Emergence of Thermodynamic Behavior in Closed Quantum Systems: A Small Spin System as an Example

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Outline

- Thermodynamics as emerging from quantum mechanics?
- Attempts to reconcile TD with QM
- Typicality and ETH
- Non-perfect applicability of the ETH and "stick-effect"
- Model and observables
- Stick-effect of magnetization difference
- Concrete quantum dynamics
- Comparison of concrete quantum dynamics to stochastic processes
- The end

Thermodynamics as emerging from quantum mechanics?

Thermodynamics

- describable in terms of few macrovariables: $V, E, T(x), \rho(x)$...
- macrovariables approach constant "equilibrium" values which are widely independent of inital values
- often there are autonomous relaxation dynamics which may be interpreted in terms of transition rates
- often one finds Langevin-type relaxation dynamics

Quantum Mechanics

- description in terms of the density matrix $\hat{\rho}$: insanely many variables
- Schroedinger equation has no fixpoint
- there is no direct stochastic interpretation of unitary quantum dynamics

Attempts to reconcile TD with QM (unsorted and incomplete)

- Addition of extra "non-unitary" superoperator terms to the Schroedinger equation (Ghirardi, Rimini, Weber / Beretta et. al. / ...). Many undefined parameters, seems in conflict with occam's razor
- Open quantum systems, environment induced decoherence. Always a "bath" required. Derivations based on weak coupling, broad spectra, often bosonic baths, uncorrelated init al conditions, etc.
- Typicality

Dynamics of the typicality approach in a nutshell:

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

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

for very many $\hat{A}$

Typicality and ETH

Since $< \hat{A}(t) >= \sum_{nm} \langle n|\hat{\rho}(0)|m\rangle\langle m|\hat{A}|n\rangle e^{-i(E_m - E_n)t}$, if $< \hat{A}(t) >$ goes to a constant value at all it has to be $A^{eq} := \sum_n \langle n|\hat{\rho}(0)|n\rangle\langle n|\hat{A}|n\rangle$

How can A^{eq} be independent of the initial state $\hat{\rho}(0)$?

This can only hold if $\langle n|\hat{A}|n\rangle$ is independent of n: Eigenstate Thermalization Hypothesis (ETH). Why should this be the case?

For drawing states $|\psi\rangle$ at random one gets

$$HA(< A >) = \frac{1}{d}\text{Tr}\{\hat{A}\}, \quad HV(< A >) = \frac{1}{d+1}(\frac{\text{Tr}\{\hat{A}^2\}}{d} - \frac{\text{Tr}\{\hat{A}\}^2}{d^2})$$

There is a typical value of $\langle\psi|\hat{A}|\psi\rangle$

If eigenstates are "typical" (w.r.t. a certain observable) the ETH holds and relaxation to values largely independent from the initial state may be expected.

Non-perfect applicability of the ETH and "stick-effect"

How "bad" is it if the ETH does not perfectly apply? Parametrize initial state by c_α e.g. according to

$$\hat{\rho}(0) = \frac{1}{d}\hat{1} + \sum_\alpha c_\alpha \hat{A}_\alpha \quad \text{with} \quad \text{Tr}\{\hat{A}_\alpha\} = 0, \; \text{Tr}\{\hat{A}_\alpha \hat{A}_\beta\} = \delta_{\alpha\beta}$$

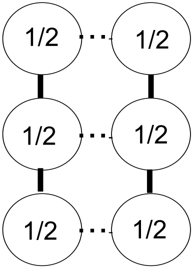
Consider e.g. the case $c_1 \neq 0$, all other $c_\alpha = 0$. Then one gets

$$< \hat{A}_1(0) >= c_1 \quad \text{and} \quad A_1^{eq} = c_1 \sum_n \langle n|\hat{A}_1|n\rangle^2$$

"stick-effect": If the ETH does not perfectly apply, observables tend to stick to their initial values, i.e. do not relax completely to their typical values.

