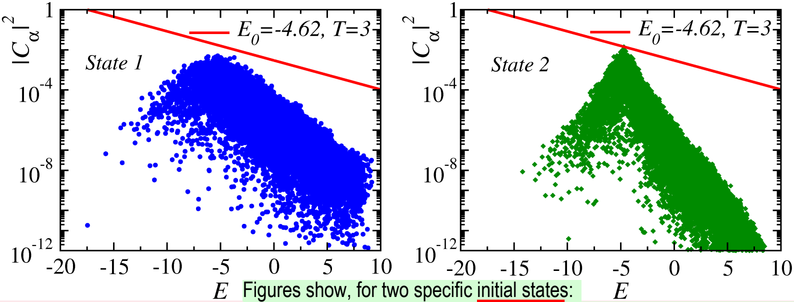


Figures show, for two specific initial states:
1) Distribution of cofficients C_a are smooth and exponential, and peaked at E_0
2) A *thermal* state with the same <E> (red line) has a very *different* distribution

MR, PRA **82**, 037601 (2010).

Eigenstate thermalization hypothesis

(this is the same as first part of p.15)

Paradox?

$$\sum_{\alpha} |C_\alpha|^2 O_{\alpha\alpha} = \langle O \rangle_{\text{microcan.}}(E_0) \equiv \frac{1}{N_{E_0,\Delta E}} \sum_{|E_0 - E_\alpha| < \Delta E} O_{\alpha\alpha}$$

Left hand side: Depends on the initial conditions through $C_\alpha = \langle \Psi_\alpha | \psi_I \rangle$
Right hand side: Depends only on the initial energy

Potential explanations:

i) For physically relevant initial conditions, $|C_\alpha|^2$ practically do not fluctuate.

ii) Large (and uncorrelated) fluctuations occur in both $O_{\alpha\alpha}$ and $|C_\alpha|^2$. A physically relevant initial state performs an unbiased sampling of $O_{\alpha\alpha}$.

MR and M. Srednicki, PRL **108**, 110601 (2012).

(see first part of p.15 for commented version)

Eigenstate thermalization hypothesis

Paradox?

$$\sum_{\alpha} |C_\alpha|^2 O_{\alpha\alpha} = \langle O \rangle_{\text{microcan.}}(E_0) \equiv \frac{1}{N_{E_0,\Delta E}} \sum_{|E_0 - E_\alpha| < \Delta E} O_{\alpha\alpha}$$

Left hand side: Depends on the initial conditions through $C_\alpha = \langle \Psi_\alpha | \psi_I \rangle$
Right hand side: Depends only on the initial energy

Eigenstate thermalization hypothesis (ETH)

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

few body observable in large system
=> averaging over many particles
(similar to averaging in a bath)

iii) The expectation value $\langle \Psi_\alpha | \hat{O} | \Psi_\alpha \rangle$ of a few-body observable $\hat{O}$ in an eigenstate of the Hamiltonian $|\Psi_\alpha\rangle$, with energy E_α, of a large interacting many-body system equals the thermal average of $\hat{O}$ at the mean energy E_α:

all Oaa on l.h.s.

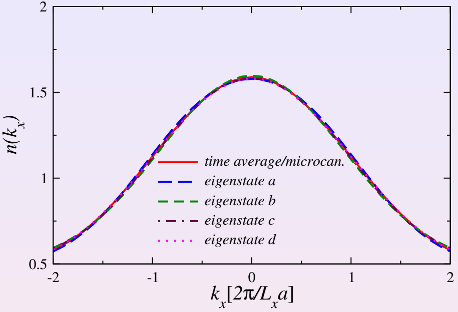
r.h.s. of (1)

(microcanonical (with energy window of +-2%))

O_aa = $\langle \Psi_\alpha | \hat{O} | \Psi_\alpha \rangle = \langle O \rangle_{\text{microcan.}}(E_\alpha)$

