Irreversible Non-Equilibrium Dynamics in Closed Finite Quantum Systems?

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Bielefeld, Feb. 1., 2016

Overview

- Background
- Numerical Example (calming)
- Typicality
- Eigenstate Thermalization Hypothesis (ETH)
- “Advanced Typicality”
- Numerical Example (odd)
- Pathological initial states
- Stochastic Trajectories from Closed Finite Quantum Systems

Thermalization in Closed Quantum Systems?

(Non-eq.) Thermodynamics

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

Quantum Mechanics

- autonomous dynamics of the wavefunction.
- no attractive fixed point (Schrödinger equation)
- Schrödinger is not Fokker-Planck

Can these two seemingly antagonistic principles be reconciled?

And if so how?

Quantum Mechanics

$$i\hbar\dot{\psi} = \hat{H}\psi$$

Heisenberg Cut

$\longrightarrow$

Classical Mechanics

$$\ddot{\vec{x}} = \vec{F}(\vec{x})$$

$\searrow$ $\swarrow$

typicality,
"ETH",
etc.

ergodicity,
mixing,
etc.

$\searrow$ $\swarrow$

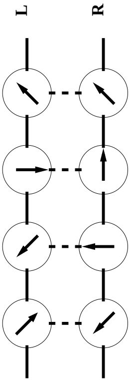
Thermodynamics

$$\dot{\rho} = -\nabla(\vec{f}\rho) + \frac{1}{2}\Delta(D\rho)$$

$$\rho_{eq} \propto e^{(-H/kT)}$$

An Instructive Numerical Experiment

“spin-ladder”



Heisenberg-type Hamiltonian:

$$\hat{H} = \sum_{ij} J_{ij}(\hat{\sigma}_x^i \hat{\sigma}_x^j + \hat{\sigma}_y^i \hat{\sigma}_y^j + 0.6\ \hat{\sigma}_z^i \hat{\sigma}_z^j),$$

Observable

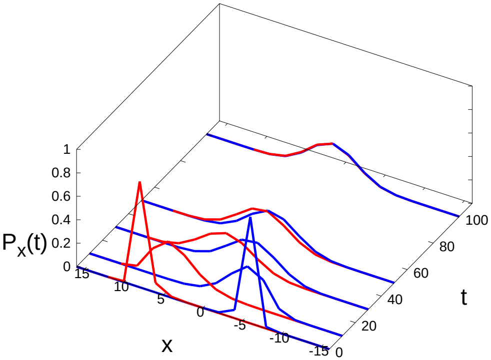
$$\hat{x} = \frac{1}{2}\left(\sum_{l \in L} \hat{\sigma}_z^l - \sum_{r \in R} \hat{\sigma}_z^r\right)$$

Roughly this may be viewed as particles hopping between the junctions of a ladder. The particles may hop along the legs and along the rungs. The particles interact. X counts the difference of particles between the legs leg. There are 16 rungs and 16 particles (“half filling”).

An Instructive Numerical Experiment

We solved the Schrödinger equation for a pure state rather concentrated in X and energy, but completely random otherwise

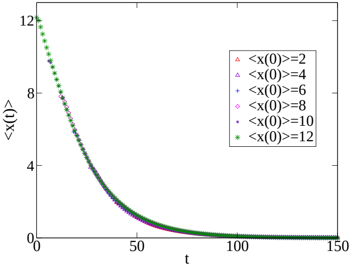
$P_X(t)$: probability to find a certain X



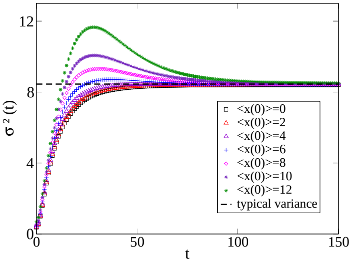
(remark: producing this data took 6h on 65 000 CPU's in Jülich)

All fluctuations/uncertainties are quantum.

time shifted $\langle \hat{x}(t) \rangle$

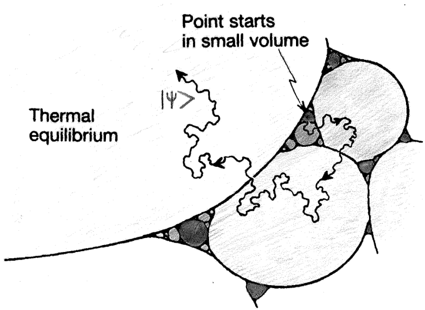


variances of x



Why Equilibrium? → "Typicality"

Pure states move through Hilbert space forever. But: Extremely many points in Hilbert space may correspond to almost the same expectation value of some observable $\langle \hat{A} \rangle$. Thus, at some point, $\langle \hat{A}(t) \rangle$ may practically come to a halt for a very long time.



