Boltzmann entropy in quantum mechanics

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Gran Sasso Science Institute, 21 September 2021

Joint work, in part, with Shelly Goldstein, Joel Lebowitz, Cornelia Vogel, Stefan Teufel, and Nino Zanghì
Introductory paper: http://arxiv.org/abs/1903.11870

Plan of the talk

- Review of Boltzmann entropy in classical mechanics
- My reaction to Tim Maudlin's talk
- The quantum case

In classical mechanics: 2 definitions of entropy

Phase space Γ, e.g., $\Gamma = \mathbb{R}^{6N} = \{(\boldsymbol{q}_1, \boldsymbol{v}_1, \ldots, \boldsymbol{q}_N, \boldsymbol{v}_N)\}$
(symmetrized) volume measure $dx = N!^{-1} d^3\boldsymbol{q}_1 \, d^3\boldsymbol{v}_1 \cdots d^3\boldsymbol{q}_N \, d^3\boldsymbol{v}_N$

Gibbs entropy

$$S_{\mathrm{G}}(\rho) = -k \int_\Gamma dx \, \rho(x) \, \log \rho(x)$$

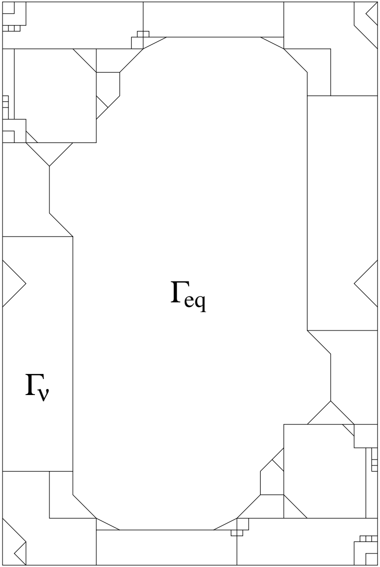
for ρ a probability density on Γ.

Boltzmann entropy

$$S_{\mathrm{B}}(X) = k \log \mathrm{vol}\, \Gamma(X)$$

for X a phase point in Γ, $\Gamma(X)$ = set of phase points that "look macroscopically the same" as X.

Classical mechanics: partition of phase space



- $\Gamma = \cup_\nu \Gamma_\nu$ "macro sets"
- Γ_ν = set of phase points that look like macro state ν
- Set $\Gamma(X) = \Gamma_\nu \ni X$, so

$S_{\mathrm{B}}(X) = S_{\mathrm{B}}(\nu) = k \log \mathrm{vol}\, \Gamma_\nu$

- Usually, in every energy shell $\Gamma_{\mathrm{mc}} = \{x : E - \Delta E < H(x) \leq E\}$ there is one macro state $\Gamma_\nu = \Gamma_{\mathrm{eq}}$ corresponding to thermal equilibrium and taking up $> 99.99\%$ of volume.

$S_{\mathrm{B}}(\mathrm{eq}) \approx k \log \mathrm{vol}\, \Gamma_{\mathrm{mc}} = S_{\mathrm{G}}(\rho_{\mathrm{mc}})$

- Generally, $S_{\mathrm{B}} \approx S_{\mathrm{G}}$ in local thermal equilibrium (including non-equilibrium stationary states).

Gibbs vs. Boltzmann entropy

But outside local thermal equilibrium, S_{B} is the more fundamental definition than S_{G}:

- Every system has an X but not a ρ.
- In thermal equil., ρ should mean a Gibbs ensemble. But outside?
- $\rho =$ an observer's knowledge or belief? (subjective)
- $\rho =$ preparation procedure?
- $\rho(x) \propto 1_{\Gamma(X)}(x)$? (An ideal observer's knowledge?)

Against subjective entropy

- Usually, we explain the fact that heat never flows from the cooler to the hotter by saying that this would decrease entropy. This explanation would not get off the ground if entropy were subjective:
- In the absence of observers, does heat flow from the cooler to the hotter?
- In the days before humans existed, did heat flow from the cooler to the hotter?
- If not, why would observers be relevant at all to the explanation of the phenomenon?
- As with explanation, so with prediction: Can we predict that heat will flow from the hotter to the cooler also in the absence of observers?
- If we don't know whether a pot is hot or cold, then

$$S_{\mathrm{G}}(\text{our knowledge}) = \tfrac{1}{2}S(\text{hot}) + \tfrac{1}{2}S(\text{cold}) + k\log 2.$$

  But in reality, the thermodynamic entropy is either $S = S(\text{hot})$ or $S = S(\text{cold})$. So $S \neq S_{\mathrm{G}}(\rho_{\text{subjective}})$.