This **ETH is sometimes true** (approximately),but **not** always

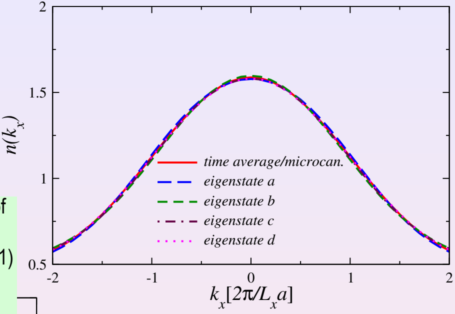
i.e. O_aa (almost) constant in small neighborhood of E_a



Momentum distribution

Eigenstates $a - d$ are the ones with energies closest to E_0

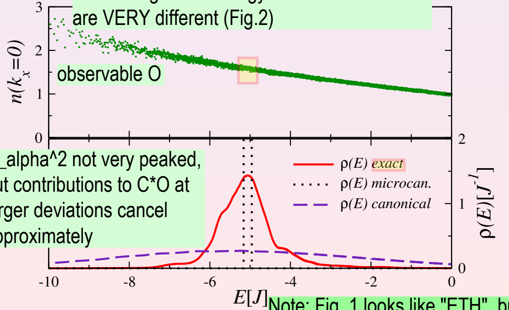
Eigenstate thermalization hypothesis



Momentum distribution

Eigenstates $a - d$ are the ones with energies closest to E_0

Figures show: the momentum distributions of (1) time average, (2) microcan., and (3) several eigenstates are very similar (Fig.1) even though their energy distributions are VERY different (Fig.2)



C_alpha^2 not very peaked, but contributions to C*O at larger deviations cancel approximately

$n(k_x = 0)$ vs energy

$$\rho(E) = \mathrm{P(E)} \times \text{dens. stat.}$$

$$P(E)_{\text{exact}} \to |C_\alpha|^2$$

$$P(E)_{\text{mic}} \to \text{constant}$$

$$P(E)_{\text{can}} \to \exp\left(-E/k_B T\right)$$

("exact" refers to initial state and time average)

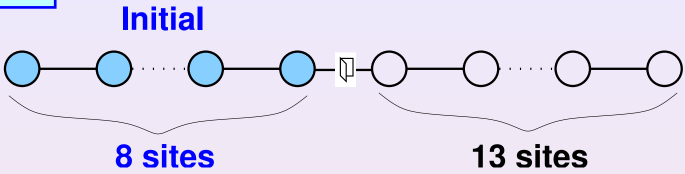
(but (0) and (iiia) are satisfied)

Note: Fig. 1 looks like "ETH", but none of the explanations (i),(ii),(iii) actually satisfied

One-dimensional integrable case

Next:
integrable case

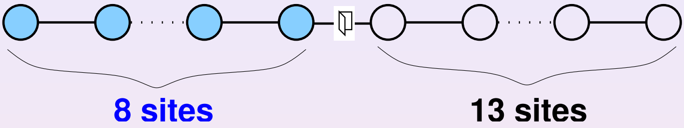
Similar experiment in one dimension



One-dimensional integrable case

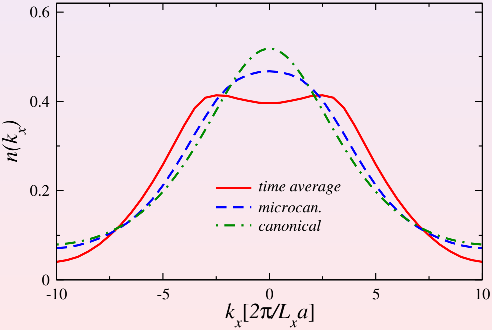
Similar experiment in one dimension

Initial

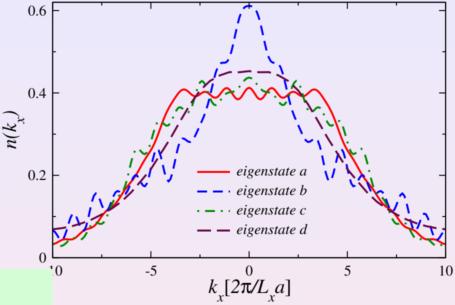


Time average vs Stat. Mech.

No thermalization!



