From unitary dynamics to statistical mechanics in isolated quantum systems

Marcos Rigol
Department of Physics
The Pennsylvania State University

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Quantum Information and Thermodynamics
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Outline

1 Motivation
   - Foundations of quantum statistical mechanics
   - Experiments with ultracold gases

2 Quantum chaos and random matrix theory
   - Classical and quantum chaos
   - Random matrix theory

3 Dynamics and thermalization (quantum chaotic systems)
   - Quantum mechanics vs statistical mechanics
   - Dynamics and equilibration
   - Thermalization
   - Eigenstate thermalization

4 Dynamics and generalized thermalization (integrable systems)
   - Generalized Gibbs ensemble (GGE)

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

Recent works (keywords)

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)
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Experiments with ultracold bosons in one dimension

Effective 1D $\delta$ potential
M. Olshanii, PRL 81, 938 (1998).

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

Lieb-Liniger parameter
\[ \gamma = \frac{mg_{1D}}{\hbar^2 \rho} \]
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Observables (density and momentum distribution functions) equilibrated to nonthermal distributions
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5. Summary
Classical chaos and integrability

Particle trajectories in a circular cavity and a Bunimovich stadium (scholarpedia)
A Hamiltonian \( H(p, q) \), with \( q = (q_1, \cdots, q_N) \) and \( p = (p_1, \cdots, p_N) \), is said to be integrable if there are \( N \) functionally independent constants of the motion \( I = (I_1, \cdots, I_N) \) in involution:

\[
\{ I_\alpha, H \} = 0, \quad \{ I_\alpha, I_\beta \} = 0, \quad \text{where} \quad \{ f, g \} = \sum_{i=1,N} \frac{\partial f}{\partial q_i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q_i}.
\]

Liouville’s integrability theorem: \( (p, q) \rightarrow (I, \Theta) \), so that \( H(p, q) \rightarrow H(I) \).
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$$\{I_\alpha, H\} = 0, \quad \{I_\alpha, I_\beta\} = 0,$$

where

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Chaos: exponential sensitivity of the trajectories to perturbations.
Semi-classical limit: Statistics of energy levels

- Berry-Tabor conjecture (1977): The statistics of level spacings of quantum systems whose classical counterpart is integrable is described by a Poisson distribution. (Energy eigenvalues behave like a sequence of independent random variables.)
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- Bohigas, Giannoni, and Schmit (1984): At high energies, the statistics of level spacings of a particle in a Sinai billiard is described by a Wigner-Dyson distribution. This was conjecture to apply to quantum systems that have a classically chaotic counterpart (violated in singular cases).
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Distribution of level spacings: rectangular and chaotic cavities

Integrability to quantum chaos transition

Spinless fermions (hard-core bosons) in one dimension

\[ \hat{H} = \sum_{i=1}^{L} \left\{ -t \left( \hat{f}_i^\dagger \hat{f}_{i+1} + \text{H.c.} \right) + V \hat{n}_i \hat{n}_{i+1} - t' \left( \hat{f}_i^\dagger \hat{f}_{i+2} + \text{H.c.} \right) + V' \hat{n}_i \hat{n}_{i+2} \right\} \]
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Level spacing distribution \((N_f = L/3)\)

L. Santos and MR, PRE 81, 036206 (2010); PRE 82, 031130 (2010).
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Random matrix theory

- Wigner (1955) & Dyson (1962): Statistical properties of the spectra of complex quantum systems (in a narrow energy window) can be predicted from the statistical properties of the spectra of random matrices (with the appropriate symmetries). It was used with great success to understand the spectra of complex nuclei.
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Distribution of level spacings for the “Nuclear Data Ensemble”

Distribution of level spacings $P(\omega)$

$P(\omega)$ can be understood using $2 \times 2$ matrices

$$
\begin{bmatrix}
\varepsilon_1 & \frac{V}{\sqrt{2}} \\
\frac{V^*}{\sqrt{2}} & \varepsilon_2
\end{bmatrix}, \quad E_{1,2} = \frac{\varepsilon_1 + \varepsilon_2}{2} \pm \frac{1}{2} \sqrt{(\varepsilon_1 - \varepsilon_2)^2 + 2|V|^2}.
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E_{1,2} = \frac{\varepsilon_1 + \varepsilon_2}{2} \pm \frac{1}{2} \sqrt{(\varepsilon_1 - \varepsilon_2)^2 + 2|V|^2}.
$$

