# Emergence of Irreversible Stochastic Behavior within Closed Finite Quantum Systems

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# Overview

Part I:
Example of the emergence of stochastic behavior: magnetization dynamics in a specific system comprising 32 spins (reasonably well established)

Part II:
Attempt to introduce a general non-equilibrium quantum entropy for closed systems (work in progress, (highly) speculative)

# Thermalization in closed quantum systems?

**(Non-eq.) Thermodynamics**

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

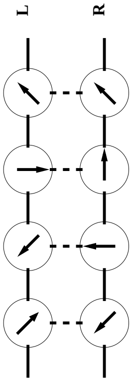
**Quantum Mechanics**

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

Quantum systems that show standard Fokker-Planck-type relaxation but are not of the "small system + large bath" type appear to be rare in the literature.

theme of this talk in a nutshell: Why and how do two cups of coffee thermalize each other?

**spin-model**




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

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

where $J_{ij} = 1$ for solid lines, $J_{ij} = \kappa = 0.2$ for dotted lines and $J_{ij} = 0$ otherwise. Total number of spins $N = 16, 32$. The $z$-component of total magnetization $S_z$ is conserved

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

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

eigenvalues of $\hat{x}$ within the subspace of vanishing total magnetization, $S_z = 0$: $X = -\frac{N}{4}, -\frac{N}{2} + 1, ..... + \frac{N}{4}$.

Assume there are rates at which mutual spin-flips, i.e., simultanous, contrariwise flips of adjacent spins occur. Let these rates be proportional to the square of the coupling constant between the adjacent spins.

Exploit local equilibrium due to time scale separation between leg-dynamics (fast) and rung-dynamics (slow) $\Rightarrow$

$$\text{Rates} \qquad R_{(X \to X \pm 1)} = \frac{\gamma \kappa^2 N}{2} \left( \frac{1}{2} \mp \frac{2X}{N} \right)^2$$

continuum limit, $N \to \infty, X \to \infty$, magnetization difference density $z := X/N$, Kramer-Moyal expansion:

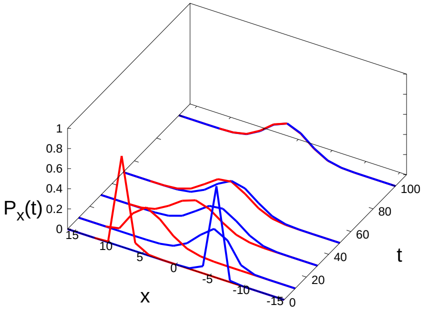
$$\partial_t p(t, z) = -\partial_z((-\partial_z U(z)p) + \frac{1}{2}\partial_z^2 (D(z)p) + \mathcal{O}(\partial_z^3)$$

$U(z) = \gamma\kappa^2 z^2$, $D(z) = \gamma\kappa^2(1/4 + 4z^2)/N$.

Almost like a Brownian particle in a parabolic potential.

# I: Numerically exact quantum description

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

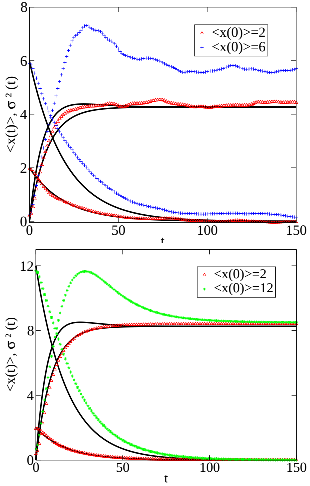



data from solving the Schroedinger equation ($N = 32$) for two pure, partially random initial states:

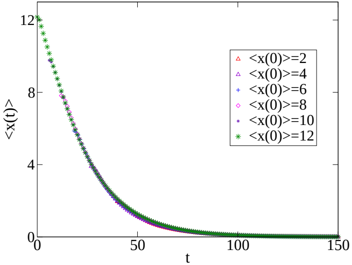
$$|\psi_X(0)\rangle = e^{-\alpha \hat{H}^2} \hat{P}_x \hat{P}(S_z = 0)|\omega\rangle,$$

(remark: taking this picture took 6h on 65 000 CPU's)