Breakdown of eigenstate thermalization

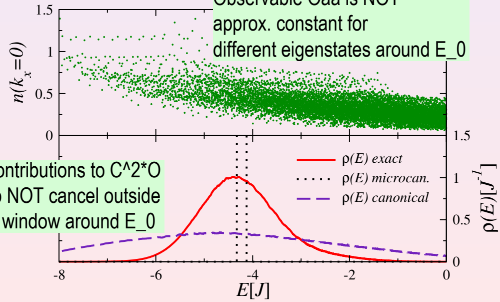


Momentum distribution

Eigenstates $a - d$ are the ones with energies closest to E_0

Very different from page 16

Observable Oaa is NOT approx. constant for different eigenstates around E_0



Contributions to C^2*O do NOT cancel outside of window around E_0

$n(k_x = 0)$ vs energy

$\rho(E) = \mathrm{P(E)} \times \mathrm{dens.\ stat.}$

$P(E)_{\text{exact}} \rightarrow |C_\alpha|^2$ ("exact" refers to time average)

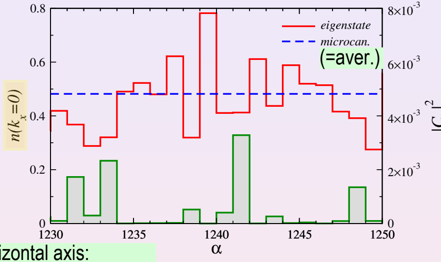
$P(E)_{\text{mic}} \rightarrow \text{constant}$

$P(E)_{\text{can}} \rightarrow \exp\left(-E/k_B T\right)$

Integrable vs Nonintegrable cases

Correlations between $n(k)$ and C_α

1D (integrable) case

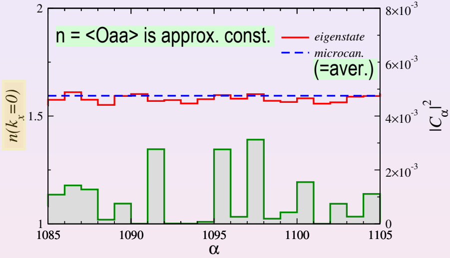


horizontal axis:
successive eigenstates
(Green bars: C_alpha)

⇓

Conservation laws play a role in integrable models.

2D (nonintegrable) case



⇓

Correlations are not relevant, ~~and they are not present~~!

==> need to use distribution with all conserved parameters: GGA "Generalized Gibbs Ensemble", see p.30

Transition between integrability and nonintegrability:

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

Outline

Relaxation dynamics of hard-core bosons in 2D

(not an integrable model)

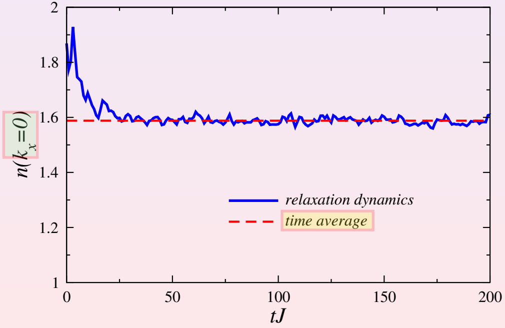
Hard-core boson Hamiltonian

$$\widehat{H} = -J \sum_{\langle i,j \rangle} \left(\hat{b}_i^\dagger \hat{b}_j + \text{H.c.} \right) + U \sum_{\langle i,j \rangle} \hat{n}_i \hat{n}_j, \qquad \hat{b}_i^{\dagger 2} = \hat{b}_i^2 = 0$$

(Same slide as last part of "page 11")

(Equivalent to spin 1/2 Quantum Heisenberg model)

Nonequilibrium dynamics in 2D



Weak n.n. $U = 0.1J$

$N_b = 5$ bosons

$N = 21$ lattice sites

Hilbert space: $D = 20349$

All states are used!

Time fluctuations

Are they small because of dephasing?