Against $S_{\mathrm{G}}(\rho_{\text{preparation}})$

- Again: Prepare a pot with chance $\frac{1}{2}$ of being hot and chance $\frac{1}{2}$ of being cold. Then

$$S_{\mathrm{G}}(\rho_{\text{preparation}}) = \tfrac{1}{2}S(\text{hot}) + \tfrac{1}{2}S(\text{cold}) + k\log 2.$$

  But in reality, the thermodynamic entropy is either $S = S(\text{hot})$ or $S = S(\text{cold})$. So $S \neq S_{\mathrm{G}}(\rho_{\text{preparation}})$.
- $S_{\mathrm{G}}(\rho)$ quantifies the width of ρ but is independent of the physical properties of the phase points x it gives weight to.

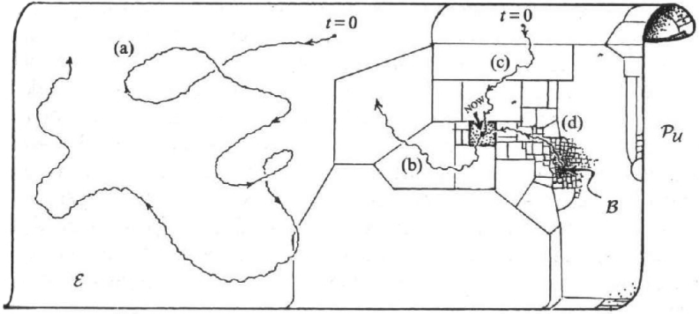
Against reference to an ideal observer

- Ex: Given a system with phase point $X \in \Gamma_\nu$, an ideal observer knows only the macro state ν, so $\rho(x) \propto 1_{\Gamma_\nu}(x)$.
- But then $S_{\mathrm{G}}(\rho) = S_{\mathrm{B}}(X)$, and there is no need to mention observers, or knowledge, or ρ.
- One could always use $S_{\mathrm{B}}(X)$ and add a narrative about beliefs of rational observers; but it would be irrelevant if observers' knowledge is irrelevant to which way heat flows.

Entropy increase, classically

- Hamiltonian flow $\Phi_t : \Gamma \to \Gamma$, $X_t = \Phi_t(X)$.
- Gibbs entropy does not increase: $S_{\mathrm{G}}(\rho_t) = S_{\mathrm{G}}(\rho_0)$ for $\rho_t = \rho \circ \Phi_{-t}$
- Boltzmann entropy usually does: Phase point typically moves to larger and larger macro sets Γ_ν.

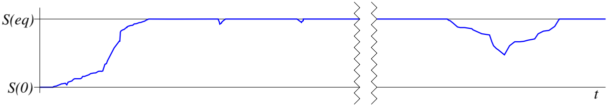
Drawing: R. Penrose



- Ex: Usually, Γ_ν is bigger than all smaller macro sets together, $\mathrm{vol}\,\Gamma_\nu \gg \mathrm{vol} \bigcup_{\nu'<\nu} \Gamma_{\nu'}$. Then, by Liouville's theorem, $\mathrm{vol}\{X \in \Gamma_\nu : S_{\mathrm{B}}(X_t) < S_{\mathrm{B}}(X)\} \ll \mathrm{vol}\,\Gamma_\nu$

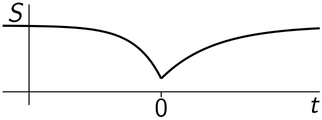
Entropy increases in both time directions

Given $\nu \neq \mathrm{eq}$, for most $X \in \Gamma_\nu$, $S_\mathrm{B}(X_t)$ increases in both time directions until it reaches the maximal value $S_\mathrm{B}(\mathrm{eq})$ (except possibly for entropy valleys that are infrequent, shallow, and short-lived). Once X_t reaches Γ_eq, it stays in there for $\sim 10^{10^{10}}$ years (except possibly for infrequent, shallow, and short-lived entropy valleys). In the long run, $S_\mathrm{B}(X_t)$ goes down again (due to Poincaré recurrence).



Theorem [Lanford 1976, Boltzmann 1872]

For a dilute hard sphere gas and large particle number, entropy increases in both time directions for most $X \in \Gamma_\nu$ for at least a short time.



So why does entropy increase in 1 direction only?

Because of a law of nature constraining the initial conditions of the universe:

Past hypothesis

The phase point of the universe at the initial time T_0 of the universe (the big bang) is typical in a certain macro set Γ_{ν_0}; ν_0 has very low entropy.

[Feynman 1965; Penrose 1979; Albert 2000]

("typical" $=$ behaves like most points in that set)

(Maybe it is helpful to avoid the word "probability.")

