

Physics 415 - Lecture 4

January 29, 2025

Summary of Classical Statistical Description

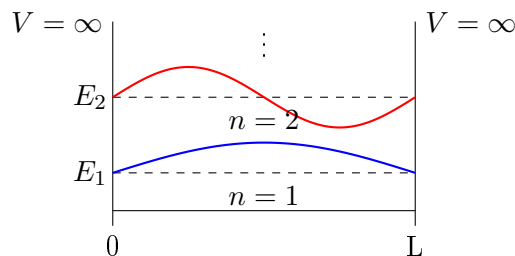
- Microstate (μ -state) \leftrightarrow Phase space cell (size h_0^S).
- **Fundamental Postulate:** An isolated system in equilibrium is equally likely to be in any of its accessible μ -states.
- Accessible states = μ -states compatible with given constraints (e.g., energy in $(E, E+\delta E)$).
- $\Omega(E)$ = number of accessible states.
- Probability of being in a specific accessible μ -state = $1/\Omega(E)$.

Quantum Mechanical (QM) Description

In QM, the main difference from the classical approach is in the identification of μ -states.

- In QM, the state of a system is described by a wave function Ψ .
- Such a quantum state may be specified by a set of "quantum numbers".

Example 1: 1D particle in a box (Length L , $V = \infty$ at boundaries).



The time-independent Schrödinger equation is:

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) = E\psi(x)$$

with boundary conditions $\psi(x=0) = \psi(x=L) = 0$. The solutions (stationary states or μ -states) are:

- Wave functions: $\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$
- Energies: $E_n = \frac{\hbar^2 \pi^2 n^2}{2mL^2}$
- Quantum number: $n = 1, 2, 3, \dots$ specifies the state.

Example 2: 1D harmonic oscillator. Schrödinger equation: $\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} kx^2\right) \psi = E\psi$.

- Allowed energies: $E_n = (n + \frac{1}{2})\hbar\omega$, where $\omega = \sqrt{k/m}$.
- Quantum number: $n = 0, 1, 2, \dots$ specifies the state.
- For a system of N decoupled oscillators, the quantum state is specified by N quantum numbers: $\{n_1, n_2, \dots, n_N\}$ with $n_i = 0, 1, 2, \dots$.

Example 3: Spin-1/2 particle. Consider a spin-1/2 particle, fixed in space (no translational DOF).

- The quantum state can be specified by the projection of spin along some axis (say z).
- Quantum number m can take values $m = \pm 1/2$.
- For N spin-1/2 particles fixed in space, the quantum state is specified by N quantum numbers: $\{m_1, m_2, \dots, m_N\}$ with $m_i = \pm 1/2$. There are 2^N possible states.

Fundamental Postulate in QM

In QM, the fundamental postulate is unchanged:

- If $\Omega(E) = \#$ of quantum states with energy in the range $(E, E + \delta E)$ (or exactly energy E if the spectrum is discrete and we consider degenerate states), then the probability that the system is in any particular accessible μ -state is $1/\Omega(E)$.

Example: Consider three spin-1/2 particles in equilibrium, in an external magnetic field H (along z). Assume the Hamiltonian only involves the interaction with the field. The energy of each spin depends on its m value:

$$\text{Energy} = \begin{cases} -\mu H & \text{if } m = +1/2 \\ +\mu H & \text{if } m = -1/2 \end{cases}$$

(μ is the magnetic moment). The μ -states are specified by $\{m_1, m_2, m_3\}$, and there are $2^3 = 8$ such states in total.

Now suppose the total energy of the system is known to be exactly $E_{\text{total}} = -\mu H$. What are the accessible states? The total energy is the sum of individual energies. We need $E_{\text{total}} = E_1 + E_2 + E_3 = -\mu H$. This requires two spins to be up ($m = +1/2$, energy $-\mu H$) and one spin to be down ($m = -1/2$, energy $+\mu H$). The accessible states are:

$$\{+1/2, +1/2, -1/2\}, \quad \{+1/2, -1/2, +1/2\}, \quad \{-1/2, +1/2, +1/2\}$$

There are 3 accessible states $\implies \Omega(E = -\mu H) = 3$.

Question: What is the probability that the first spin has $m_1 = +1/2$? We need to count the number of accessible states where $m_1 = +1/2$. These are the first two states listed above. $\Omega(E; m_1 = +1/2) = 2$. The probability is $P(m_1 = +1/2) = \frac{\Omega(E; m_1 = +1/2)}{\Omega(E)} = \frac{2}{3}$. Note also $P(m_1 = -1/2) = \frac{\Omega(E; m_1 = -1/2)}{\Omega(E)} = \frac{1}{3}$.

