From unitary dynamics to statistical mechanics in isolated quantum systems

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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

\[ g_{1D} = \frac{2\hbar a_s \omega_\perp}{1 - C a_s \sqrt{\frac{m \omega_\perp}{2\hbar}}} \]
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Girardeau '60, Lieb and Liniger '63

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$$\gamma_{\text{eff}} = \frac{mg_{1D}}{\hbar^2 \rho}$$
Absence of thermalization in 1D?

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**Experiment**

**Theory**

Marcos Rigol (Penn State)
Dynamics in quantum systems
May 4, 2015
Absence of thermalization in 1D?


\[ \gamma = \frac{mg_{1D}}{\hbar^2 \rho} \]

\( g_{1D} \): Interaction strength
\( \rho \): 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

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4 Summary
Exact results from quantum mechanics

If the initial state is not an eigenstate of $\hat{H}$

$$|\psi_0\rangle \neq |\alpha\rangle \quad \text{where} \quad \hat{H}|\alpha\rangle = E_\alpha|\alpha\rangle \quad \text{and} \quad E_0 = \langle \psi_0 | \hat{H} | \psi_0 \rangle,$$

then a generic observable $O$ will evolve in time following

$$O(\tau) \equiv \langle \psi(\tau) | \hat{O} | \psi(\tau) \rangle \quad \text{where} \quad |\psi(\tau)\rangle = e^{-i\hat{H}\tau} |\psi_0\rangle.$$
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What is it that we call thermalization?

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

One can rewrite

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

Taking the infinite time average (diagonal ensemble $\hat{\rho}_{DE} \equiv \sum_\alpha |C_\alpha|^2 |\alpha\rangle \langle \alpha|$

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

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 $\hat{H}_0$. At $\tau = 0$

$$\hat{H}_0 \rightarrow \hat{H} = \hat{H}_0 + \hat{W} \quad \text{with} \quad \hat{W} = \sum_j \hat{w}(j) \quad \text{and} \quad \hat{H}|\alpha\rangle = E_\alpha |\alpha\rangle.$$
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The width of the weighted energy density $\Delta E$ is then

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

or

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

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 $\propto N$

$$\Delta \epsilon = \frac{\Delta E}{W} \xrightarrow{N \rightarrow \infty} \frac{1}{\sqrt{N}},$$

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

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Relaxation dynamics of hard-core bosons in 2D

Hard-core boson Hamiltonian

\[
\hat{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, \quad \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!
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and taking the infinite time average (diagonal ensemble)

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Statistical description after relaxation

Canonical calculation

\[ O = \text{Tr} \left\{ \hat{O} \hat{\rho} \right\} \]
\[ \hat{\rho} = Z^{-1} \exp \left( -\hat{H} / k_B T \right) \]
\[ Z = \text{Tr} \left\{ \exp \left( -\hat{H} / k_B T \right) \right\} \]
\[ E_0 = \text{Tr} \left\{ \hat{H} \hat{\rho} \right\} \quad T = 1.9 J \]
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E_0 = \text{Tr} \left\{ \hat{H} \hat{\rho} \right\} \quad T = 1.9J
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Microcanonical calculation

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

with \( E_0 - \Delta E < E_\alpha < E_0 + \Delta E \)

\( N_{\text{states}} \) : # of states in the window
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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

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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 \( O_{\alpha\alpha} \).

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

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 \( E_\alpha \), of a large interacting many-body system equals the thermal average of \( \hat{O} \) at the mean energy \( E_\alpha \):

\[ \langle \Psi_{\alpha} | \hat{O} | \Psi_{\alpha} \rangle = \langle O \rangle_{\text{microcan.}}(E_\alpha) \]
Eigenstate thermalization hypothesis

Momentum distribution

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

\[
n(k_x = 0) \text{ vs energy}
\]

\[
\rho(E) = P(E) \times \text{dens. stat.}
\]

\[
P(E)_{\text{exact}} \rightarrow |C_\alpha|^2
\]

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

\[
P(E)_{\text{can}} \rightarrow \exp\left(-\frac{E}{k_B T}\right)
\]
One-dimensional integrable case

Similar experiment in one dimension

Initial

8 sites

13 sites
One-dimensional integrable case

Similar experiment in one dimension

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No thermalization!
Momentum distribution

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

Are they small because of dephasing?