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

time average

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

sqrt(N^2) results when the exponential
is randomly distributed (why should it be?)
Then all phases cancel,
i.e. only alpha=alpha' contributes

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

sqrt(N^2) results when the exponential
is randomly distributed (why should it be?)
Then all phases cancel,
i.e. only alpha=alpha' contributes

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

$$\overline{\langle \hat{O}\rangle} = \sum_{\alpha} |C_{\alpha}|^2 O_{\alpha\alpha}$$

$$\sim \sum_{\alpha} \frac{1}{N_{\text{states}}} O_{\alpha\alpha} \sim O^{\text{typical}}_{\alpha\alpha}$$

Time fluctuations

Are they small because of dephasing?

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

NOT the time average!
(see page 8)

from subtraction

(when C_alpha is sharply peaked)

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

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

$$\overline{\langle \hat{O}\rangle} = \sum_{\alpha} |C_{\alpha}|^2 O_{\alpha\alpha}$$

(when ETH is valid):

$$\sim \sum_{\alpha} \frac{1}{N_{\text{states}}} O_{\alpha\alpha} \sim O^{\text{typical}}_{\alpha\alpha}$$

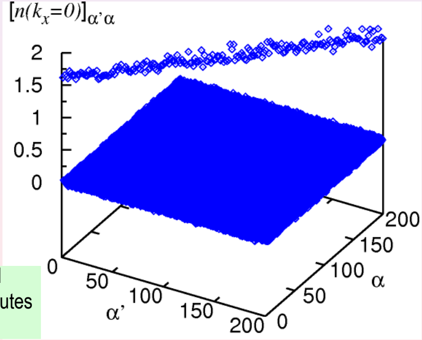
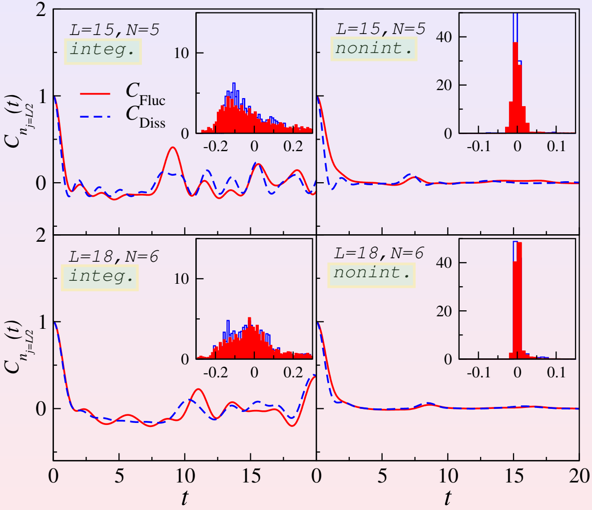


Figure shows that indeed only alpha=alpha' contributes to the expectation value

Fluctuation-dissipation theorem (dipolar bosons)

Occupation in the center of the trap ($n_{j=L/2}$)



Hamiltonian

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

$$+V \sum_{j<l} \frac{\hat{n}_j \hat{n}_l}{|j-l|^3} + g \sum_j x_j^2 \hat{n}_j$$

"dipolar IA" trap

magnetic atoms, polar molecules

Relaxation dynamics

$$O(t) = C(t) O(t=0)$$

where

$$C(t) = \frac{\overline{O(t+t')O(t')}}{\overline{(O(t'))^2}}$$

Srednicki, JPA **32**, 1163 (1999).

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

Outline

Bose-Fermi mapping

Hard-core boson Hamiltonian in an external potential

$$\hat{H} = -J \sum_i \left(\hat{b}_i^\dagger \hat{b}_{i+1} + \text{H.c.} \right) + \sum_i v_i \ \hat{n}_i$$

Constraints on the bosonic operators

$$\hat{b}_i^{\dagger 2} = \hat{b}_i^2 = 0$$

Bose-Fermi mapping

Hard-core boson Hamiltonian in an external potential

1 dim

$$\hat{H} = -J \sum_i \left(\hat{b}_i^\dagger \hat{b}_{i+1} + \text{H.c.} \right) + \sum_i v_i \, \hat{n}_i$$

Here: no density-density interaction !

