# Entropy increase in k-step Markovian, decoherent quantum dynamics

More work on a "tired old question" (Charles Bennett)

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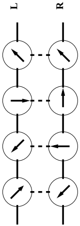
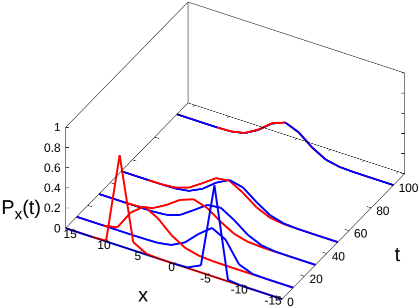
# “Irreversible” behavior in closed quantum systems: an example

anisotropc Heisenberg spin-ladder, weakly coupled leggs, $N = 32$




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

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




Data from solving the Schroedinger equation for two pure, partially random initial states! (H. de Raedt, K. Michielsen)

It is possible to find a positive (transition) matrix $W_{XY}$ such that

$$P_X((n+1)\tau) \approx \sum_Y W_{XY} P_Y(n\tau)$$

# 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: $S^{I}_{VN} = -\mathrm{Tr}\{\hat{\rho} \ln \hat{\rho}\}$. 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: $S^{II}_{VN} = -\sum_n \langle \hat{\Pi}_n \rangle \ln \frac{\langle \hat{\Pi}_n \rangle}{\mathrm{Tr}\{\hat{\Pi}_n\}}$. 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": $S_{SP} = -\sum_a \mathrm{Tr}\{\hat{\rho}_a \ln \hat{\rho}_a\}$, $a$:"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 !**

# My current concept of entropy, POVM's and consistency

This concept is not especially quantum. It just holds in the quantum case as well. Entropy is eventually taken to be a function of a sequence of measurements.

Measurements are represented by operators $\hat{A}_n$ (POVM's), such that: $\sum_n \hat{A}_n^+ \hat{A}_n = \hat{1}$

probability to measure $n$: $p(n) = \text{Tr}\{\hat{\rho}\hat{A}_n^+ \hat{A}_n\}$

def: $\mathcal{A}_n \hat{\rho} := \hat{A}_n \hat{\rho} \hat{A}_n^+$

post-measurement state $\hat{\rho}'$: $\hat{\rho}' = \frac{\mathcal{A}_n \hat{\rho}}{p(n)}$

def: $e^{-i\hat{H}t}\hat{\rho}e^{i\hat{H}t} := \mathcal{U}_\tau \hat{\rho}$

probability to measure the sequence $i, j, ...n$ at subsequent time-steps $\tau$: $p(ij..n) := \text{Tr}\{\mathcal{A}_n \mathcal{U}_\tau ... \mathcal{A}_j \mathcal{U}_\tau \mathcal{A}_i \hat{\rho}\}$

**assumption 1**: Sequences of measurements are decoherent, "consistent", etc. This means e.g.,

$$\text{Tr}\{\mathcal{A}_n \mathcal{U}_{2\tau} \mathcal{A}_i \hat{\rho}\} = \sum_j \text{Tr}\{\mathcal{A}_n \mathcal{U}_\tau \mathcal{A}_j \mathcal{U}_\tau \mathcal{A}_i \hat{\rho}\}$$

This relates to the third Kolmogorov axiom.

informal formulation:

probability to get first $i$ and later $n$ $= \sum_j$ probabilities to get first $i$ then $j$ then $n$

# Conditional (transition) probabilities

The consistency allows for the interpretation of the above expressions as conventional probabilities. The system dynamics does not depend on whether it is being watched. Unlike the double-slit, etc.