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

$$\sim \sqrt{N_{\text{states}}^2} O_{\text{typical}} \sim O_{\text{typical}}$$

Time fluctuations

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\[ \langle \hat{O}(t) \rangle - \langle \hat{O}(t) \rangle = \sum_{\alpha', \alpha} C_{\alpha, \alpha'}^* C_{\alpha} e^{i(E_{\alpha'} - E_{\alpha})t} O_{\alpha' \alpha} \sim \sum_{\alpha', \alpha} e^{i(E_{\alpha'} - E_{\alpha})t} \frac{1}{N_{\text{states}}} O_{\alpha' \alpha} \]

\[ \sim \sqrt{\frac{N_{\text{states}}^2}{N_{\text{states}}} O_{\alpha' \alpha}} \sim O_{\alpha' \alpha}^{\text{typical}} \]

Time average of \( \langle \hat{O} \rangle \)

\[ \langle \hat{O} \rangle = \sum_{\alpha} |C_{\alpha}|^2 O_{\alpha \alpha} \]

\[ \sim \sum_{\alpha} \frac{1}{N_{\text{states}}} O_{\alpha \alpha} \sim O_{\alpha' \alpha}^{\text{typical}} \]

One needs: \( O_{\alpha' \alpha}^{\text{typical}} \ll O_{\alpha \alpha}^{\text{typical}} \)
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\[
\sim \frac{\sqrt{N_{\text{states}}^2}}{N_{\text{states}}} O^{\text{typical}}_{\alpha' \alpha} \sim O^{\text{typical}}_{\alpha' \alpha}
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Bose-Fermi mapping

Hard-core boson Hamiltonian in an external potential

\[ \hat{H} = -J \sum_i \left( \hat{b}_i^\dagger \hat{b}_{i+1} + \text{H.c.} \right) + \sum_i v_i \hat{n}_i, \quad \text{constraints} \quad \hat{b}_i^\dagger^2 = \hat{b}_i^2 = 0 \]
Bose-Fermi mapping

Hard-core boson Hamiltonian in an external potential

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\[ \Downarrow \]

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

\[ \sigma_i^+ = f_i^\dagger \prod_{\beta=1}^{i-1} e^{-i\pi \hat{f}_\beta^\dagger \hat{f}_\beta}, \quad \sigma_i^- = \prod_{\beta=1}^{i-1} e^{i\pi \hat{f}_\beta^\dagger \hat{f}_\beta} f_i \]
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Exact Green’s function

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

Computation time \( \sim L^2 N^3 \)

3000 lattice sites, 300 particles

Relaxation dynamics in an integrable system

Statistical description after relaxation

Thermal equilibrium

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

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

\[ E = \text{Tr} \left\{ \hat{H} \hat{\rho} \right\}, \quad N_b = \text{Tr} \left\{ \hat{N}_b \hat{\rho} \right\} \]

MR, PRA 72, 063607 (2005).
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\[ Z = \text{Tr} \left\{ \exp \left[ - \left( \hat{H} - \mu \hat{N}_b \right) / k_B T \right] \right\} \]

\[ E = \text{Tr} \left\{ \hat{H} \hat{\rho} \right\}, \quad N_b = \text{Tr} \left\{ \hat{N}_b \hat{\rho} \right\} \]

MR, PRA 72, 063607 (2005).

Integrals of motion

(underlying noninteracting fermions)

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

\[ \left\{ \hat{I}_m^f \right\} = \left\{ \hat{\gamma}_m^{f \dagger} \hat{\gamma}_m^f \right\} \]
Statistical description after relaxation

Thermal equilibrium

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Generalized Gibbs ensemble

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

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

\[ \langle \hat{I}_m \rangle_{\tau=0} = \text{Tr} \left\{ \hat{I}_m \hat{\rho}_c \right\} \]
Summary

- Thermalization occurs in generic isolated systems
  - ★ Finite size effects

Eigenstate thermalization hypothesis

\[ \langle \Psi_\alpha | \hat{O} | \Psi_\alpha \rangle = \langle O \rangle \text{ microcan.} \]

Small time fluctuations $\leftarrow$ smallness of off-diagonal elements

Time plays only an auxiliary role

Integrable systems are different

(Generalized Gibbs ensemble)

Thermalization and ETH break down close integrability (finite system)

★ Quantum equivalent of KAM?
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- Thermalization occurs in generic isolated systems
  - Finite size effects

- Eigenstate thermalization hypothesis
  - $\langle \Psi_\alpha | \hat{O} | \Psi_\alpha \rangle = \langle O \rangle_{\text{microcan.}}(E_\alpha)$
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- Eigenstate thermalization hypothesis
  - \( \langle \Psi_\alpha | \hat{O} | \Psi_\alpha \rangle = \langle O \rangle_{\text{microcan.}} (E_\alpha) \)
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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).