Constraints on the bosonic operators

$$\hat{b}_i^{\dagger 2} = \hat{b}_i^2 = 0$$

Since n_i = b^dagger_i b_i, this Hamiltonian is bilinear in creation and annihilation operators and the eigenstates are products of single particle states. (Special case v_i=const: momentum space states)

$$\Downarrow$$

Map to spins and then to fermions (Jordan-Wigner transformation)

$$\sigma_i^+ = \hat{f}_i^\dagger \prod_{\beta=1}^{i-1} e^{-i\pi \hat{f}_\beta^\dagger \hat{f}_\beta}, \quad \sigma_i^- = \prod_{\beta=1}^{i-1} e^{i\pi \hat{f}_\beta^\dagger \hat{f}_\beta} \hat{f}_i$$

= (-1)^(number of fermions before site i)
==> in 1d provides for anticommutation

$$\Downarrow$$

Mapping results in

Non-interacting fermion Hamiltonian

Signs cancel as long as fermions cannot hop past each other !

$$\hat{H}_F = -J \sum_i \left(\hat{f}_i^\dagger \hat{f}_{i+1} + \text{H.c.} \right) + \sum_i v_i \, \hat{n}_i^f$$

(This is an integrable model)

One-particle density matrix

One-particle Green's function

$$G_{ij} = \langle \Psi_{HCB} | \sigma_i^- \sigma_j^+ | \Psi_{HCB} \rangle = \langle \Psi_F | \prod_{\beta=1}^{i-1} e^{i\pi \hat{f}_\beta^\dagger \hat{f}_\beta} \hat{f}_i \hat{f}_j^\dagger \prod_{\gamma=1}^{j-1} e^{-i\pi \hat{f}_\gamma^\dagger \hat{f}_\gamma} | \Psi_F \rangle$$

$\Downarrow$

For non-neighboring sites i,j each interchange of fermions gives a sign -> need to cancel by e-factors

Time evolution

$$|\Psi_F(\tau)\rangle = e^{-i\hat{H}_F \tau/\hbar} |\Psi_F^I\rangle = \prod_{\delta=1}^{N} \sum_{\sigma=1}^{L} P_{\sigma\delta}(\tau) \hat{f}_\sigma^\dagger \, |0\rangle$$

One-particle density matrix

One-particle Green's function

$$G_{ij} = \langle \Psi_{HCB} | \sigma_i^- \sigma_j^+ | \Psi_{HCB} \rangle = \langle \Psi_F | \prod_{\beta=1}^{i-1} e^{i\pi \hat{f}_\beta^\dagger \hat{f}_\beta} \hat{f}_i \hat{f}_j^\dagger \prod_{\gamma=1}^{j-1} e^{-i\pi \hat{f}_\gamma^\dagger \hat{f}_\gamma} | \Psi_F \rangle$$

For non-neighboring sites i,j each interchange of fermions gives a sign -> cancelled by e-factors

$$\Downarrow$$

Time evolution

from an initial Fock state

remains a Fock state, which can be written as:

$$|\Psi_F(\tau)\rangle = e^{-i\hat{H}_F \tau/\hbar} |\Psi_F^I\rangle = \prod_{\delta=1}^{N} \sum_{\sigma=1}^{L} P_{\sigma\delta}(\tau) \hat{f}_\sigma^\dagger \, |0\rangle$$

$$\Downarrow$$

Fock state: prod_k (c^dagger_k)^(n_k) /0>
= prod_k sum_x e^(i k x n_k) c^dagger_x /0>
= prod_n (sum_x e^(i k_n x) c^dagger_x /0>
= prod_n sum_x P_(k_n x) c^dagger_x /0>

Exact Green's function

$$G_{ij}(\tau) = \det\left[\left(\mathbf{P}^l(\tau) \right)^\dagger \mathbf{P}^r(\tau) \right]$$

Here "k" numbers the single particle eigenstates (= momentum states when v_i=const in Hamiltonian)