For systems that are invariant under time reversal, $\hat{H}$ can be written as a real matrix. Draw $\varepsilon_1$, $\varepsilon_2$, and $V$ from a Gaussian distribution with zero mean and variance $\sigma$.

$$
P(\omega \equiv E_1 - E_2) = \frac{1}{(2\pi)^{3/2}\sigma^3} \int d\varepsilon_1 \int d\varepsilon_2 \int dV \delta \left( \sqrt{(\varepsilon_1 - \varepsilon_2)^2 + 2V^2} - \omega \right)$$

$$
\times \exp \left( -\frac{\varepsilon_1^2 + \varepsilon_2^2 + V^2}{2\sigma^2} \right).
$$

Wigner Surmise (Wigner-Dyson distribution)

$$
P(\omega) = A_{\beta} \omega^\beta \exp\left[ -B_{\beta} \omega^2 \right],
$$

where $\beta = 1$ (GOE) and $\beta = 2$ (GUE).
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\]

Calculating the integrals (change of variables plus cylindrical coordinates)

\[
P(\omega) = \frac{\omega}{2\sigma^2} \exp \left[ -\frac{\omega^2}{4\sigma^2} \right]
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Exact results from quantum mechanics

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

$$|\psi_{\text{ini}}\rangle \neq |\alpha\rangle \quad \text{where} \quad \hat{H}|\alpha\rangle = E_\alpha|\alpha\rangle \quad \text{and} \quad E = \langle \psi_{\text{ini}} | \hat{H} | \psi_{\text{ini}} \rangle,$$

then observables $\hat{O}$ evolve in time:

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

$$\overline{O(\tau)} = O(E) = O(T) = O(T, \mu).$$
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One can rewrite

$$O(\tau) = \sum_{\alpha, \beta} C^*_\alpha C_\beta e^{i(E_\alpha - E_\beta)\tau} O_{\alpha\beta} \quad \text{using} \quad |\psi_{\text{ini}}\rangle = \sum_\alpha C_\alpha |\alpha\rangle.$$

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 $C_\alpha = \langle \alpha | \psi_{\text{ini}} \rangle$. 
Energy fluctuations after a sudden quench

Initial state $|\psi_{\text{ini}}\rangle = \sum_\alpha C_\alpha |\alpha\rangle$ is an eigenstate of $\hat{H}_{\text{ini}}$. At $t = 0$

$$\hat{H}_{\text{ini}} \rightarrow \hat{H} = \hat{H}_{\text{ini}} + \hat{W} \quad \text{with} \quad \hat{W} = \sum_j \hat{w}(j) \quad \text{and} \quad \hat{H}|\alpha\rangle = E_\alpha |\alpha\rangle.$$
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The energy fluctuations after a quench, $\Delta E$, are:

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

or

$$\Delta E = \sqrt{\sum_{j_1, j_2 \in \sigma} [\langle \psi_{\text{ini}} | \hat{w}(j_1) \hat{w}(j_2) | \psi_{\text{ini}} \rangle - \langle \psi_{\text{ini}} | \hat{w}(j_1) | \psi_{\text{ini}} \rangle \langle \psi_{\text{ini}} | \hat{w}(j_2) | \psi_{\text{ini}} \rangle]^N \xrightarrow{\infty} \sqrt{N},$$

where $N$ is the total number of lattice sites.

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

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

so, as in traditional ensembles, it vanishes in the thermodynamic limit.