(Deeper explanations of the past hypothesis have been proposed by [Carroll et al. 2004; Barbour et al. 2013])

My reaction to Tim's talk

Tim's boundary entropy S_∂

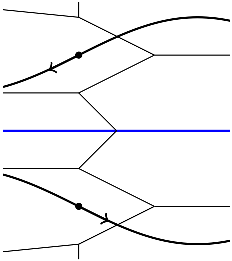
- TRUE: For reasonable entropy curves $t \mapsto S(t)$ to come out, it is necessary that the macro sets bordering on very small macro sets are small. It is equally necessary for $S_{\mathrm{B}} = k \log V$ and $S_\partial = k \log B(V)$. And it is actually the case for reasonable partitions of realistic examples.
- Claim of Tim's: For typical trajectories, S_∂ is higher than now in the future and lower in the past. (A past hypothesis is not needed.)
- That seems true in Hades as Tim described it.
- Is it true in stat mech phase space?
- I have 2 reservations:

Reservation 1

- velocity reversal mapping
  $R : \Gamma \to \Gamma$,

  $$R(\boldsymbol{q}_1, \boldsymbol{v}_1, \ldots, \boldsymbol{q}_N, \boldsymbol{v}_N) := (\boldsymbol{q}_1, -\boldsymbol{v}_1, \ldots, \boldsymbol{q}_N, -\boldsymbol{v}_N)$$

- It seems reasonable that $R\Gamma_\nu = \Gamma_{\nu'}$ for some ν'.
- Since R is volume-preserving and surface-area-preserving, $S_{\mathrm{B}}(RX) = S_{\mathrm{B}}(X)$ and $S_\partial(RX) = S_\partial(X)$.



- $(RX)_t = R(X_{-t})$, $S_\partial((RX)_t) = S_\partial(X_{-t})$.
- Thus, there are as many trajectories with decreasing $t \mapsto S_\partial(t)$ as with increasing.
- With a past hypothesis, this is not a problem. But without a past hypothesis, it conflicts with the claim that typical trajectories have increasing S_∂.

Reservation 2

- Lanford's 1975 theorem on the validity of the Boltzmann eq, together with Boltzmann's H theorem, shows that for most $X \in \Gamma_\nu$, $\nu \neq \mathrm{eq}$, S_{B} increases in both time directions (for at least a short time).
- Tim made it plausible that usually $S_\partial \approx S_{\mathrm{B}}$.
- Thus, it is plausible that for most $X \in \Gamma_\nu$, S_∂ increases in both time directions, contrary to the claim that typical trajectories have increasing S_∂.

In sum, I doubt that the past hypothesis can be avoided.

The quantum case

Entropy in quantum mechanics

- Hilbert space $\mathscr{H}$, unit sphere $\mathbb{S}(\mathscr{H}) = \{\psi \in \mathscr{H} : \|\psi\| = 1\}$
- Hamiltonian $\hat{H} = \sum_\alpha E_\alpha |\phi_\alpha\rangle\langle\phi_\alpha|$
- micro-canonical subspace

$$\mathscr{H}_{\mathrm{mc}} = \operatorname{ran} 1_{(E-\Delta E, E]}(\hat{H}) = \operatorname{span}\{\phi_\alpha : E - \Delta E < E_\alpha \leq E\}$$

Quantum analog of Gibbs entropy

von Neumann entropy $S_{\mathrm{vN}} = -k \operatorname{tr}(\hat{\rho} \log \hat{\rho})$, $\hat{\rho}$ = density matrix

Does not increase under unitary evolution. Like Gibbs entropy, applicable in thermal equil. (and non-eq. stationary states) but not always outside.

Quantum analog of Boltzmann entropy

Orthogonal decomposition $\mathscr{H} = \oplus_\nu \mathscr{H}_\nu$ into "macro spaces" $\mathscr{H}_\nu$
(replaces partition $\Gamma = \cup_\nu \Gamma_\nu$)
quantum Boltzmann entropy $S_{\mathrm{qB}}(\nu) = k \log \dim \mathscr{H}_\nu$

[Einstein 1914; von Neumann 1929; Griffiths 1994; Maes et al. 2006; Lebowitz 2008; Goldstein et al. 2010]

Properties of S_{qB}

- $\dim \mathscr{H}_{\mathrm{eq}} / \dim \mathscr{H}_{\mathrm{mc}} > 0.9999$ thermal equilibrium space
- So within $\mathscr{H}_{\mathrm{mc}}$, $S_{\mathrm{qB}}(\mathrm{eq}) = \max_\nu S_{\mathrm{qB}}(\nu)$.
- $S_{\mathrm{qB}}(\mathrm{eq}) \approx k \log \dim \mathscr{H}_{\mathrm{mc}} = S_{\mathrm{vN}}(\hat{\rho}_{\mathrm{mc}})$, which is known to yield the correct entropy value in thermal equilibrium
- So again, $S_{\mathrm{qB}} \approx S_{\mathrm{vN}}$ in thermal equilibrium
- S_{qB} is an extensive/additive quantity: 2 systems $\mathscr{S}_1, \mathscr{S}_2$, negligible interaction, $\mathscr{H} = \mathscr{H}_{\mathscr{S}_1 \cup \mathscr{S}_2} = \mathscr{H}_{\mathscr{S}_1} \otimes \mathscr{H}_{\mathscr{S}_2}$, $\nu = (\nu_1, \nu_2)$ with $\mathscr{H}_\nu = \mathscr{H}_{\nu_1} \otimes \mathscr{H}_{\nu_2}$. Then