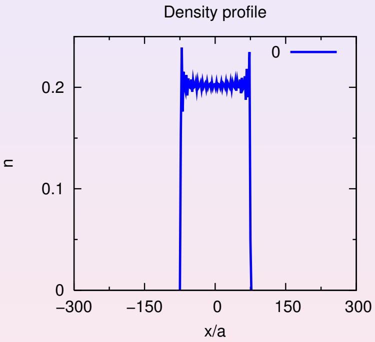
Computation time $\sim L^2 N^3$

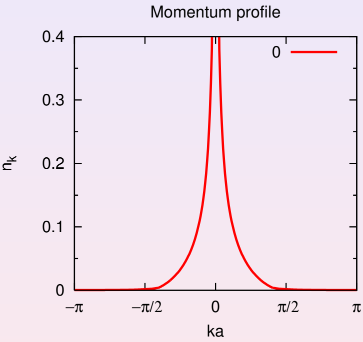
3000 lattice sites, 300 particles

MR and A. Muramatsu, PRL **93**, 230404 (2004); PRL **94**, 240403 (2005).

Relaxation dynamics in an integrable system

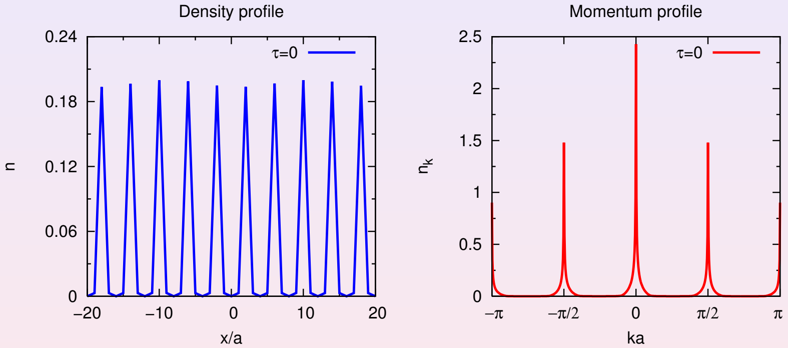
Initial state:
center part of system filled at approx. constant density





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

State after long time relaxation:
combination of (a few) eigenstates



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

Outline

Statistical description after relaxation (integrable system)

Thermal equilibrium

$$\hat{\rho} = Z^{-1} \exp\left[-\left(\hat{H} - \mu \hat{N}_b\right)/k_B T\right]$$

$$Z = \mathrm{Tr}\left\{\exp\left[-\left(\hat{H} - \mu \hat{N}_b\right)/k_B T\right]\right\}$$

$$E = \mathrm{Tr}\left\{\hat{H}\hat{\rho}\right\}, \quad N_b = \mathrm{Tr}\left\{\hat{N}_b\hat{\rho}\right\}$$

MR, PRA **72**, 063607 (2005).

Statistical description after relaxation

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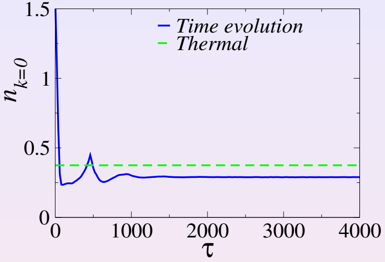
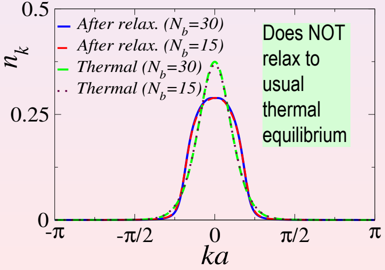
Evolution of $n_{k=0}$



n_k after relaxation



Does NOT relax to usual thermal equilibrium

Statistical description after relaxation

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MR, PRA **72**, 063607 (2005).

