Quantum typicality: what is it and what can be done with it?

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Outline

- Thermal relaxation in closed quantum systems?
- Typicality in a nutshell
- Numerical experiment: model, observables and results
- Typicality in formulas
- Spin transport in the Heisenberg chain
- Eigenstate thermalization hypothesis
Thermal relaxation in closed quantum systems?

Why it exists: We see it in system we assume to be closed.

Why it does not exist: There are issues with the underlying theory:

(Non-eq.) Thermodynamics

- autonomous dynamics of a few macrovariables
- attractive fixed point, equilibrium
- often describable by master equations, Fokker-Planck equations, stochastic processes, etc.

Quantum Mechanics

- autonomous dynamics of the wave function (number of parameters: insane)
- no attractive fixed point (Schroedinger equation)
- Schroedinger equation is no rate equation

Quantum systems that explicitly exhibit relaxation but are not of the “small system + large bath” type appear to be rare in the literature.

To cut it short: Why and how do two cups of coffee thermalize each other?
Typicality in a nutshell

The naive view on relaxation i.e. 2nd law of thermodynamics:

\[
\hat{\rho}_0 = |\psi\rangle\langle\psi| \quad \text{evolves into} \quad \hat{\rho}_{eq} = \frac{1}{Z} e^{-\frac{\hat{H}}{kT}} \quad \text{or} \quad \hat{\rho}_{eq} \approx \frac{1}{Z} \delta(\hat{H} - E)
\]

problem: invariance of Von Neuman-entropy

\textit{traditional cure: open quantum systems} \Rightarrow this requires:
large, doable, broad band environment (usually oscillators), adequate weak
coupling (Van-Hove structure), applicability of projection techniques, specific
initial states: factorizing, thermal bath, etc.

Typicality:

\[
\hat{\rho}_0 = |\psi\rangle\langle\psi| \quad \text{does not evolve into} \quad \hat{\rho}_{eq} = \frac{1}{Z} e^{-\frac{\hat{H}}{kT}}, \quad \hat{\rho}_{eq} \approx \frac{1}{Z} \delta(\hat{H} - E)
\]

but \[ \langle \psi | \hat{A}(t) | \psi \rangle \] evolves into \[ \approx \text{Tr}\{\hat{\rho}_{eq} \hat{A}\}\]

for many (all?) \( \hat{A}, |\psi\rangle \) ............ \textit{Can this be true?}
Numerical experiment: model and observables

**Heisenberg-type Hamiltonian:** A ladder with anisotropic, XXZ-type couplings which are strong along the legs and weak along the rungs:

\[
\hat{H} = \sum_{ij} J_{ij} (\hat{\sigma}_i^x \hat{\sigma}_j^x + \hat{\sigma}_i^y \hat{\sigma}_j^y + 0.6 \hat{\sigma}_i^z \hat{\sigma}_j^z),
\]

\(J_{ij} = 1\) for solid lines, \(J_{ij} = \kappa = 0.2\) for dotted lines and \(J_{ij} = 0\) otherwise. Total number of spins: \(N = 32\). The \(z\)-component of total magnetization \(S_z = \sum_i \hat{\sigma}_i^z\) is conserved.

We analyze: “magnetization difference” \(\hat{x}\)

\[
\hat{x} = \left( \sum_{l \in L} \hat{\sigma}_z^l - \sum_{r \in R} \hat{\sigma}_z^r \right)
\]

eigenvalues of \(\hat{x}\) within the subspace of vanishing total magnetization, \(S_z = 0\): \(X = -16, -14, \ldots , +16\).
Numerical experiment: results

\( \hat{x} \): z-magnetization difference between legs

\( P_X(t) \): probability to find a certain \( X \)

H. de Raedt, K. Michielsen (Juelich)

![Graph showing time-shifted \( \langle \hat{x}(t) \rangle \)]

![Graph showing variances of \( x \)]

Data from solving the Schroedinger equation \((N = 32)\) for two pure, partially random initial states:

\[
|\psi_X(0)\rangle = e^{-\alpha \hat{H}^2} \hat{P}_x \hat{P}(S_z = 0) |\omega\rangle,
\]

Remark: taking this picture took 6h on 65 000 CPU’s. Thanks to:

J.Gemmer quantum typicality
“static typicality”

\[ <A> := \frac{\text{Tr}\{\hat{A}\}}{d} \text{ expectation value of the maximally mixed state} \]

\[ |\omega\rangle \text{ uniform random states sampled according to the unitary invariant measure} \]

\[ \text{HA}[\langle \omega | \hat{A} | \omega \rangle] =<A> \quad \text{HV}[\langle \omega | \hat{A} | \omega \rangle] = \frac{1}{d+1} ( <A^2> - <A>^2 ) \]