Model and observables

spin-model



Heisenberg-type Hamiltonian:

$$\hat{H} = \sum_{ij} J_{ij}((\hat{\sigma}_x^i \hat{\sigma}_x^j + \hat{\sigma}_y^i \hat{\sigma}_y^j) + 0.6\ \hat{\sigma}_z^i \hat{\sigma}_z^j), \quad J_{ij} = 1 \text{ or } 0.15$$

conserves z-component of total magnetization:
$\hat{M}_z = \sum_i \hat{\sigma}_z^i$
analyzed variable: magnetization difference $\hat{x}$

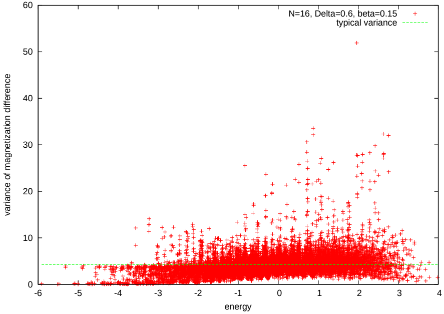
$$\hat{x} = \sum_{i \in L} \hat{\sigma}_z^i - \sum_{j \in R} \hat{\sigma}_z^j$$

eigenvalues of $\hat{x}$ within the $M_z = 0$ subspace:
$x_i = -\frac{N}{2}, -\frac{N}{2} + 2, \dots. + \frac{N}{2}$.
We concretely consider (for a start):
$\hat{A}_1 \propto \hat{x}$ (mean) and $\hat{A}_2 \propto \hat{x}^2 - \frac{\mathrm{Tr}\{\hat{x}^2\}}{d}$((deviation) of variance)

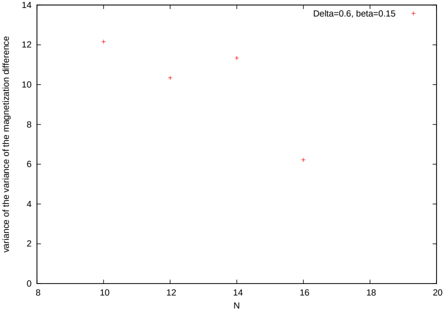
Stick-effect of magnetization difference

Stick-effect of mean magnetization difference: $\langle n|\hat{x}|n\rangle = \langle n|\hat{A}_1|n\rangle = 0$: perfect ETH by symmetrie. Stick-effect of variance of magnetization difference $\langle n|\hat{x}^2|n\rangle$

variances for $N = 16$



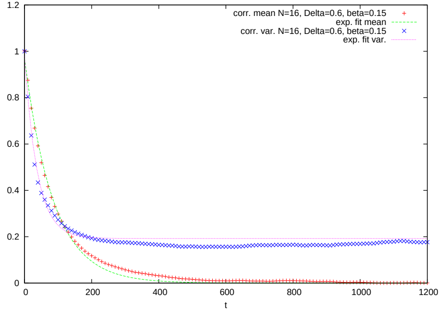
skaling of variances



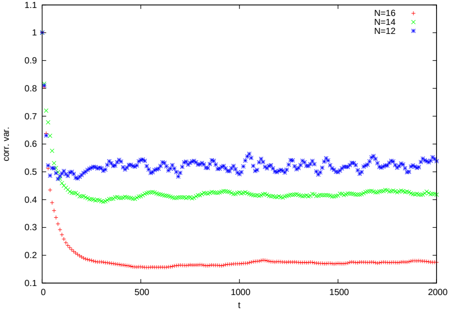
There is a non-negligible stick-effect for systems up to 16 spins. ETH applies much less acurately than for states drawn at random (eigenstates of random Hamiltonians). However, one may guess that the stick-effect vanishes for $N \to \infty$

In order to analyze the dynamics we compute the temporal correlation functions of mean and variance: $C_1(t) = \mathrm{Tr}\{\hat{A}_1(t)\hat{A}_1\}$ and $C_2(t) = \mathrm{Tr}\{\hat{A}_2(t)\hat{A}_2\}$

dynamics for $N = 16$



variance dynamics for various N



Up to the stick-effect there seems to be more or less exponential decay. The ratio of the relaxation rates of second to first moment of the magnetization difference ist found to be 2.2. How is that a signature of thermodynamic behavior in a more far reaching sense?

Consider a linear stochastic process, e.g. of the Ornstein-Uhlenbeck or Langevin type:

$$dX_t = -RX_t dt + D dW_t \quad \text{with} \quad \overline{dW_t dW_s} = \delta_{ts} dt$$

For this one gets

$$< x(t) >=< x(0) > e^{-Rt}, \quad < x^2(t) > -\frac{D^2}{2R} =< x^2(0) > e^{-2Rt}$$

That means: Numerics from the Schroedinger equation for this model indicate that the relaxation of the magnetization difference is (to some extend) in accord with the above stochastic proccess.

The end

Seems like some features of thermodynamics may be found in the quantum dynamics of a closed spin system.

Questions:

- How generic is this approach? Does it apply to all sorts of thermodynamics including things like the heat-death end of the universe?
- How may entropy be defined within such a scheme?
- What about fluctuation-theorems?
- ....and many more.

Thank you very much for your attention!