$$S_{\mathrm{qB}}(\nu) = S_{\mathrm{qB}}(\nu_1) + S_{\mathrm{qB}}(\nu_2)\,.$$

Thermalization of closed quantum systems

Some references [Deutsch 1991; Tasaki 1998; Gemmer et al. 2004; Popescu et al. 2005; Goldstein et al. 2005; Reimann 2008; Rigol et al. 2008];

key words "canonical typicality" and "eigenstate thermalization hypothesis" (ETH).

- An individual, closed, macroscopic quantum system $\mathscr{S}$ in a pure state ψ_t that evolves unitarily will often behave as if in thermal equilibrium: relevant observables yield their thermal equilibrium values up to small deviations with probabilities close to 1.
- These works support the idea that the approach to thermal equilibrium need not have anything to do with an observer's ignorance. $\mathscr{S}$ is always in a pure state, so $S_{\mathrm{vN}} = 0$ at all times.
- An "individualist" version of approach to thermal equilibrium:

Theorem [Goldstein et al. 2010]

Consider $\dim \mathscr{H}_{\mathrm{mc}} \gg 1$, $\dim \mathscr{H}_{\mathrm{eq}} / \dim \mathscr{H}_{\mathrm{mc}} \approx 1$, either H with random eigenbasis or $\mathscr{H}_\nu$'s in random directions. Then $\forall \psi \, \forall \varepsilon > 0 \, \exists t > 0$: $\psi_t \in \varepsilon$-neighborhood of $\mathscr{H}_{\mathrm{eq}}$ (in fact, for *most* t in the long run).

- In two flavors: "macroscopic" thermal equilibrium (MATE) $\psi \in \mathscr{H}_{\mathrm{eq}}$ and "microscopic" thermal equilibrium (MITE) $\mathrm{tr}_{\mathrm{bath}} |\psi\rangle\langle\psi| \approx \hat{\rho}_{\mathrm{can}}$. [Goldstein et al. 2015]

Quantum past hypothesis

The wave function of the universe at the initial time T_0 of the universe (the big bang) is typical in the unit sphere of a certain macro space $\mathscr{H}_{\nu_0}$; $S_{\mathrm{qB}}(\nu_0)$ is very low.

Increase of quantum Boltzmann entropy (1)

Just as the classical macro sets Γ_ν have vastly different volumes, the quantum macro spaces $\mathscr{H}_\nu$ have vastly different dimensions, and as phase space volume is conserved classically, dimensions of subspaces are conserved under unitary evolution.

It follows, e.g., that if macro states ν follow an autonomous, deterministic evolution law $\nu \mapsto \nu_t$, then S_{qB} increases:

$$\text{if } e^{-i\hat{H}t}\mathscr{H}_\nu \subseteq \mathscr{H}_{\nu'}, \text{ then } S_{\mathrm{qB}}(\nu') \geq S_{\mathrm{qB}}(\nu).$$

Increase of quantum Boltzmann entropy (2)

- Most $\psi \in \mathscr{H}$ don't lie in any particular $\mathscr{H}_\nu$ but are a superposition of contributions from different $\mathscr{H}_\nu$.
- Different from the classical case, where every x lies in *some* Γ_ν.
- So, most ψ don't have an entropy value. They are in a superposition of different entropy values.
- It is natural to define the entropy operator

$$\hat{S} = \sum_\nu S_{\mathrm{qB}}(\nu)\, P_\nu$$

with P_ν the projection to $\mathscr{H}_\nu$.

What could it even mean to say that $\log \dim \mathscr{H}_\nu$ increases with time?

I will present some options.

