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 thermodynamcis:

QM: $\hat{\rho}_0 = |\psi\rangle\langle\psi|$ evolves into $\hat{\rho}_{eq} = \frac{1}{Z} \mathrm{e}^{-\frac{\hat{H}}{kT}}$ 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:
large, doable, broad band environment (usually oscillators), adequate weak coupling (Van-Hove structure), applicability of projection techniques, specific initial states: factorizing, thermal bath, etc.

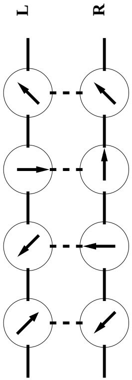
Typicality:

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

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

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

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" $\hat{x}$

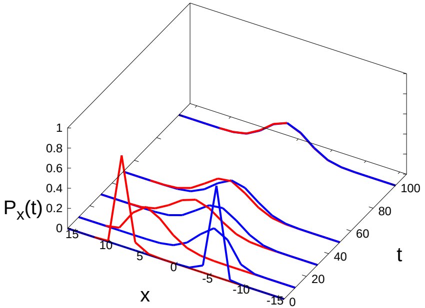
$$\hat{x} = \left(\sum_{l \in L} \hat{\sigma}_z^l - \sum_{r \in R} \hat{\sigma}_z^r \right)$$

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

Numerical experiment: results

Phys. Rev. E, 89, 042113, (2014)

$\hat{x}$: z-magnetization difference between legs
$P_X(t)$: probability to find a certain X



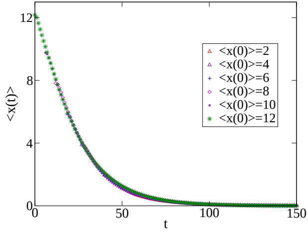
data from solving the Schroedinger equation ($N = 32$) for two pure, partially random initial states:

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

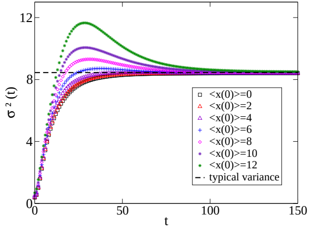
(remark: taking this picture took 6h on 65 000 CPU's. Thanks to:

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

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

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 "equilibrium" expectation values overwhelmingly often.*

"dynamical typicality"

$|\psi\rangle := \sqrt{\hat{\rho}d}|\omega\rangle$: "taylored", non-uniform random states,

$$\langle\psi|\hat{A}(t)|\psi\rangle \approx \mathrm{Tr}\{\hat{A}(t)\hat{\rho}\}$$

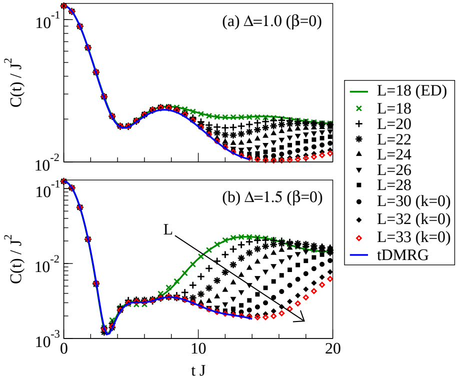
The statisitcal variance of $\langle\psi|\hat{A}(t)|\psi\rangle$ decreases as $1/d_{\text{eff}}$ where the latter is the inverse of the largest eigenvalue of $\hat{\rho}$.
$\Rightarrow$ *Very many different pure states exhibit dynamics of expectation values close to those of corresponding mixed states*
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"

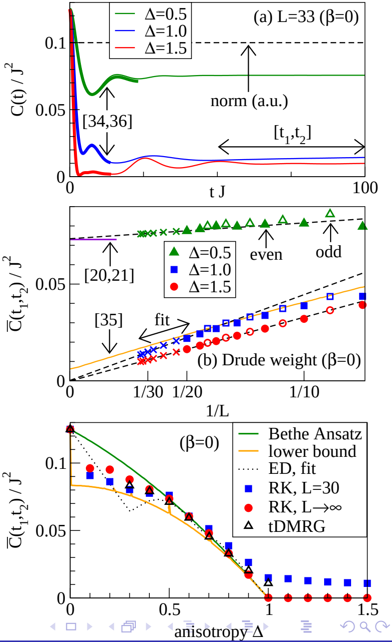
Spin transport in the anisotropic Heisenberg chain (PRL., 112, 120601, (2014))

