Emergence of Thermal Equilibrium

Entanglement between System and Environment I

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Motivation

- discrepancy between quantum mechanics and emergent phenomena, thermodynamics
- First attempts to justify thermodynamics by quantum mechanics: **quantum statistical mechanics**.

What Are We Talking about?

- Entanglement between System and Environment I:
  Averaging over possible quantum states yields thermodynamics.
- Entanglement between System and Environment II:
  How can thermodynamics be derived without averaging and the a priori assumption of equipartition?
- Entanglement between System and Environment III:
  How is thermal equilibrium achieved?

Outline

Outline

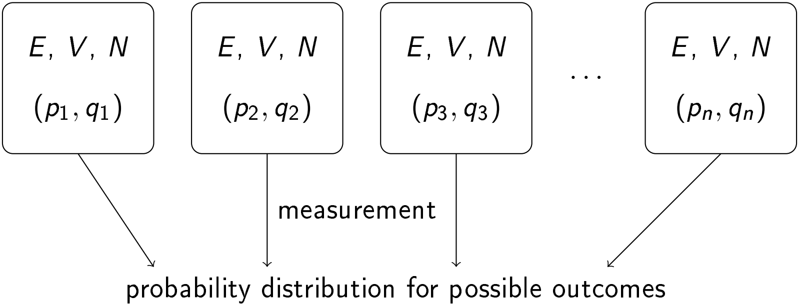
Definitions

Definition

An ensemble is a collection of systems with certain common macroscopic properties, but which are all in different states.
The ensemble average of a quantity is the average of this quantity over all systems in the ensemble.

Example

Microcanonical ensemble



The Microcanonical Ensemble

- E, V, N fixed
- **Postulate:** Every state compatible with E, V and N has the same probability.
- This yields a state density

$$\rho(p,q) = \begin{cases} \frac{1}{h^{3N} N!}, & \text{if } E < H(p,q) < E + \Delta \\ 0, & \text{otherwise.} \end{cases}$$

- Define the total number of states with energy between E and $E + \Delta$ by

$$\Gamma = \Gamma(E) = \int \mathrm{d}^{3N}p\, \mathrm{d}^{3N}q\, \rho(p,q)$$
$$= \frac{1}{h^{3N} N!} \int_{E<H(p,q)<E+\Delta} \mathrm{d}^{3N}p\, \mathrm{d}^{3N}q.$$

The Microcanonical Ensemble

- The quantity

$$S = k_B \log \Gamma$$

can be proven to be extensive and maximal for a closed system. It is thus identified with the **entropy**.

- We now get thermodynamics by defining

$$\frac{1}{T} = \left.\frac{\partial S}{\partial E}\right|_{V,N},$$

$$p = T \left.\frac{\partial S}{\partial V}\right|_{E,N},$$

$$\mu = T \left.\frac{\partial S}{\partial N}\right|_{E,V}.$$

The Canonical Ensemble

- System (E_A, V_A, N_A) in thermal contact with a large system (E_B, V_B, N_B) ("heat reservoir")
  - $(E_A, V_A, N_A) \ll (E_B, V_B, N_B)$
  - The composite system is isolated: $E \leq E_A + E_B \leq E + 2\Delta$, $E = const.$
  - V_A, V_B, N_A, N_B are constant.

The Canonical Ensemble

- For E_A, E_B fixed, we have $\Gamma(E) = \Gamma_A(E_A)\Gamma_B(E_B)$.
- In general:

$$\begin{aligned} \Gamma(E) &= \sum_{i=1}^{E/\Delta} \Gamma_A(E_i)\Gamma_B(E - E_i) \\ S(E) &= k_B \log \Gamma(E) \\ &\approx k_B \log \Gamma_A(\bar{E})\Gamma_B(E - \bar{E}), \end{aligned}$$

where $\Gamma_A(\bar{E})\Gamma_B(E - \bar{E})$ is the maximal summand of $\Gamma(E)$.

The Canonical Ensemble

- As $\bar{E} \ll E$, we can expand

$$\Gamma_B(E - \bar{E}) \approx const \cdot e^{-\bar{E}/k_B T_B}$$

- In equilibrium, $T_A = T_B \equiv T$.
- The probability for (p_A, q_A) with $H_A(p_A, q_A) = \bar{E}$ is proportional to $\Gamma_B(E - \bar{E})$.
- We get:

$$\rho(p, q) = \frac{1}{h^{3N} N!} e^{-H(p,q)/k_B T}$$

  and can define the **free energy** to be

$$F(V, T, N) = -k_B T \log Z_N(V, T),$$

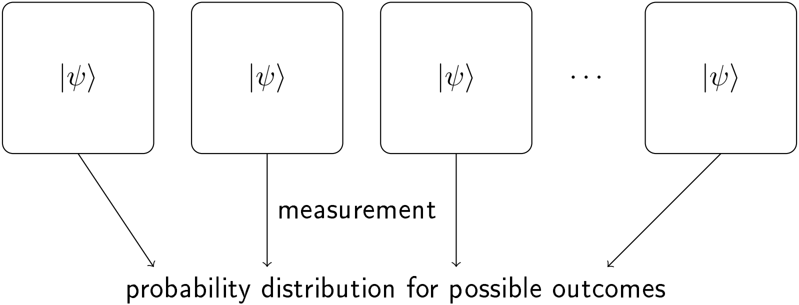
  where

$$Z_N(V, T) = \int \mathrm{d}^{3N} p \, \mathrm{d}^{3N} q \, \rho(p, q).$$

Outline

Quantum Statistical Mechanics

- Setup: A large number of systems all prepared **in the same quantum state**.
- **Quantum Statistics** describe the distribution of outcomes of a certain measurement on these systems.
- intrinsic uncertainty
- density function replaced by density operator ρ



A Theorem

Theorem

Let $\mathcal{H} \cong \mathbb{C}^n$ be a subset of the Hilbert Space for System A,
F an hermitian operator corresponding to some measurement on A.
Let $\mathcal{A}$ denote averaging over all $|\psi\rangle \in \mathcal{H}$. Then

$$\sqrt{\mathcal{A}[(\langle\psi|F|\psi\rangle - \frac{1}{n}\operatorname{tr} F)^2]} = \frac{1}{\sqrt{n+1}} \underbrace{\sqrt{\frac{1}{n}\operatorname{tr}(F^2) - \frac{1}{n^2}(\operatorname{tr} F)^2}}_{\leq \max_i |f_i|}.$$

Proof.

On the board. □

Meaning: Most of the states behave nearly like an ensemble when F is applied on them.

A Theorem

Corollary

Let $|\psi\rangle \in \mathcal{H} \cong \mathbb{C}^n$ *and a set of real numbers* $\{f_i\}_{i=1,\dots,n}$ *be fixed. Let* $\mathcal{B}$ *denote averaging over all possible orthonormal bases* $\{|e_i\rangle\}$ *of* $\mathcal{H}$*. Then*

$$\sqrt{\mathcal{B}[(\langle\psi|F|\psi\rangle - \frac{1}{n}\operatorname{tr} F)^2]} = \frac{1}{\sqrt{n+1}}\sqrt{\frac{1}{n}\operatorname{tr}(F^2) - \frac{1}{n^2}(\operatorname{tr} F)^2},$$

where $F = \sum_i f_i |e_i\rangle\langle e_i|$.

Proof.

Follows immediately from the proof of the theorem. □

Meaning: The majority of measurements performed on some state $|\psi\rangle$ yield nearly the same results as if applied on the ensemble corresponding to $\mathcal{H}$.

A Theorem

- Theorem and corollary also hold for higher moments: in particular, the standard deviation of the distribution is very close to the standard deviation of the ensemble.

Some Words on Ergodicity ...

- Bocchieri and Loinger also showed that the average over time behaves very similarly:
  The average over time and over all initial state vectors yields almost the same distribution as the ensemble, the standard deviation is small.
- **Upshot:** "[...] for the 'overwhelming majority' of the initial states of the system the distribution laws of quantum statistical mechanics hold at the 'overwhelming majority' of time instants."
- any measurement takes finite time: time average

Justification of the Microcanonical Ensemble

- System: E, V, N fixed (as before)
- $\mathcal{H} = \mathcal{H}_{E,E+\Delta} = \{|\psi\rangle : H|\psi\rangle = E'|\psi\rangle$, where $E \leq E' \leq E+\Delta\}$
- By the theorem, the distribution measured will be very close to the distribution predicted by the microcanonical ensemble for almost all $|\psi\rangle \in \mathcal{H}$, if $n \gg 1$.
- By the corollary, whatever state the system is in, most measurements will yield almost the same distribution as for the microcanonical ensemble.
- define entropy S, get thermodynamics

Justification of the Canonical Ensemble

- A small system (E_A, V_A, N_A) **interacts weakly** with a large system (E_B, V_B, N_B), so the interaction can be treated as a perturbation.
- $E \leq E_A + E_B \leq E + 2\Delta$
- The composite system is in an entangled state!
- **As we consider the small system only, we have to trace out the large system. This leads to a mixed state and we get our canonical ensemble!**

Outline

Summary

- For large systems in equilibrium, quantum statistics lead roughly to the same result as classical statistics: thermodynamics.
- This is shown by **averaging** over all possible states.
- **Disadvantages**:
  - not true for all states and all measurements
  - canonical case: weak-interaction assumption required
- **Outlook:**
  - new approach without averaging, without equiprobability postulate, based on entanglement alone
  - What happens if the system is not in equilibrium?

Literature

- P. Bocchieri, A. Loinger:
  Ergodic Foundation of Quantum Statistical Mechanics
- S. Lloyd:
  Chapter 3: Pure Quantum Statistical Mechanics and Black Holes
  in *Black Holes, Demons and the Loss of Coherence*
- K. Huang: *Statistical Mechanics*