formulation of conditional probabilities:
def: $d(ij..k) := \mathrm{Tr}\{\mathcal{A}_k \mathcal{U}_\tau ... \mathcal{A}_j \mathcal{U}_\tau \mathcal{A}_i\}$
probability to measure $l$ given one has measured $i, j..k$ without any prior knowledge:

$$w(l|ij...k) = \frac{d(ij...kl)}{d(ij...k)}$$

This allows for a definition of k-step Markovianity:

e.g., 3-step $w(l|......ijk) = w(l|ijk)$ or 1-step $w(l|......ijk) = w(l|k)$

**assumption 2**: The system is $k$-step Markovian for all measurement sequences with $k$ being finite.

def: Label ordered sequences of $k$ measurements by greek letters, $\alpha, \beta, ...,$ call them "macrostates".
def: Let $w(\beta|\alpha)$ be the transition probability from $\alpha$ to $\beta$ through performing only **one** more measurement, regardeless of $k$, e.g.,
$w(\beta = jkl|\alpha = ijk) = w(l|ijk)$.

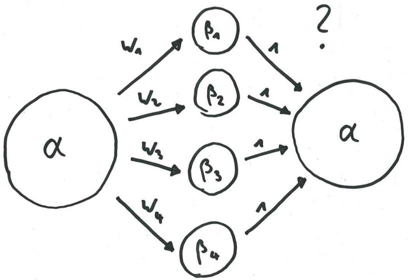
# Results: entropy definition and statement 1

def.: My currently favoured entropy: $S(\alpha) := \ln d(\alpha)$, $\alpha$ being the actual macrostate of the system.

statement 1.:

$$w(\beta|\alpha) \leq \frac{d(\beta)}{d(\alpha)} = e^{S(\beta)-S(\alpha)}$$

Unfortunately this does not yet imply irreversibility:



Fortunately there is a second statement.

# Results: statement 2, second law as a deal

statement 2.:
Introduce some normalized $d(\alpha)$ called $g(\alpha)$ through $g(\alpha) := \frac{d(\alpha)}{\sum_\beta d(\beta)}$
Consider the function $L(t)$

$$L(t) := \sum_\alpha -p(\alpha)\ln p(\alpha) + p(\alpha)\ln g(\alpha).$$

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 tells whether or not some dynamics is indeed irreversible.

My point of view on this: there are two types of entropy to be considered, "knowledge entropy" $S_k := \sum_\alpha -p(\alpha)\ln p(\alpha)$ and "mean system entropy" $\bar{S}_s := \sum_\alpha p(\alpha)\ln g(\alpha)$ so the above statement reads:

$$S_k(t') + \bar{S}_s(t') \geq S_k(t) + \bar{S}_s(t)$$

There is a trade-off: if knowledge entropy is supposed to shrink, mean system entropy has to rise. So in this sense the second law is a prize we have to pay for living in a predictable world..........back to physics!

statement 3.: Systems and sets of macrostates that fit into this scheme feature (unique) equilibrium probability distributions. Those are $p_{\text{eq}}(\alpha) = g(\alpha)$.

If the eigenstate thermalization hypothesis (ETH) would apply to the observable (say, on the energy shell to which the dynamics is restricted) i.e., e.g. for $k = 1$, $\langle i|\hat{A}_n^+ \hat{A}_n|i\rangle \approx \langle j|\hat{A}_n^+ \hat{A}_n|j\rangle$ and if furthermore the non-resonance condition would apply, then elementary quantum mechanics predict the same equilibrium probabilities. $\Rightarrow$ ETH and non-resonance condition are prerequisites for the above two assumptions to hold.

Landauer's principle as a consequence of statement 2: Consider erasure of one bit. Knowledge entropy before erasure: $S_k^i = \ln 2$. Knowledge entropy after erasure: $S_k^f = 0$. $\Rightarrow \Delta S_k = -\ln 2$. This requires $\Delta \bar{S}_s \geq \ln 2$. The easiest way to do this is by heating up some environment by work. $\Rightarrow \Delta W \geq T \ln 2$

**Thank you for your attention, I am looking forward to lively discussions!**

(This talk can be found on our webpage, I'll be happy to explain the proofs of the statements to anybody who is interested.)