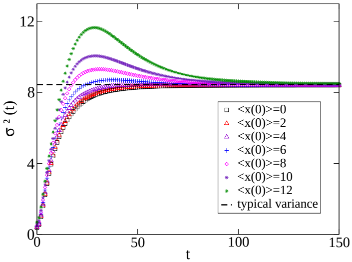
mean and variance of $x$ for $N = 16$ (top) and $N = 32$ (bottom)




Bigger is better ! (but only close to equilibrium) time shifted $\langle \hat{x}(t) \rangle$




variances of $x$

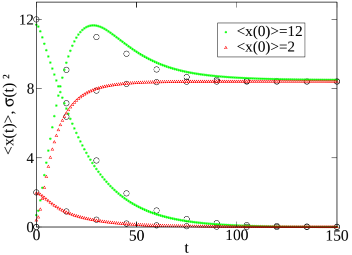



Is there any stochastic process with "autonomous $\langle \hat{x}(t) \rangle$-dynamics" that describes the quantum data at all?

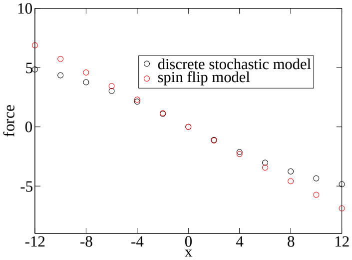
$$w_{XY}(\tau) := |\hat{P}_X e^{-i\tau\hat{H}}|\psi_Y\rangle|^2$$

$$\vec{P} := \{P_X\} \; W := \{w_{XY}\}$$

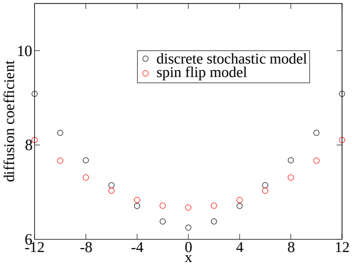
$$\vec{P}(n\tau) = W(\tau)^n \vec{P}(0)$$



# I: Comparison of naive and less naive models




"force": finite change of $\langle \hat{x}(t) \rangle$ during time $\tau = 15$ given that one started at some sharp $X$



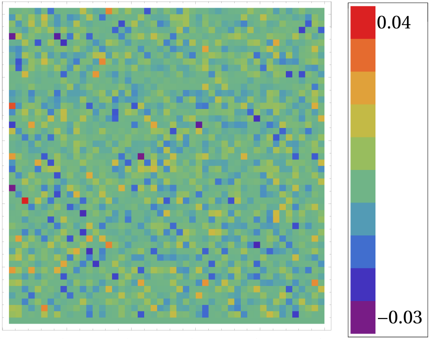

"diffusion coefficient": finite change of $\sigma^2(t)$ during time $\tau = 15$ given that one started at some sharp $X$

It can be shown that a Nakajima-Zwanzig-type projection approach with

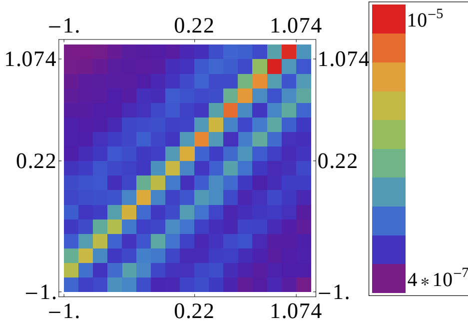
$$\mathcal{P}\hat{\rho} = \mathrm{Tr}\{\hat{P}_X \hat{\rho}\} \frac{\hat{P}_X}{\mathrm{Tr}\{\hat{P}_X\}} \quad \Rightarrow \mathcal{P}^2 = \mathcal{P}$$

yields to leading order the rates of the naive model (under the assumption of equal correlation times and time scale separation). However, unless you know that the transition matrix looks more or less random, that is not good enough. Better check:

“random” transition matrix elements




systematic coarse grained weights



# II: Thermodynamic entropy in quantum mechanics?

**Everybody is entitled to their own opinion!**
I would like to have (for a start):
0. Entropy to be defined in equilibrium and non-equilibrium.
1. Entropy defined as function that can be shown to be in some sense non-decreasing on the basis of some underlying theory (this is different from entropy being close to maximum on an endless time average).
2. Entropy as converging to the standard equilibrium value in standard physical scenarios.

