Typicality in Statistical Mechanics and the arrow of time

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Time flies like an arrow; fruit flies like a banana

– A. Oettinger

Statistical Mechanics

- Classical mechanics: reversible: Hamilton's equations:

$$\dot{q} = \partial_p H(q,p), \quad \dot{p} = -\partial_q H(q,p)$$

symmetric under $(q,p,t) \leftrightarrow (q,-p,-t)$.

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- Real world: irreversible. How is this possible?
- There are (very (**very!**)) many particles ($\gtrsim 10^{23}$).
- L. Boltzmann: random particle configurations (microcanonical ensemble), entropy:

$$S = k_B \log W.$$

Microcanonical Ensemble

- Phase space: N particles in 3D, in bounded set Ω:

$$(\mathbf{q}, \mathbf{p}) \equiv (q_1, \cdots, q_N; p_1, \cdots, p_N) \in \Omega^N \times \mathbb{R}^{3N}$$

- Hamiltonian:

$$H(\mathbf{q}, \mathbf{p}) = \sum_{i=1}^{N} \frac{1}{2m_i} \mathbf{p}_i^2 + V(\mathbf{q}).$$

- Energy shell: Fix ΔU small: for $U \in \mathbb{R}$:

$$\Sigma_U := \{(\mathbf{q}, \mathbf{p}) : \ H(\mathbf{q}, \mathbf{p}) \in [U - \Delta U, U + \Delta U]\}$$

- Uniform distribution on Σ_U: ρ_U: microcanonical distribution.

Microcanonical Ensemble

- Phase point of system: randomly sampled from the microcanonical distribution ρ_U.
- Can compute many quantities: e.g. ideal gas:

$$p = \frac{2U}{3V}$$

- Why does this work?

Unsatisfactory explanation number 1: Ergodicity

- Ergodicity and mixing: The trajectory under the Hamiltonian dynamics uniformly covers the energy shell:

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T dt\ f(\mathbf{q}(t),\mathbf{p}(t)) = \frac{1}{\mathrm{Vol}(\Sigma_U)}\int_{\Sigma_U} d\mathbf{q}d\mathbf{p}\ f(\mathbf{q},\mathbf{p})$$

left: time average, right: average over the microcanonical distribution.

- Problem: T needs to be extremely large in order to get anywhere near the limit: $\gtrsim 10^{10^{23}}$ s (life span of the universe: 4×10^{17} s).

Unsatisfactory explanation number 2: Uncertainty

- Uniform distribution because the observer does not know the exact state in phase space.
- Problem: fundamental theories cannot depend on the knowledge of observers.
- Would the entropy of a gas change if we knew the position of all its molecules?

Satisfactory explanation: Typicality

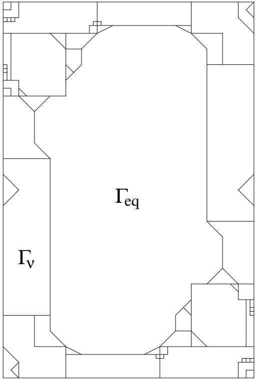
- Macroscopic observables: $M_1, \cdots, M_\ell$ (e.g. energy, pressure, volume, mass).
- M_i: coarse-grained functions on phase space (take discrete values (this is not really necessary, but it makes things easier)).
- $\Gamma_1, \cdots, \Gamma_\nu$: level sets of $\mathbf{M} \equiv (M_1, \cdots, M_\ell)$. That is, $\mathbf{M}$ is constant on the sets Γ_j.
- The Γ_j partition the energy shell:

$$\Gamma_1 \sqcup \cdots \sqcup \Gamma_\nu = \Sigma_U$$

- Γ_j: "Macrostate".

Typicality

- If 1 macrostate dominates the energy shell: Equilibrium Macrostate



Picture: [Goldstein, Lebowitz, Tumulka, Zanghì, 2019]

Typicality

- The points in the equilibrium macrostate are indistinguishable from a macroscopic point of view.
- Therefore, for all macroscopic observables M_i, and a point $(\mathbf{q}_0, \mathbf{p}_0) \in \Gamma_{\mathrm{eq}}$,

$$M_i(\mathbf{q}_0, \mathbf{p}_0) = \frac{1}{\mathrm{Vol}(\Gamma_{\mathrm{eq}})} \int_{\Gamma_{\mathrm{eq}}} d\mathbf{q} d\mathbf{p} \; M_i(\mathbf{q}, \mathbf{p}).$$

- If the macrostate is sufficiently large,

$$M_i(\mathbf{q}_0, \mathbf{p}_0) \approx \frac{1}{\mathrm{Vol}(\Sigma_U)} \int_{\Sigma_U} d\mathbf{q} d\mathbf{p} \; M_i(\mathbf{q}, \mathbf{p})$$

that is, the microcanonical average.

Typicality

- In summary: the microcanonical average of M_i is its value at a typical point, that is, a point whose M_i values are the same as for most points in the energy shell.
- Note: this is different from a random point of the energy shell. The point is not sampled from a distribution.
- This is called the "Individualist" point of view, as opposed to the "Ensemblist" view.
- Questions:
  - Is the choice of M_i and the coarse graining arbitrary?
  - Can one prove that one macrostate dominates?