In a high dimensional Hilbert space almost all possible states feature very similar expectation values for observables with bound spectra. \( \Rightarrow \text{It is no surprise to find these “equilibrium” expectation values overwhelmingly often.} \)

“dynamical typicality”

\[ |\psi\rangle := \sqrt{\hat{\rho} d} |\omega\rangle \text{ “taylored”, non-uniform random states,} \]

\[ \langle \psi | \hat{A}(t) | \psi \rangle \approx \text{Tr}\{\hat{A}(t)\hat{\rho}\} \]

The statistics variance of \( \langle \psi | \hat{A}(t) | \psi \rangle \) decreases as \( 1/d_{\text{eff}} \) where the latter is the inverse of the largest eigenvalue of \( \hat{\rho} \).

\( \Rightarrow \text{Very many different pure states exhibit dynamics of expectation values close to those of corresponding mixed states} \)

If \( \hat{\rho} \) is of “exponential form”, e.g., \( \hat{\rho} \propto e^{-\beta(\hat{H} - \bar{E})^2 - \alpha(\hat{A} - A_0)^2} \) or \( \hat{\rho} \propto e^{-\beta \hat{H} - \alpha \hat{A}} \) than one may infer dynamics of mixed states from “pure state propagation”
Spin transport in the anisotropic Heisenberg chain (PRL, 112, 120601, (2014))

Linear response $\Rightarrow$ conductivity from current autocorrelation function

here: infinite temperature, i.e., $\hat{\rho} := \hat{J}/d$, $\hat{A} := \hat{J}$

$C(t) \propto \text{Tr}\{\hat{J}(t)\hat{J}\}$
**Eigenstate thermalization hypothesis (ETH)**

ETH: Eigenstates of some Hamiltonian $\hat{H}$ that are close in energy feature expectation values of some observable $\hat{A}$ that are close to each other.

$$E_n \approx E_m \rightarrow \langle n | \hat{A} | n \rangle \approx \langle m | \hat{A} | m \rangle$$

Jochen’s formulation: “Eigenstates belong to the set of typical states”

If ETH applies:
- Expectation values from microncanonical ensembles are close to expectation values of individual eigenstates
- Initial state independent (ISI) equilibration:

$$\langle \hat{A}(t) \rangle = \sum_{n,m} \rho_{nm} A_{mn} e^{i(E_n - E_m) t}$$

If the oscillating terms behave like “white noise” for $\tau$ large enough

$$\langle \hat{A}(\tau) \rangle = \sum_n \rho_{nn} A_{nn}^{\text{ETH}} \approx A_{nn}$$

But does ETH apply? Have to check by exact diagonalization, or.......
\( \hat{A} := \hat{x}^2 \): width of the magnetization distribution

\[
\hat{\rho} \propto e^{-\alpha (\hat{H} - U)^2} \quad \bar{A} := \sum_n \rho_{nn} A_{nn} \approx \langle \psi | \hat{A} | \psi \rangle
\]

\[
\Sigma^2 + \bar{A}^2 := \sum_n \rho_{nn} A_{nn}^2 \approx \text{Re}[\langle \psi(\tau) | \hat{A} | \psi'(\tau) \rangle]
\]

ETH applies!

\( \Sigma \) scales approx like \( \hat{H} \) was a random matrix.
Is ISI equilibration always driven by ETH?

Back to the two cups of coffee: Temperature differences between macroscopic object always equilibrate, regardless of the objects ⇒ ETH always fulfilled? We investigate energy differences \( \hat{A} = \hat{H}_L - \hat{H}_R \) between all sorts of coupled “spin-objects”

Seems like the ETH is indeed always fulfilled, but what about “integrable” systems?
Consider energy difference dynamics in a clean Heisenberg chain w.r.t. 1:2 partition using initial states like

$$|\psi(0)\rangle \propto e^{-\alpha \hat{H}^2 - \beta (\hat{A} - N_L)^2} |\omega\rangle$$

There appears to be ISI equilibration for large systems.

Check scaling of $\Sigma$.

The ETH is violated w.r.t. the bare $\Sigma$.

Define “scaled” ETH parameter $\Sigma/\delta$:

$$\delta^2 = \text{Tr} \left\{ \frac{1}{Z} \hat{A}^2 e^{-\alpha \hat{A}^2} \right\} - \text{Tr} \left\{ \frac{1}{Z} e^{-\alpha \hat{H}^2} \right\}^2$$

The scaled ETH parameter appears to vanish in the limit of large systems.

(erratum: $D \Rightarrow A$)
People who truly did the work: R. Steinigeweg, H. de Raedt, K. Michielsen A. Khodja, D. Schmidtke, C. Gogolin ....

Thank you for your attention!

The talk itself as well as the mentioned papers may be found on our webpage.