**Some candidates:**

- Von Neumann I: $S^{I}_{VN} = -\text{Tr}\{\hat{\rho} \ln \hat{\rho}\}$. Does not change under unitary dynamics.
- "diagonal energy-Shannon": $S_{DS} = -\sum_n P_n \ln P_n$, $P_n := \langle n|\hat{\rho}|n\rangle$. Does not change in non-driven systems.
- Von Neumann II: $S^{II}_{VN} = -\sum_n \langle \hat{\Pi}_n \rangle \ln \frac{\langle \hat{\Pi}_n \rangle}{\text{Tr}\{\hat{\Pi}_n\}}$. Von Neumann shows: $S^{II}_{VN} \geq S^{I}_{VN}$. But $S^{II}_{VN}$ does not change in non-driven systems.
- "sum of parts entropy": $S_{SP} = -\sum_a \text{Tr}\{\hat{\rho}_a \ln \hat{\rho}_a\}$, $a$:"subsystems". Rigourously clear definition is lacking. No statement of the form $S(t_2) \geq S(t_1)$ if $t_2 \geq t_1$
- "fluctuation theorem inspired": $e^{\Delta S} = \frac{W_{if}}{W_{fi}}$. $i, f$: initial/final states. What precisely are these? What about 2. ?
- **Please add more !**

Choose a "level of observation" i.e., an (set of) observable $\hat{x} = \sum_n X_n \hat{\pi}_n$ such that: $\hat{\pi}_n = \hat{A}_n^+ \hat{A}_n$ and $\sum_n \hat{\pi}_n = \hat{1}$ (POVM-scheme)

probability to measure outcome $n$: $p(n) = \text{Tr}\{\hat{\rho}\hat{\pi}_n\}$

Assume that the dynamics of the quantum system is such that a sequence of past measurement outcomes determines a probability for a future measurement outcome:

$$p(l,(s+1)\tau) = \sum_{g,\ldots,j,k} w(l|g\ldots jk) p(k,s\tau \wedge j,(s-1)\tau \wedge \ldots\ldots \wedge g,(s-K+1)\tau)$$

e.g., $K = 1 \Rightarrow p(l,(s+1)\tau) = \sum_k w(l|k) p(k,s\tau)$

This implies two conditions on the quantum dynamics:
**1. consistency, 2. K-step Markovianity**

def.: label ordered sequences of $K$ measurements by greek letters, $\alpha, \beta, \ldots$, call them "macrostates".

$$d(\alpha) := \text{Tr}\{\hat{\pi}_k(0)\hat{\pi}_j(-\tau)\ldots\ldots\hat{\pi}_g(-K+1)\tau)\} \quad K = 1 : d(k) = \text{Tr}\{\hat{\pi}_k\}$$

If 1.,2. hold the following statements can be shown to result:

equilibrium distribution $$p_{eq}(\alpha) \propto d(\alpha) \quad (1)$$

fluctuation theorem $$\frac{w(\alpha|\beta)}{w(\beta|\alpha)} = \frac{d(\alpha)}{d(\beta)} = e^{(\ln(d(\alpha)) - \ln(d(\beta)))} \quad (2)$$

irreversibility $$L(t) := \sum_{\alpha} -p(\alpha) \ln p(\alpha) + p(\alpha) \ln d(\alpha). \quad (3)$$

This function $L(t)$ is strictly non-decreasing in time, i.e.,

$$L(t') \geq L(t) \quad \text{if} \quad t' \geq t$$

This motivates the definition of $S(\alpha) := \ln(d(\alpha))$ as a "system entropy". If $\sum_{\alpha} -p(\alpha) \ln p(\alpha)$ is considered a "lack of knowledge entropy", then (3) implies that the sum of the two entropies can never decrease. (1) is in accord with, typicality, eigenstate thermalization hypothesis, etc. (2) is in accord with Landauers principle.

Most of the material from Part I has been published. If you are interested in any references, ask me or simply visit our webpage.

The talk itself may also be found on our webpage.

# Thank you for your attention !