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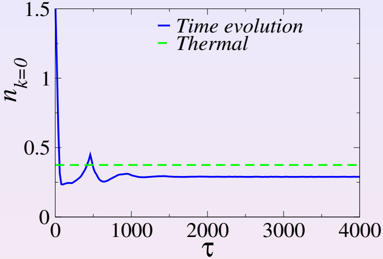


Integrals of motion

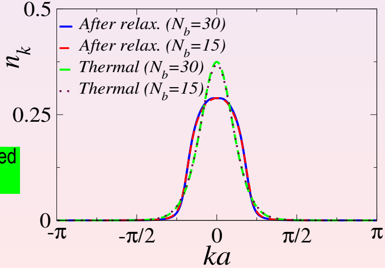
(underlying noninteracting fermions)

$$\hat{H}_F \hat{\gamma}_m^{f\dagger}|0\rangle = E_m \hat{\gamma}_m^{f\dagger}|0\rangle$$

$$\left\{\hat{I}_m^f\right\} = \left\{\hat{\gamma}_m^{f\dagger}\hat{\gamma}_m^f\right\}$$

Many local conserved quantities I^f_m

n_k after relaxation



Statistical description after relaxation

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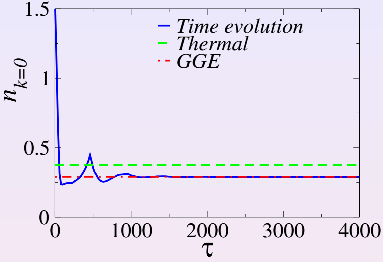
MR, PRA **72**, 063607 (2005).

Evolution of $n_{k=0}$



Generalized Gibbs ensemble

$$\hat{\rho}_c = Z_c^{-1} \exp\left[-\sum_m \lambda_m \hat{I}_m\right]$$

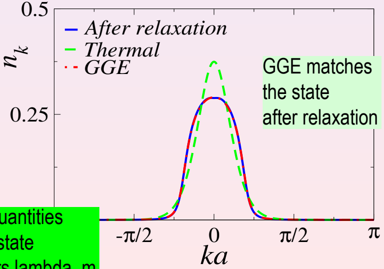
instead of e^(- H/T)

$$Z_c = \mathrm{Tr}\left\{\exp\left[-\sum_m \lambda_m \hat{I}_m\right]\right\}$$

$$\langle \hat{I}_m \rangle_{\tau=0} = \mathrm{Tr}\left\{\hat{I}_m \hat{\rho}_c\right\}$$

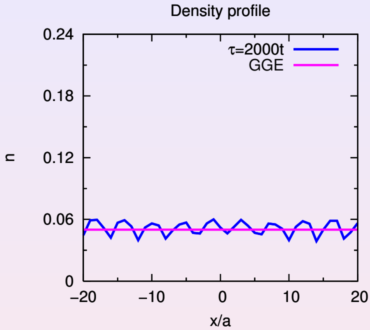
Values of local quantities I_m in the initial state fix the parameters lambda_m

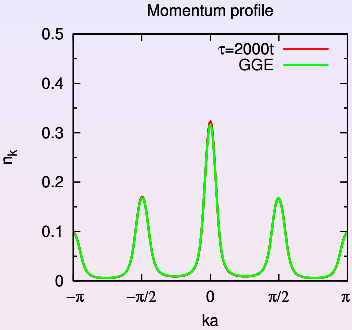
n_k after relaxation



GGE matches the state after relaxation

Statistical description after relaxation





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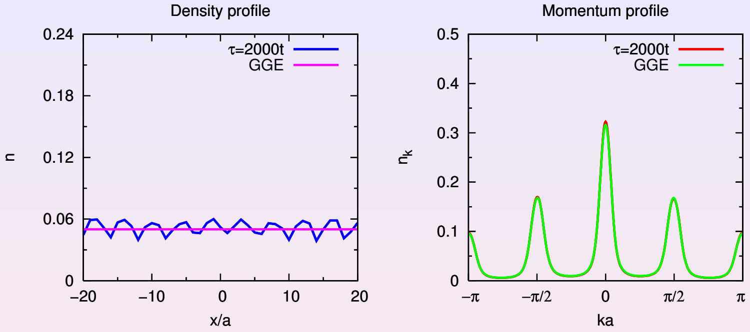

Why does the GGE work?

Generalized eigenstate thermalization:

A. C. Cassidy, C. W. Clark, and MR, Phys. Rev. Lett. **106**, 140405 (2011).
K. He, L. F. Santos, T. M. Wright, and MR, Phys. Rev. A **87**, 063637 (2013).
J.-S. Caux and F. H. L. Essler, Phys. Rev. Lett. 110, 257203 (2013).