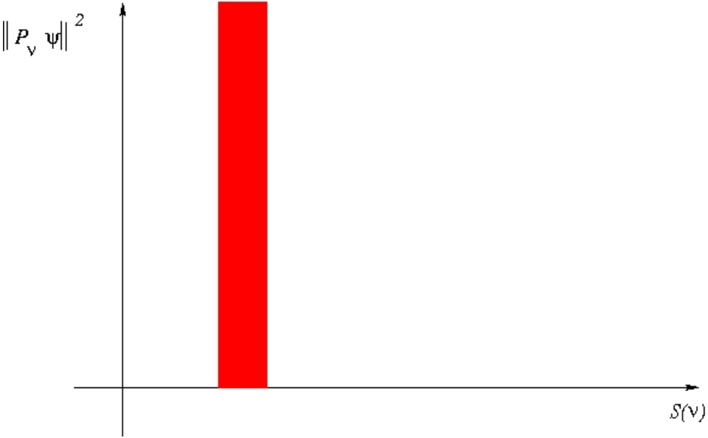
Right-moving distributions

- Every $\psi \in \mathbb{S}(\mathscr{H})$ defines a distribution weight $p_\nu = \|P_\nu \psi\|^2$ for each $\mathscr{H}_\nu$.
- Order macro states by their sizes: $\nu < \nu' \;\Leftrightarrow\; \dim \mathscr{H}_\nu < \dim \mathscr{H}_{\nu'}$
- Def: A distribution $\tilde{p}$ lies to the right of p ($p \preceq \tilde{p}$) $\quad :\Leftrightarrow$ $\forall \nu_0 : \;\sum_{\nu \geq \nu_0} p_\nu \leq \sum_{\nu \geq \nu_0} \tilde{p}_\nu$.
- Def: A family $p(t)_{0 \leq t \leq T}$ is right-moving $\Leftrightarrow \forall t_1 \leq t_2 : \; p(t_1) \preceq p(t_2)$.

Conjecture

In realistic cases and for most $\psi \in \mathbb{S}(\mathscr{H}_{\nu_0})$, $p(t) = \|P_\nu \psi_t\|^2$ is an (approximately) right-moving family up to the time T when ψ_T is mostly concentrated in $\mathscr{H}_{\mathrm{eq}}$.

Conjecture:



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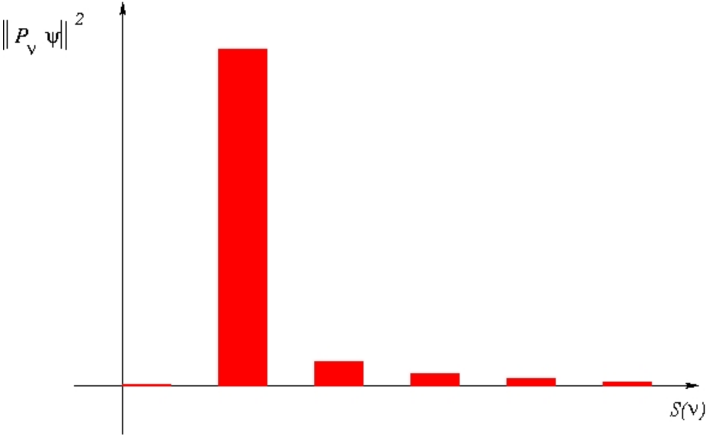

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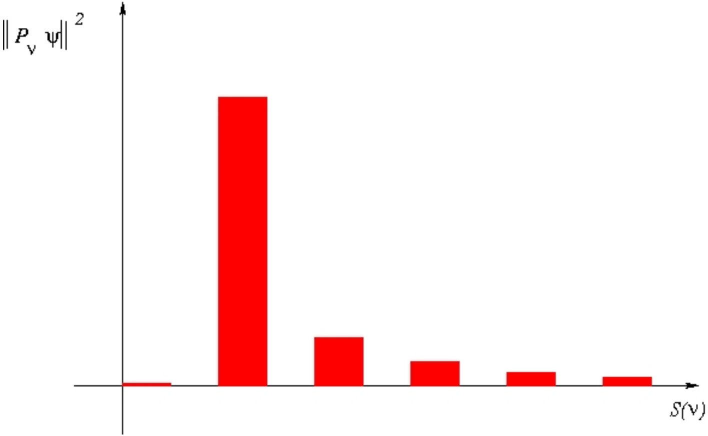

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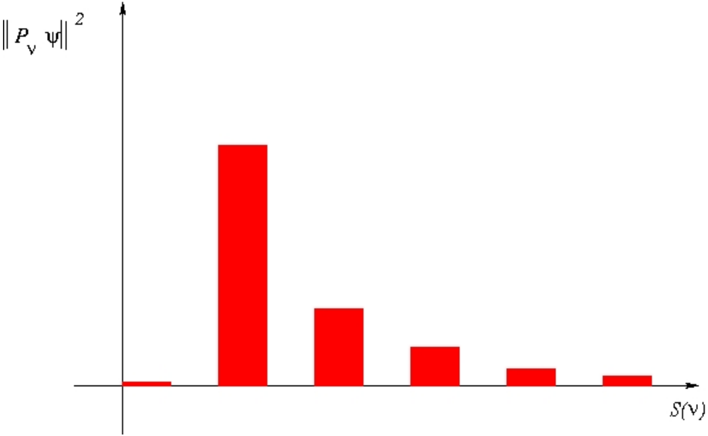