Example: Boltzmann

- N spheres that collide elastically, at low density.
- Partition configuration space into ℓ boxes of volume V/ℓ. N_i: number of particles in box $i \in \{1, \cdots, \ell\}$.
- Fix a coarse graining length ΔM, and define the Macroscopic observables M_i as the occupation fraction of the i-th box, coarse grained over a length ΔM:

$$M_i := \left\lfloor \frac{N_i}{N \Delta M} \right\rfloor \Delta M$$

- As we will now argue, the equilibrium macrostate is that of constant density:

$$\Gamma_{\mathrm{eq}} := \{(\mathbf{q}, \mathbf{p}) : \ M_i = \tfrac{1}{\ell}\}.$$

Example: Boltzmann

- The probability distribution of N_i is binomial (either the particles go in the i-th box or they do not):

$$\mathbb{P}(N_i) = \binom{N}{N_i} \left(\frac{1}{\ell}\right)^{N_i} \left(1 - \frac{1}{\ell}\right)^{N-N_i}$$

- By the De Moivre-Laplace theorem, if $N \to \infty$ and $N_i \propto \frac{N}{\ell}$,

$$\mathbb{P}(N_i) \sim \frac{e^{-\frac{(N_i-\mu)^2}{2N\sigma^2}}}{\sqrt{2N\pi}\sigma}, \quad \mu := \frac{N}{\ell}, \quad \sigma^2 := \frac{1}{\ell}\left(1 - \frac{1}{\ell}\right)$$

Example: Boltzmann

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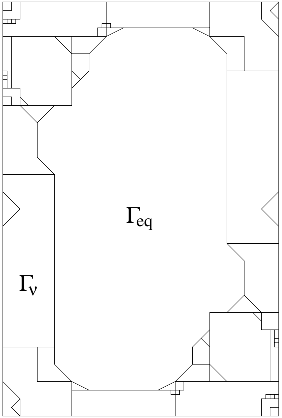
- So the probability that M_i deviates by more than ΔM is the probability that N_i deviates by more than $N\Delta M$, which is

$$1 - \int_{-N\Delta M}^{N\Delta M} dx \; \frac{e^{-\frac{x^2}{2N\sigma^2}}}{\sqrt{2N\pi}\sigma} \sim \frac{\sigma\sqrt{2}e^{-\frac{\Delta M^2 N}{2\sigma^2}}}{\Delta M\sqrt{N\pi}}$$

- Thus the probability that M_i deviates from $\frac{1}{\ell}$ is exponentially small in N. As N gets larger Γ_{eq} fills the energy shell, independently of the choice of ℓ or ΔM.

Irreversibility



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Irreversibility

- If the configuration is initially in the equilibrium macrostate Γ_{eq}, it will stay there for a very long time (infinite in the limit $N \to \infty$).
- If the configuration is initially in another Γ_j, it is likely to leave the small macrostate to go to a larger one.
- Defining the entropy of a state $(\mathbf{q}, \mathbf{p}) \in \Gamma_j$ by

$$k_B \log \mathrm{Vol}(\Gamma_j)$$

  entropy always increases.
- Question: can one prove this?

Quantum Statistical Mechanics

- Replace phase space with “states”: normalized wavefunctions ψ: uniquely defined up to a phase.
- Convenient analog of probability on state space: density matrix:

$$\rho = \sum_i c_i \left|\varphi_i\right\rangle \left\langle\varphi_i\right|, \quad \sum_i c_i = 1$$

  where $|\varphi_i\rangle$ is a basis of the Hilbert space and $|\varphi_i\rangle \langle\varphi_i|$ is the projector onto the basis element, and $c_i \geqslant 0$.

- Microcanonical density matrix: if $\mathcal{D}$ is the dimension of the Hilbert space.

$$\rho_{\mathrm{mc}} = \frac{1}{\mathcal{D}} \sum_i \left|\varphi_i\right\rangle \left\langle\varphi_i\right|$$

Quantum Typicality

- Given a density matrix ρ, the average of an observable A is

$$\langle A \rangle_\rho := \mathrm{Tr}(\rho A).$$

- "Pure state": corresponds to a single wavefunction

$$\rho_{\mathrm{pure}} = |\psi\rangle \langle\psi| \,.$$

- Macrostate: set of states, which yield the same coarse-grained values of macroscopic observables.
- Equilibrium macrostate: $\rho_{\mathrm{eq}} = |\psi_{\mathrm{eq}}\rangle \langle\psi_{\mathrm{eq}}|$ (pure state)

$$\mathrm{Tr}(\rho_{\mathrm{mc}} A) = \mathrm{Tr}(\rho_{\mathrm{eq}} A).$$

Further reading

S. Goldstein, J.L. Lebowitz, R. Tumulka, N. Zanghì - *Gibbs and Boltzmann Entropy in Classical and Quantum Mechanics*, Statistical Mechanics and Scientific Explanation, pp. 519-581, 2020
doi:10.1142/9789811211720_0014, arXiv:1903.11870.