Summary

- Thermalization occurs in generic isolated systems
  ★ Finite size effects

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  ★ Finite size effects
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  ★ $\langle \Psi_\alpha | \hat{O} | \Psi_\alpha \rangle = \langle O \rangle_{\text{microcan.}}(E_\alpha)$

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  ★ Quantum equivalent of KAM?

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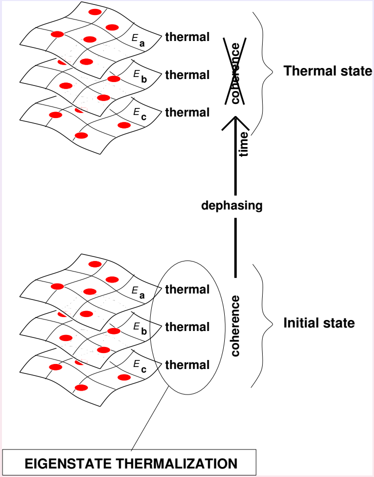
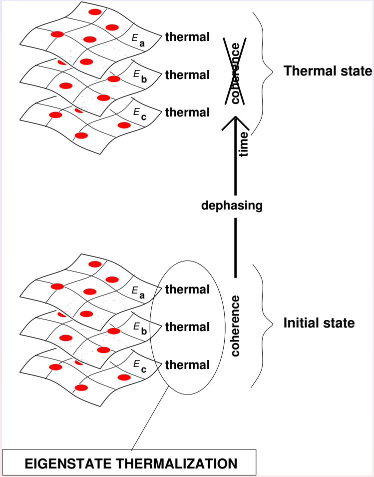


Summary

- Thermalization occurs in generic isolated systems
  ★ Finite size effects
- Eigenstate thermalization hypothesis
  ★ $\langle \Psi_\alpha | \hat{O} | \Psi_\alpha \rangle = \langle O \rangle_{\text{microcan.}}(E_\alpha)$
- Thermalization and ETH break down close integrability (finite system)
  ★ Quantum equivalent of KAM?
- Small time fluctuations $\leftarrow$ smallness of off-diagonal elements
- Time plays only an auxiliary role
- Integrable systems are different (Generalized Gibbs ensemble)

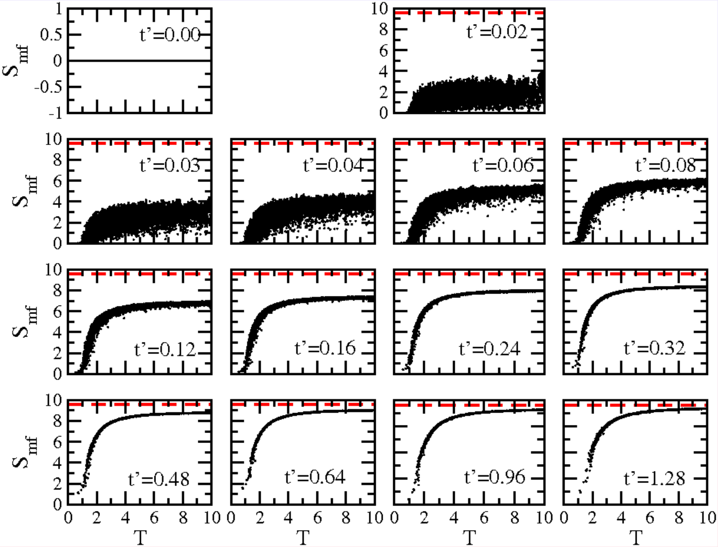


Collaborators

- Vanja Dunjko (U Mass Boston)
- Alejandro Muramatsu (Stuttgart U)
- Maxim Olshanii (U Mass Boston)
- Lea F. Santos (Yeshiva U)
- Mark Srednicki (UC Santa Barbara)
- Former group members: Kai He, Ehsan Khatami

Supported by:

Information entropy ($S_j = -\sum_{k=1}^{D} |c_j^k|^2 \ln |c_j^k|^2$)



L.F. Santos and MR, PRE **81**, 036206 (2010); PRE **82**, 031130 (2010).