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Numerical experiments in one dimension

Hard-core boson Hamiltonian

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

Nonequilibrium dynamics in 1D (density-density structure factor)

\[
N_b = 8 \text{ hard-core bosons}
\]

\[
N = 24 \text{ lattice sites}
\]

Fix \( t' = V' \) and "quench"

\[
t_{\text{ini}} = 0.5, V_{\text{ini}} = 2 \\
\rightarrow t_{\text{fin}} = 1, V_{\text{fin}} = 1
\]

Integrated results for $L = 24$, $N_b = 8$

Relative difference

$$\delta N(\tau) = \frac{\sum_{k} |N(k, \tau) - N_{DE}(k)|}{\sum_{k} N_{DE}(k)}$$
Integrated results for \( L = 24, \ N_b = 8 \)

Relative difference

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Scaling of the integrated results with system size

Relative difference

\[ \delta N(\tau) = \frac{\sum_k |N(k, \tau) - N_{DE}(k)|}{\sum_k N_{DE}(k)} \]

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Canonical calculation

\[
O_{CE} = \text{Tr} \left\{ \hat{O} \hat{\rho}_{CE} \right\}
\]

\[
\hat{\rho}_{CE} = Z_{CE}^{-1} \exp \left( -\hat{H} / k_B T \right)
\]

\[
Z_{CE} = \text{Tr} \left\{ \exp \left( -\hat{H} / k_B T \right) \right\}
\]

\[
E = \text{Tr} \left\{ \hat{H} \hat{\rho}_{CE} \right\} \quad T = 3.0
\]
Statistical description after relaxation (nonintegrable)

Canonical calculation

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E = \text{Tr} \left\{ \hat{H} \hat{\rho}_{CE} \right\} \quad T = 3.0
\]

### Microcanonical calculation

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

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

\( N_{\text{states}} \): # of states in the window
Thermalization and the lack thereof at integrability

Relative difference

$$\sum_k \left| N_{DE}(k) - N_{ME}(k) \right| \over \sum_k N_{DE}(k)$$

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Eigenstate thermalization

Paradox?

\[ \sum_{\alpha} |C_{\alpha}|^2 O_{\alpha\alpha} = \frac{1}{N_{E,\Delta E}} \sum_{|E - E_{\alpha}| < \Delta E} O_{\alpha\alpha} \]

Left hand side: Depends on the initial conditions through \( C_{\alpha} = \langle \alpha | \psi_{\text{ini}} \rangle \)
Right hand side: Depends only on the energy
Eigenstate thermalization

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**Right hand side:** Depends only on the energy

**Eigenstate thermalization hypothesis (ETH): diagonal part**

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

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

\[ \langle \alpha | \hat{O} | \alpha \rangle = O_{\text{ME}}(E_{\alpha}) \]
ETH – away from integrability \((t' = V' = 0.24)\)

Structure factor

Eigenstates with energies closest to \(E\)

![Graph showing Structure factor and Eigenstates]

There is no eigenstate thermalization at the edges of the spectrum (there is no quantum chaos either)
ETH – away from integrability \((t' = V' = 0.24)\)

**Structure factor**

Eigenstates with energies closest to \(E\)

There is no eigenstate thermalization at the edges of the spectrum (there is no quantum chaos either)

\(N(k = \pi)\) vs eigenstate energy
Breakdown of ETH at integrability ($t' = V' = 0$)

Structure factor

Eigenstates with energies closest to $E$

In finite systems, eigenstate thermalization breaks down close to integrable points (there is no quantum chaos either). Quantum KAM?
Breakdown of ETH at integrability \((t' = V' = 0)\)

Structure factor

Eigenstates with energies closest to \(E\)

\[
egin{align*}
\text{ka} & \quad 0 \quad 0.1 \quad 0.2 \quad 0.3 \\
N(k) & \quad \text{Diagonal} \quad \text{eigenstate 1} \quad \text{eigenstate 2} \quad \text{eigenstate 3}
\end{align*}
\]

\(N(k=\pi)\) vs eigenstate energy

In finite systems, eigenstate thermalization breaks down close to integrable points (there is no quantum chaos either). Quantum KAM?
Diagonal part of ETH (2D AF-TFIM)

Hamiltonian: \( \hat{H} = J \sum_{\langle i,j \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z + g \sum_i \hat{\sigma}_i^x + \varepsilon \sum_i \hat{\sigma}_i^z \),

Smallness of the time fluctuations

Relative difference

\[ \delta N(\tau) = \frac{\sum_k |N(k, \tau) - N_{DE}(k)|}{\sum_k N_{DE}(k)} \]

