(Dynamical) quantum typicality: What is it and what are its physical and computational implications ?

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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 should occur: We see it in system we assume to be closed.

Why it should not occur: 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?

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

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

problem: invariance of Von Neuman-entropy
traditional cure: open quantum systems $\Rightarrow$ this requires:

- environment
- special structure of structure of environment: large, broad band (oscillator) bath
- adequate weak coupling, applicability of projection techniques
- specific initial states: factorizing, thermal bath.....
- etc.

Typicality:

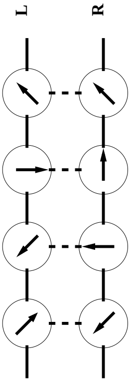
$$\hat{\rho}_0 = |\psi\rangle\langle\psi| \quad \text{does not evolve into} \quad \hat{\rho}_{eq} = \frac{1}{Z}e^{-\frac{\hat{H}}{kT}}, \; \hat{\rho}_{eq} = \frac{1}{Z}\hat{\delta}(\hat{H} - E)$$

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

for many (all?) $\hat{A}$ .... **Can this be true?**

Numerical experiment: model and observables

spin-model



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

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

$J_{ij} = 1$ 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 $S_z = \sum_i \hat{\sigma}_z^i$ is conserved

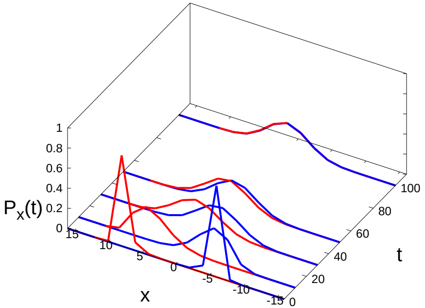
We analyze: "magnetization difference" $\hat{x}$

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

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



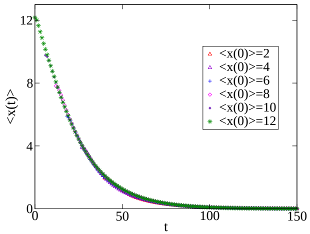
data from solving the Schroedinger equation ($N = 32$) for two pure, partially random initial states:

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

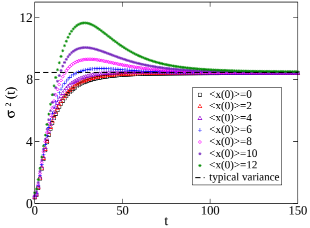
(remark: taking this picture took 6h on 65 000 CPU's. Thanks to:

H. de Raedt, K. Michielsen (Juelich))

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



variances of x



“static typicality”

$< A > := \mathrm{Tr}\{\hat{A}\}/d$: expectation value of the maximally mixed state
$|\omega\rangle$ uniform random states sampled according to the unitary invariant measure

$$\mathrm{HA}[\langle\omega|\hat{A}|\omega\rangle] = < A > \qquad \mathrm{HV}[\langle\omega|\hat{A}(t)|\omega\rangle] = \frac{1}{d+1}\left(< A^2 > - < A >^2\right)$$

In a high dimensional Hilbert space almost all possible states feature very similar expectation values for observables with bound spectra. $\Rightarrow$ *It is no surprise to find these expectation values eventually.*

“dynamical typicality”

$|\psi\rangle := \sqrt{\hat{\rho} d}\,|\omega\rangle$: “taylored”, non-uniform random states, $\hat{A} \rightarrow \hat{B}(t)$

$$\mathrm{HA}[\langle\psi|\hat{B}(t)|\psi\rangle] = \mathrm{Tr}\{\hat{B}(t)\hat{\rho}\} \qquad \mathrm{HV}[\langle\psi|\hat{B}(t)|\psi\rangle] \leq \frac{\mathrm{Tr}\{\hat{B}^2(t)\hat{\rho}\}}{d_{\mathrm{eff}}}$$

d_{eff}: inverse of the largest eigenvalue of $\hat{\rho}$, interpreted as “effective dimension”
$\Rightarrow$ *Very many different pure states exhibit very similar dynamics of expectation values*

"correlation functions"

$|\psi\rangle := \sqrt{\hat{\rho} d}|\omega\rangle$: "taylored", non-uniform random states,
$\hat{A} \rightarrow \hat{C}(t) := \frac{1}{2}(\hat{B}(t)\hat{B} + \hat{B}\hat{B}(t))$

$$\mathrm{HA}[\langle\psi|\hat{C}(t)|\psi\rangle] = \mathrm{Tr}\{\hat{C}(t)\hat{\rho}\} \qquad \mathrm{HV}[\langle\psi|\hat{C}(t)|\psi\rangle] \leq \frac{\mathrm{Tr}\{\hat{C}^2(t)\hat{\rho}\}}{d_{\text{eff}}}$$

What to do practically?