Drawing pure states $|\omega\rangle$ " at random" yields a probability distribution for the $\langle \hat{A} \rangle$

$$\mathrm{mean}[\langle \omega | \hat{A} | \omega \rangle] = \mathrm{Tr}\{\hat{A}\}/d$$

$$\mathrm{variance}[\langle \omega | \hat{A} | \omega \rangle] = \frac{\sigma_A^2}{d+1}$$

σ_A^2 variance of the spectrum of $\hat{A}$
d: dimension of the respective Hilbertspace

As a consequence there is also a most frequent local density matrix $\hat{\rho}_S$ for a total set-up comprising a system S and an environment E. For generic spectra of E an weak coupling one gets $\hat{\rho}_S \propto \mathrm{e}^{-\frac{\hat{H}_S}{kT}}$ ("canonical typicaltiy")

These typicality considerations are only based on measures in Hilbert space and completely ignore the specific Hamiltonian and initial state

Why Equilibrium? → "Eigenstate Thermalization Hypothesis"

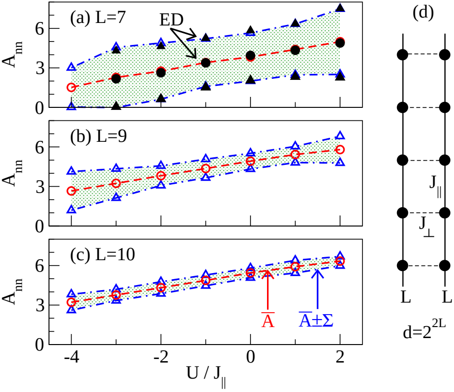
The speakers personal version of the ETH: Expectation values of some observable $\hat{A}$ as resulting from energy eigenstates of some Hamiltonian $\hat{H}$ are close, if the energies are close.

Long time averages of states from a narrow energy shell:

$$\overline{\langle\psi(t)|\hat{A}|\psi(t)\rangle} = \sum_n |\langle\psi(0)|n\rangle|^2 \langle n|\hat{A}|n\rangle$$

$$\overset{\text{ETH}}{\approx} \quad \langle n|\hat{A}|n\rangle$$

→ independent of initial state



- For quantum systems with no direct classical counterpart the ETH is a hypothesis
- In very many instances the ETH is found to hold
- ETH holds ⇔ eigenstates are typical
- Statement concerns long time averages

What has the time average got to do with the actual value?

- Assume every frequency $\omega_{nm} := E_n - E_m$ occurs only once, "non-resonance condition"
- Assume $\overline{|\langle\psi(0)|n\rangle|^4 << 1}$, "broad energy participation"

$\Rightarrow \langle\psi(t)|\hat{A}|\psi(t)\rangle \approx \overline{\langle\psi(t)|\hat{A}|\psi(t)\rangle}$ for an overwhelmingly large fraction of instances in time from any interval T with $T > 1/\omega_{\mathrm{min}}$.

Is the ETH really important?

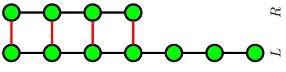
The long time average $\overline{\langle\psi(t)|\hat{A}|\psi(t)\rangle} = \sum_n |\langle\psi(0)|n\rangle|^2 \langle n|\hat{A}|n\rangle$ depends on: The initial state $|\psi(0)\rangle$, the Hamiltonian $\hat{H}$ and the observable $\hat{A}$. If any of the three is drawn "at random" w.r.t. the two others the outcome is extremely likely to be $\overline{\langle\psi(t)|\hat{A}|\psi(t)\rangle} = \mathrm{Tr}\{\hat{A}\}/d$

- $\hat{A}$ random w.r.t. $\hat{H}$ → ETH holds,
- $|\psi(0)\rangle$ random w.r.t. $\hat{A}$: boring
- $|\psi(0)\rangle$ non-random w.r.t $\hat{H}$?

Is this the end of the story?

Do "non-contrived" exceptions exist?

Now $\hat{x}$ quantifies differences of local energies rather than magnetization/particles.