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Time fluctuations

Are they small because of dephasing?

\[ O(t) - \overline{O(t)} = \sum_{\alpha, \beta} C^{*}_\alpha C_\beta e^{i(E_\alpha - E_\beta)t} O_{\alpha \beta} \sim \sum_{\alpha, \beta} \frac{e^{i(E_\alpha - E_\beta)t}}{N_{\text{states}}} O_{\alpha \beta} \]

\[ \sim \sqrt{\frac{N_{\text{states}}^2}{N}} O^{\text{typical}}_{\alpha \beta} \sim O^{\text{typical}}_{\alpha \beta} \]

Dephasing is not enough. One needs \( O^{\text{typical}}_{\alpha \beta} \ll O^{\text{typical}}_{\alpha \alpha} \).
Time fluctuations

Are they small because of dephasing?

\[ O(t) - \overline{O(t)} = \sum_{\alpha, \beta} C_\alpha^* C_\beta e^{i(E_\alpha - E_\beta)t} O_{\alpha\beta} \sim \sum_{\alpha, \beta} \frac{e^{i(E_\alpha - E_\beta)t}}{N_{\text{states}}} O_{\alpha\beta} \]

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

Time average of \( O(t) \)

\[ \overline{O(t)} = \sum_{\alpha} |C_\alpha|^2 O_{\alpha\alpha} \]

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

Dephasing is not enough. One needs \( O_{\text{typical}}^{\alpha\beta} \ll O_{\text{typical}}^{\alpha\alpha} \)

MR, PRA 80, 053607 (2009).
Time fluctuations

Are they small because of dephasing?

\[ O(t) - \overline{O(t)} = \sum_{\alpha, \beta, \alpha \neq \beta} C_\alpha^* C_\beta e^{i(E_\alpha - E_\beta)t} O_{\alpha\beta} \sim \sum_{\alpha, \beta, \alpha \neq \beta} \frac{e^{i(E_\alpha - E_\beta)t}}{N_{\text{states}}} O_{\alpha\beta} \]

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

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Time fluctuations

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\]

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

Time average of \( O(t) \)

\[
\overline{O(t)} = \sum_\alpha |C_\alpha|^2 O_{\alpha\alpha}
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\[
\sim \sum_\alpha \frac{1}{N_{\text{states}}} O_{\alpha\alpha} \sim O_{\alpha\alpha}^{\text{typical}}
\]

Dephasing is not enough. 
One needs \( O_{\alpha\beta}^{\text{typical}} \ll O_{\alpha\alpha}^{\text{typical}} \)

MR, PRA 80, 053607 (2009).
Eigenstate thermalization hypothesis


\[ O_{\alpha\beta} = O(E)\delta_{\alpha\beta} + e^{-S(E)/2} f_{O}(E, \omega) R_{\alpha\beta} \]

where \( E \equiv (E_{\alpha} + E_{\beta})/2 \), \( \omega \equiv E_{\alpha} - E_{\beta} \), \( S(E) \) is the thermodynamic entropy at energy \( E \), and \( R_{\alpha\beta} \) is a random number with zero mean and unit variance.
Eigenstate thermalization hypothesis


\[ O_{\alpha\beta} = O(E)\delta_{\alpha\beta} + e^{-S(E)/2}O(E,\omega)R_{\alpha\beta} \]

where \( E \equiv (E_\alpha + E_\beta)/2 \), \( \omega \equiv E_\alpha - E_\beta \), \( S(E) \) is the thermodynamic entropy at energy \( E \), and \( R_{\alpha\beta} \) is a random number with zero mean and unit variance.

Off-diagonal matrix elements [histogram of \( (|O_{\alpha\beta}| - |O_{\alpha\beta}|_{\text{ave}})/|O_{\alpha\beta}|_{\text{ave}} \)]

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):

\[
(\psi_i^\alpha)^* (\psi_i^\beta) = \frac{1}{D} \delta_{\alpha\beta}.
\]
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): $(\psi_i^\alpha)^* (\psi_i^\beta) = \frac{1}{D} \delta_{\alpha\beta}$.