Compute $|\psi(t)\rangle := e^{-i\hat{H}t/\hbar}\sqrt{\hat{\rho} d}|\omega\rangle$, $|\psi'(t)\rangle := e^{-i\hat{H}t/\hbar}\hat{B}\sqrt{\hat{\rho} d}|\omega\rangle$

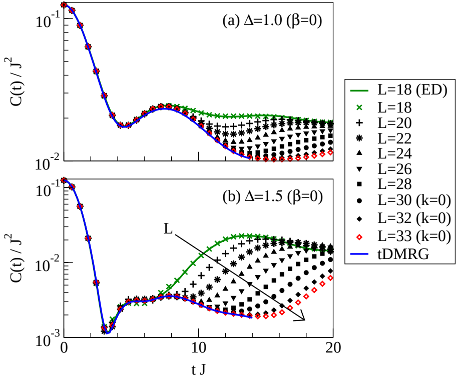
$$\langle\psi(t)|\hat{B}|\psi(t)\rangle \approx \mathrm{Tr}\{\hat{B}(t)\hat{\rho}\} \qquad \mathrm{Re}[\langle\psi(t)|\hat{B}|\psi'(t)\rangle] \approx \mathrm{Tr}\{\frac{1}{2}(\hat{B}(t)\hat{B}+\hat{B}\hat{B}(t))\hat{\rho}\}$$

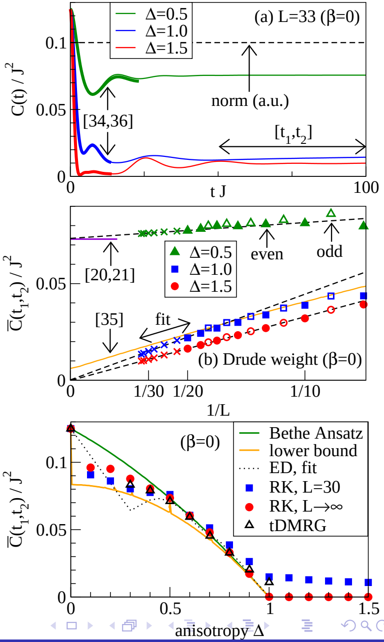
If $\hat{\rho}$ is of "exponential form", e.g., $\hat{\rho} \propto e^{-\beta(\hat{H}-\bar{E})^2-\alpha(\hat{B}-\bar{B})^2}$ or $\hat{\rho} \propto e^{-\beta\hat{H}-\alpha\hat{B}}$ than everything can be done based on "pure state propagation"

Linear response ⇒ conductivity from current autocorrelation function

here: infinite temperature, i.e., $\hat{\rho} \propto \hat{1}$, $\hat{B} \to \hat{J}$

$C(t) \propto \mathrm{Tr}\{\hat{J}(t)\hat{J}\}$





Eigenstate thermalization hypothesis (ETH)

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

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

Jochen's formulation: "Eigenstates belong to the set of typical states"

If ETH applies:

- Expecation values from microncanonical ensembles are close to expecation values of individual eigenstates

- Initial state independent equilibration:

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

If the oscillating terms behave like "white noise" for τ large enough

$$\langle \hat{B}(\tau)\rangle = \sum_{n} \rho_{nn} B_{nn} \overset{\text{ETH}}{\approx} B_{nn}$$

But does ETH apply? Have to check by exact diagonalization, or.......

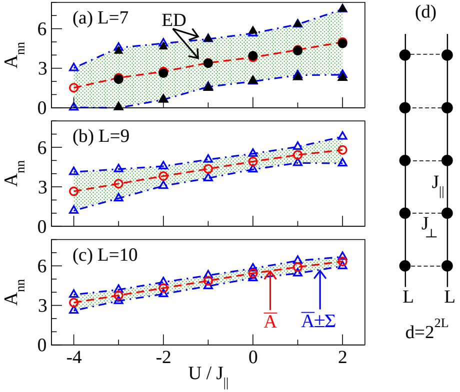
ETH check for the Heisenberg ladder

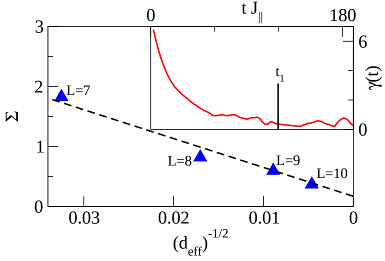
(Phys. Rev. Lett., 112, 130403, (2014))

$\hat{A} := \hat{x}^2$: width of the magnetization distribution

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

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





ETH applies!

Σ scales approx like $\hat{H}$ was a random matrix.

more people involved in this: R. Steinigeweg, A. Khodja, H. Niemeyer, D. Schmidtke, C. Gogolin ....

Thank you for your attention!

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