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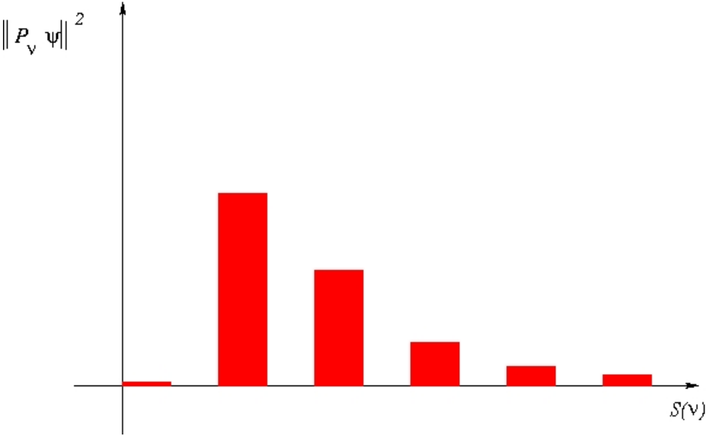

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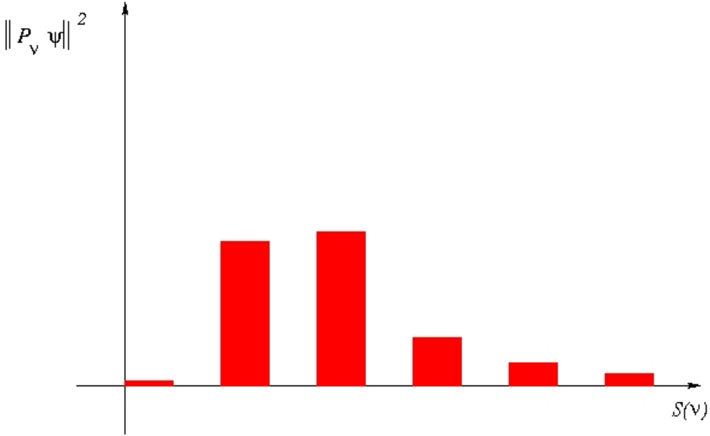

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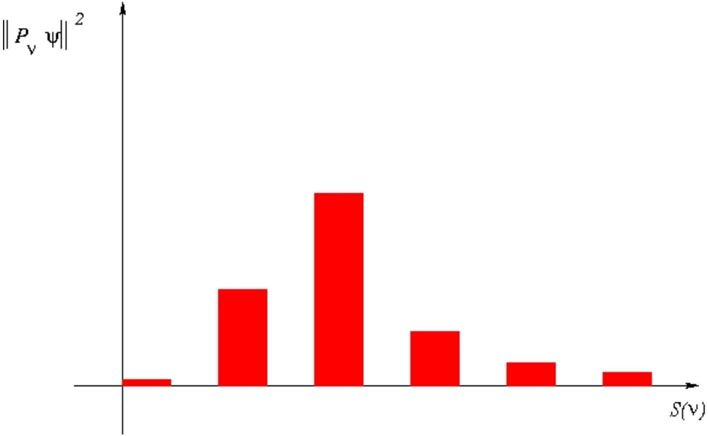

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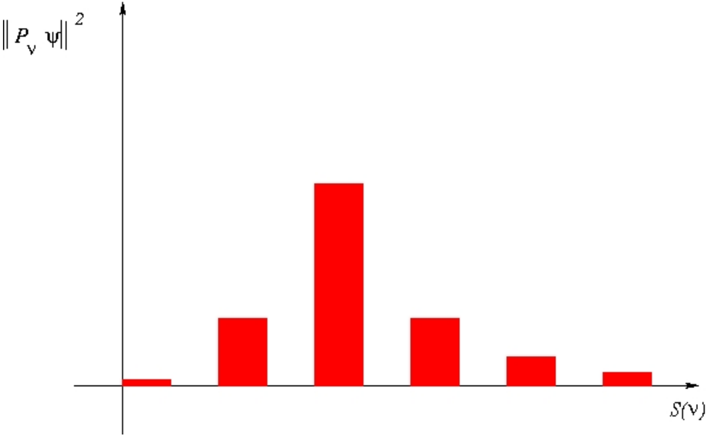

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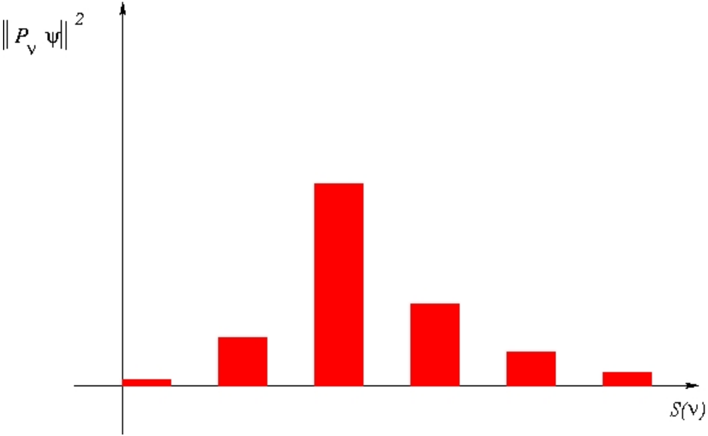