Linear response $\Rightarrow$ conductivity from current autocorrelation function

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

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





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:

- Expecation 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 τ large enough

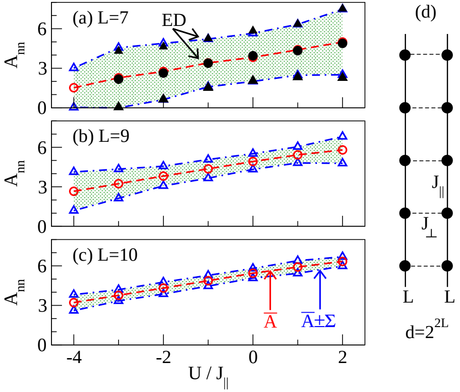
$$\langle \hat{A}(\tau)\rangle = \sum_{n} \rho_{nn} A_{nn} \overset{\text{ETH}}{\approx} A_{nn}$$

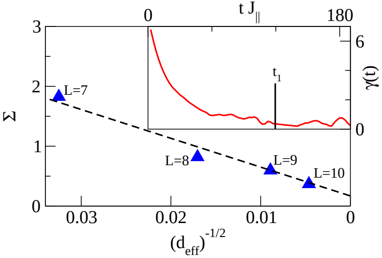
But does ETH apply? Have to check by exact diagonalization, or.......

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

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

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



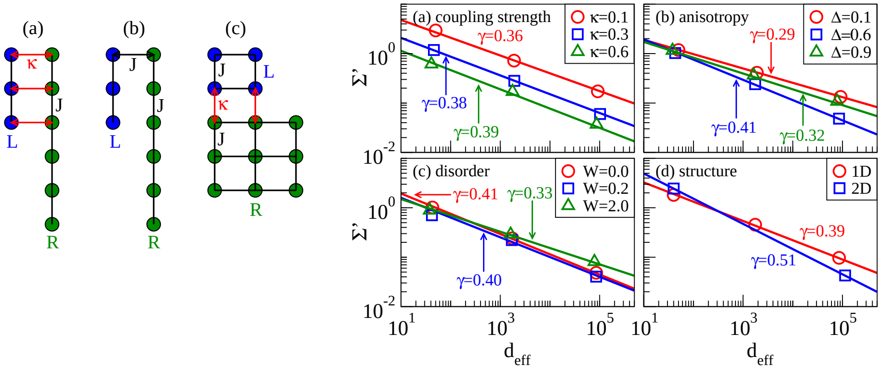


ETH applies!

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

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 ?

Is ISI equilibration always driven by ETH?

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 Σ

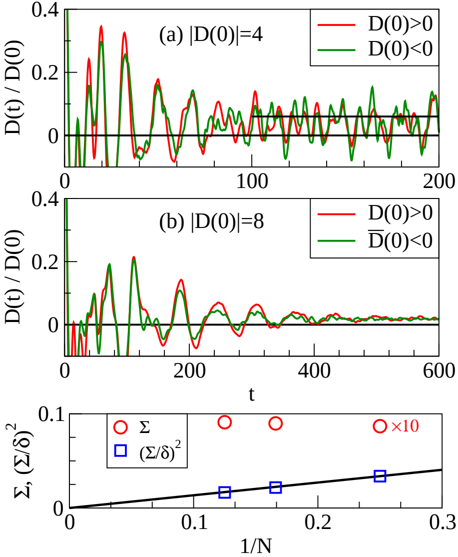
The ETH is violated w.r.t. the bare Σ.

Define "scaled" ETH parameter Σ/δ:

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

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.