This means that (to leading order):

\[ \overline{O_{\alpha\alpha}} = \frac{1}{D} \sum_i O_i \equiv \bar{O}, \quad \text{while} \quad \overline{O_{\alpha\beta}} = 0 \quad \text{for} \quad \alpha \neq \beta. \]
Let \( \hat{O} = \sum_i O_i |i \rangle \langle i| \), where \( \hat{O} |i \rangle = O_i |i \rangle \),

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\]

where \( |\alpha\rangle \) and \( |\beta\rangle \) are eigenstates of a random matrix. Averaging over \( |\alpha\rangle \) and \( |\beta\rangle \) (random orthogonal unit vectors in arbitrary bases):

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\]

One can further show that (\( \eta = 2 \) for GOE and \( \eta = 1 \) for GUE):

\[
\overline{O_{\alpha\alpha}^2} - \overline{O_{\alpha\alpha}}^2 = \eta |O_{\alpha\beta}|^2 = \frac{\eta}{D^2} \sum_i O_i^2 \equiv \frac{\eta}{D} \overline{O^2}.
\]
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):

\[
(\psi_i^\alpha)^* (\psi_i^\beta) = \frac{1}{D} \delta_{\alpha\beta}.
\]

This means that (to leading order):

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

One can further show that (\( \eta = 2 \) for GOE and \( \eta = 1 \) for GUE):

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

Combining these results one can write

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

where \( R_{\alpha\beta} \) is a random variable (real for GOE and complex for GUE).
Hamiltonian: \( \hat{H} = -J \sum_{\langle i,j \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z + g \sum_i \hat{\sigma}_i^x \).
Outline

1 Motivation
   - Foundations of quantum statistical mechanics
   - Experiments with ultracold gases

2 Quantum chaos and random matrix theory
   - Classical and quantum chaos
   - Random matrix theory

3 Dynamics and thermalization (quantum chaotic systems)
   - Quantum mechanics vs statistical mechanics
   - Dynamics and equilibration
   - Thermalization
   - Eigenstate thermalization

4 Dynamics and generalized thermalization (integrable systems)
   - Generalized Gibbs ensemble (GGE)

5 Summary
Relaxation dynamics in an integrable HCB system

Relaxation dynamics in an integrable HCB system

Generalized Gibbs ensemble (GGE)

Thermal equilibrium

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

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

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

MR, PRA 72, 063607 (2005).
Generalized Gibbs ensemble (GGE)

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MR, PRA 72, 063607 (2005).

Evolution of \( n_{k=0} \)

\[ \begin{align*}
\tau & \quad 0 \quad 1000 \quad 2000 \quad 3000 \quad 4000 \\
n_{k=0} & \quad 0 \quad 0.5 \quad 1 \quad 1.5 \\
\end{align*} \]

\( n_{k=0} \) after relaxation

\[ \begin{align*}
\alpha & \quad -\pi \quad -\pi/2 \quad 0 \quad \pi/2 \quad \pi \\
n_k & \quad 0 \quad 0.25 \quad 0.5 \\
\end{align*} \]
Generalized Gibbs ensemble (GGE)

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MR, PRA 72, 063607 (2005).

Integrals of motion

(underlying noninteracting fermions)

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

\[ \left\{ \hat{I}_m \right\} = \left\{ \hat{\gamma}_m^{f\dagger} \hat{\gamma}_m^f \right\} \]
Generalized Gibbs ensemble (GGE)

Thermal equilibrium

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MR, PRA 72, 063607 (2005).

Generalized Gibbs ensemble

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

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

\[ \text{Tr} \left\{ \hat{I}_m \hat{\rho}_{\text{GGE}} \right\} = \langle \hat{I}_m \rangle_{\tau=0} \]
Generalized Gibbs ensemble (GGE)

Thermal equilibrium

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

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MR, PRA 72, 063607 (2005).