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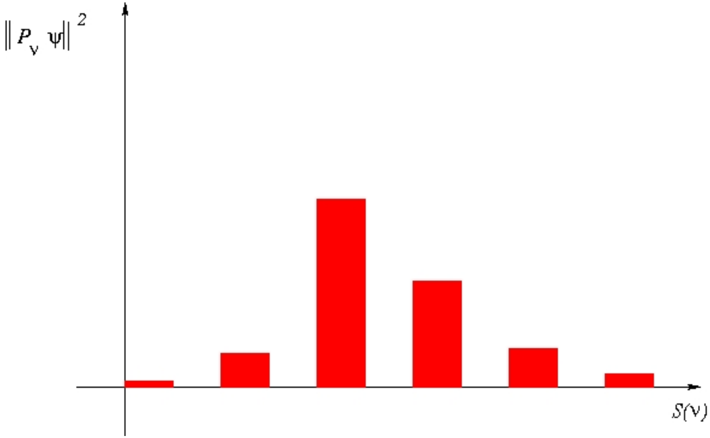

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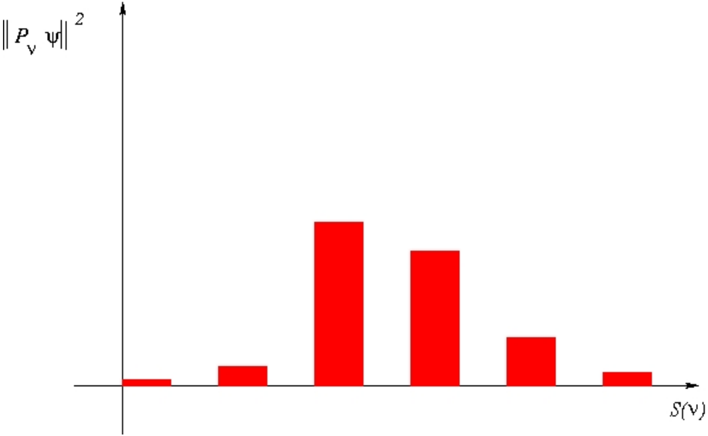

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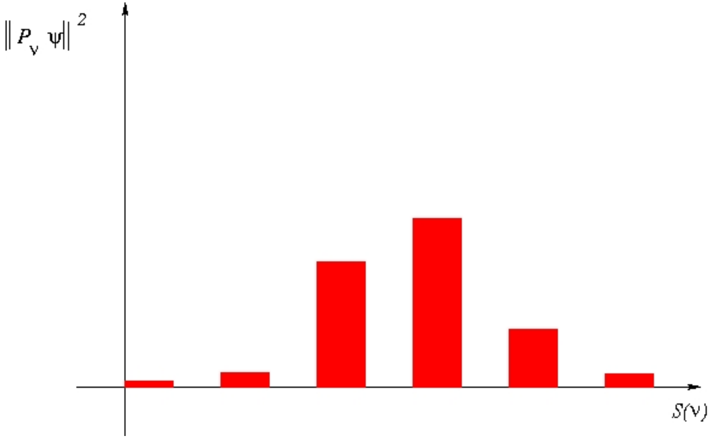

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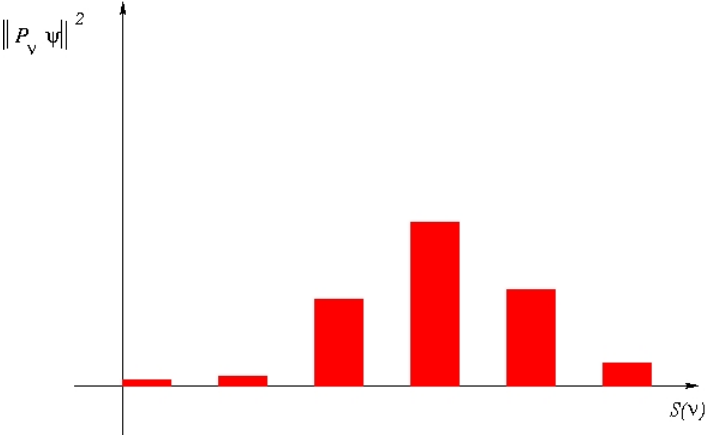