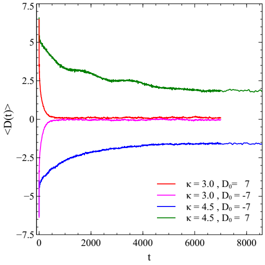
Rung coupling stronger than leg coupling by a factor of ≈ 4

Initial state along the lines of Jayne's principle:

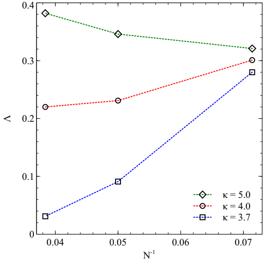
$$\hat{\rho}(0) \propto e^{(-\alpha(\hat{H}-E_0)^2-\beta(\hat{x}-X_0)^2}$$

At large couplings, there appears to be a "stick effect"

$\langle x(t) \rangle$ for different coupling strengths

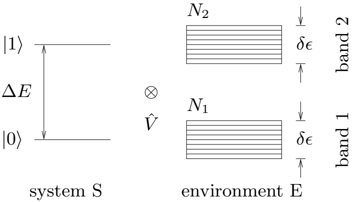


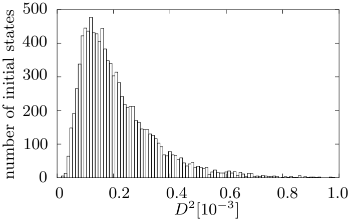
$\langle x(0) \rangle / \langle x(\tau) \rangle$ vs. inverse system size

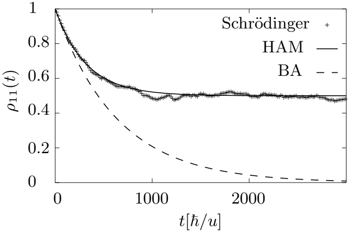


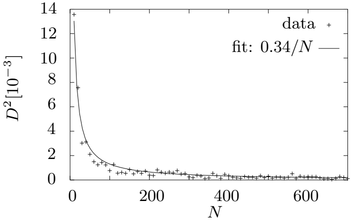
Pathological initial states? → "Dynamical Typicality"

(Pure) states that move away from equilibrium must exist. Are they frequent?









D^2 : mean squared deviations from $t = 0$ to $t = 2000$. We choose $\rho_{11} = 3/4$.
Top right: $N = 500$
Meanwhile this is reasonably understood also in terms of (somewhat involved) formulas.

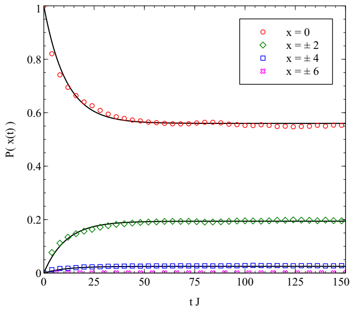
Not everything that looks stochastic is stochastic!

Stochastic processes feature
- insensitivity against observation/measurement/decoherence
- independence of the distant past

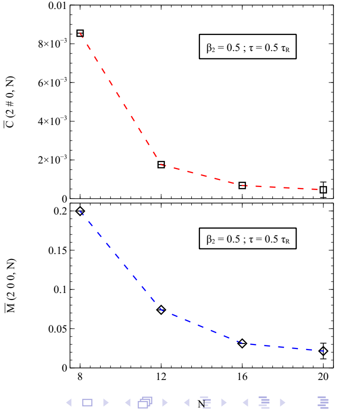
x: particle difference between left and right

$$P_x(t+\tau) = \sum_y W(x|y) P_y(t+\tau) \quad ?$$

probability dynamics



top: sensitivity against decoherence
bottom: dependence on the past



The End

Bottom line: There is considerable progress concerning concepts and numerical examples. Nevertheless, questions like:
- How can the Eigenstate Thermalization Hypothesis be worked into a Eigenstate Thermalization Theorem,
- what is entropy and why does it almost always increase, etc.
remain open
Some names in the business:

- **Typicality:** von Neumann, Schrödinger, Bocchieri, Lloyd, Goldstein, Short, Reimann, Eisert, Gemmer,....
- **ETH:** Deutsch, Srednicki, Rigol, Moessner, ...
- **Equilibration Time Scales:** Short, Reimann, ...
- **Relaxation Dynamics and Numerical Experiments:** Jensen, De Raedt, Steinigeweg, Gemmer, ...
- ... and many more.

The presented data is (published) work done by:
Robin Steinigeweg (Osnabrück), Daniel Schmidtke (Osnabrück),
Abdellah Khodja (Oran, Algeria)

Thank you for your attention !