The constraint

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

results in

\[ \lambda_m = \ln \left[ \frac{1 - \langle \hat{I}_m \rangle_{\tau=0}}{\langle \hat{I}_m \rangle_{\tau=0}} \right] \]

Evolution of \( n_{k=0} \)

Evolution of \( n_k \) after relaxation

After relax. (\( N_b = 30 \))

After relax. (\( N_b = 15 \))

Thermal (\( N_b = 30 \))

Thermal (\( N_b = 15 \))
Generalized Gibbs ensemble (GGE)

**Thermal equilibrium**

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

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Generalized Gibbs ensemble (GGE)

Density profile
\[ \tau = 2000t \]

Momentum profile
\[ \tau = 2000t \]

Why does the GGE work?
Generalized eigenstate thermalization:
Relevant to generalized thermodynamic Bethe ansatz approaches:
Generalized Gibbs ensemble (GGE)

Why does the GGE work?

Generalized eigenstate thermalization:

Relevant to generalized thermodynamic Bethe ansatz approaches:
Generalized eigenstate thermalization (1D-TFIM)

Weight of eigenstate expectation values in the diagonal ensemble

Generalized eigenstate thermalization (1D-TFIM)

Weight of eigenstate expectation values in the diagonal ensemble

Weight of eigenstate expectation values in the GGE


Marcos Rigol (Penn State) Dynamics in quantum systems September 18, 2017 39/44
Equilibration and thermalization occur 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 at, and close to (finite L), integrability
★ Quantum equivalent of KAM?

Small time fluctuations ← smallness of off-diagonal elements

Time plays only an auxiliary role

Integrable systems are different (Generalized Gibbs ensemble)
Equilibration and thermalization occur in generic isolated systems

Finite size effects

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Equilibration and thermalization occur in generic isolated systems
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Eigenstate thermalization hypothesis
★ \[ \langle \Psi_\alpha | \hat{O} | \Psi_\alpha \rangle = \langle O \rangle_{\text{microcan.}}(E_\alpha) \]

Thermalization and ETH break down at, and close to (finite \( L \)), integrability
★ Quantum equivalent of KAM?
Equilibration and thermalization occur 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 at, and close to (finite $L$), integrability

- Quantum equivalent of KAM?

Small time fluctuations $\leftrightarrow$ smallness of off-diagonal elements
Summary

- Equilibration and thermalization occur 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 at, and close to (finite \( L \)), integrability
  - ★ Quantum equivalent of KAM?
- Small time fluctuations \( \leftrightarrow \) smallness of off-diagonal elements
- Time plays only an auxiliary role
Summary

- Equilibration and thermalization occur in generic isolated systems
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  ★ Quantum equivalent of KAM?
- Small time fluctuations ↔ smallness of off-diagonal elements
- Time plays only an auxiliary role
- Integrable systems are different (Generalized Gibbs ensemble)
Collaborators

- Luca D’Alessio (Exa Corporation)
- Vanja Dunjko (U Mass Boston)
- Deepak Iyer (Bucknell)
- Yariv Kafri (Technion)
- Ehsan Khatami (San Jose State U)
- Rubem Mondaini (CSRC, Beijing)
- Maxim Olshanii (U Mass Boston)
- Anatoli Polkovnikov (Boston U)
- Guido Pupillo (U Strasbourg)
- Lea F. Santos (Yeshiva U)
- Mark Srednicki (UC Santa Barbara)
- Lev Vidmar (Penn State)

Supported by:
Coherence after quenches in Bose-Fermi mixtures

S. Will, D. Iyer, and MR

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Coherence after quenches in Bose-Fermi mixtures

\[ \langle \hat{c}^\dagger_j \hat{c}^\dagger_0 \rangle(t) = n_F \sin[\pi n_F j] e^{2n_B [\cos(U_{FB} t / \hbar) - 1]} / j, \]

\( n_F \) and \( n_B \) are the fermion and boson fillings.

S. Will, D. Iyer, and MR
Coherence after quenches in Bose-Fermi mixtures

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Dynamics in quantum systems

September 18, 2017
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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).
Fluctuation-dissipation theorem (dipolar bosons)

Occupation in the center of the trap \(n_j = L/2\)

Hamiltonian

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

magnetic atoms, polar molecules

Relaxation dynamics

\[
O(t) = C(t)O(t = 0)
\]

where

\[
C(t) = \frac{O(t + t')O(t')}{(O(t'))^2}
\]

Srednicki, JPA 32, 1163 (1999).