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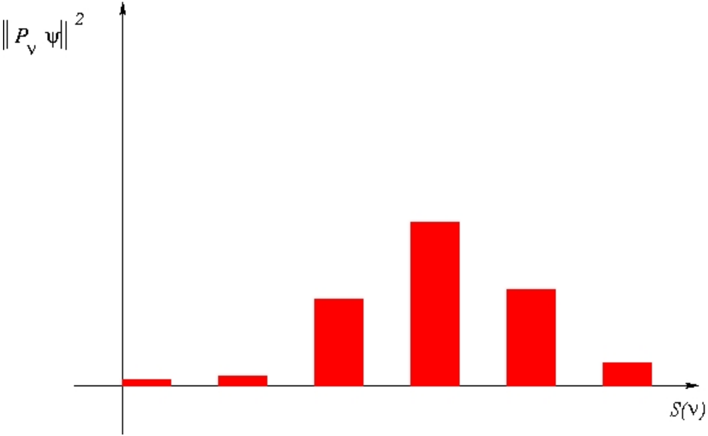

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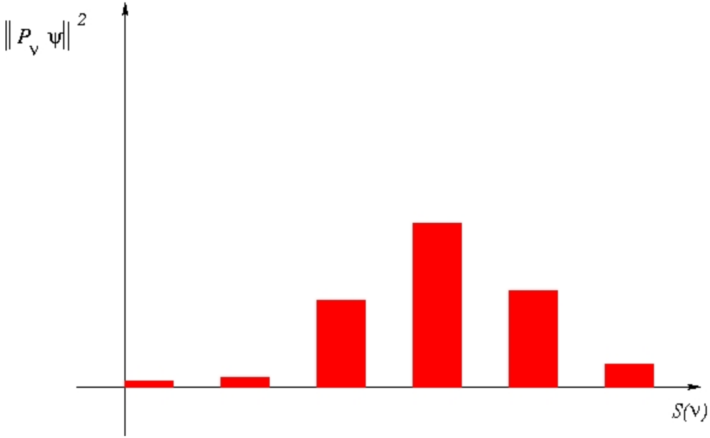

Macroscopic Superpositions

- For a macroscopic superposition ψ (e.g., Schrödinger's cat), most of us think that only one of the macroscopically different contributions corresponds to reality.
- Here, the foundations of stat mech meet the foundations of quantum mech.
- Copenhagen: unclear
- Everett: many worlds
- GRW: spontaneous collapse
- Bohm: particle positions AND wave function

Doesn't that define a history $t \mapsto S_{\mathrm{qB}}(t)$? Is it increasing?

In Bohmian mechanics,

there is a fact about whether Schrödinger's cat is alive:
$\psi = 2^{-1/2}\big(|\text{dead}\rangle + |\text{alive}\rangle\big)$ but $Q = Q_{\text{dead}}$ or $Q = Q_{\text{alive}}$. $Q \sim |\psi|^2$

$$S(Q,\psi) = S_\nu \quad \Leftrightarrow \quad Q \in \text{support}(P_\nu \psi)\,.$$

Q does not *always* select a unique macro state ν (and thus a unique entropy $S_{\mathrm{qB}}(\nu)$), but it does in practically relevant cases.

Let (Q_t, ψ_t) define a ν_t; then $t \mapsto \nu_t$ is a stochastic jump process whose Markovization should be close to

Bell's process [Bell 1986]

Given $\sum_x P_x = I$, define the Markov jump process X_t to have initial distribution $\text{Prob}(X_0 = x) = \langle \psi_0 | P_x | \psi_0 \rangle$ and jump rates

$$\sigma_t(x \to x') = \frac{2\,\mathrm{Im}^+ \langle \psi_t | P_{x'} H P_x | \psi_t \rangle}{\langle \psi_t | P_x | \psi_t \rangle}$$

Then $\text{Prob}(X_t = x) = \langle \psi_t | P_x | \psi_t \rangle$ for all t.

Set

$$R_{\nu\nu'}(t) = -iP_{\nu_0} e^{iHt}(P_\nu H P_{\nu'} - P_{\nu'} H P_\nu) e^{-iHt} P_{\nu_0} \,,$$

which is a self-adjoint operator.

Proposition

Suppose that whenever $\nu < \nu'$ and $t \in [0, T]$, the sum of positive eigenvalues of $R_{\nu\nu'}(t)$ far exceeds the absolute sum of negative ones. Then, for most $\psi \in \mathbb{S}(\mathscr{H}_{\nu_0})$ and with probability near 1, the Bell process for ν_t has increasing $S_{\mathrm{qB}}(\nu_t)$ (except possibly for infrequent, shallow, and short-lived entropy valleys).

The hypothesis may seem plausible if H is expected to have far more significant transition elements $\nu \to \nu'$ than $\nu' \to \nu$. It would be of interest to verify this hypothesis for some models.

Corollary

In that case, $p(t) = \|P_\nu \psi_t\|^2$ is (approximately) right-moving.

Consequence

In that case, S_{qB} predominantly increases along the Bohmian history.

Thank you for your attention