Question: What is the mean value of the magnetic moment (μ_z) of the first spin? The moment is $+\mu$ if $m_1 = +1/2$ and $-\mu$ if $m_1 = -1/2$.

$$\overline{\mu_{z,1}} = P(m_1 = +1/2)(+\mu) + P(m_1 = -1/2)(-\mu) = \frac{2}{3}(+\mu) + \frac{1}{3}(-\mu) = \frac{1}{3}\mu$$

Density of States

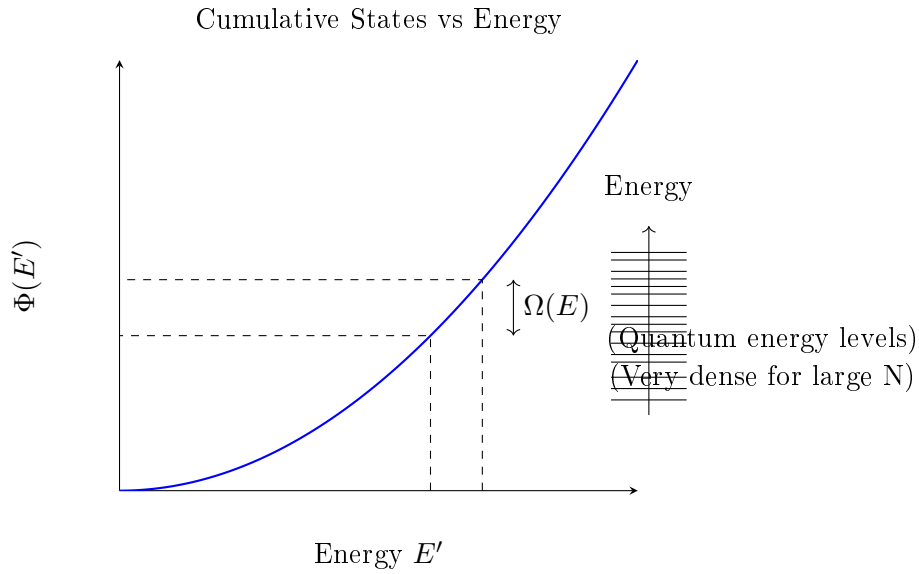
The number of accessible states $\Omega(E)$ plays a central role in statistical physics. We now examine its behavior, especially when the number of DOF becomes large ($N \gg 1$).

$\Omega(E) = \#$ of accessible states with energy in $(E, E + \delta E)$. Note that $\Omega(E)$ depends on the chosen energy "width" δE . It is useful to write:

$$\Omega(E) = \omega(E)\delta E$$

where $\omega(E)$ is the "density of states" (DOS) = $\#$ of states per unit energy range at energy E . $\omega(E)$ is independent of δE (assuming δE is small enough that $\omega(E)$ is roughly constant over the interval, but large enough to contain many states).

Another way to think about $\omega(E)$: Let $\Phi(E)$ = total $\#$ of states with energy $\leq E$.



When the number of particles is large, energy levels are very dense, and we can treat $\Phi(E)$ as a smooth function of E . Then $\Omega(E) = \Phi(E + \delta E) - \Phi(E)$. For small δE :

$$\Omega(E) \approx \frac{d\Phi(E)}{dE} \delta E$$

Comparing with $\Omega(E) = \omega(E)\delta E$, we have:

$$\omega(E) = \frac{d\Phi(E)}{dE}$$

Dependence of $\Omega(E)$ (or $\omega(E)$) on E and N

How does $\Omega(E)$ depend on energy E and number of particles N in a macroscopic system?

Example: Classical monatomic ideal gas.

- "Monatomic": particles have no internal DOF (like rotation or vibration).
- "Ideal gas": neglect interactions between atoms.

Consider N monatomic particles enclosed in volume V . The Hamiltonian is purely kinetic:

$$H(\vec{x}_1, \dots, \vec{x}_N, \vec{p}_1, \dots, \vec{p}_N) = \sum_{i=1}^N \frac{|\vec{p}_i|^2}{2m}$$

We want the number of states $\Omega(E)$ with energy in $(E, E + \delta E)$. This corresponds to the volume of phase space satisfying:

$$E \leq \sum_{i=1}^N \frac{|\vec{p}_i|^2}{2m} \leq E + \delta E$$

The phase space volume element is $d^3\vec{x}_1 \dots d^3\vec{x}_N d^3\vec{p}_1 \dots d^3\vec{p}_N$. The volume is:

$$\text{Vol}(E, \delta E) = \int_{E \leq H \leq E + \delta E} d^{3N}\vec{x} d^{3N}\vec{p}$$

The inequality defining the integration region only depends on momenta \vec{p}_i , not coordinates \vec{x}_i . The integral over coordinates gives:

$$\int d^3\vec{x}_1 \dots d^3\vec{x}_N = \left(\int d^3\vec{x} \right)^N = V^N$$

So, the phase space volume is:

$$\text{Vol}(E, \delta E) = V^N \int_{E \leq \sum \frac{p_i^2}{2m} \leq E + \delta E} d^{3N}\vec{p}$$

The integral is over the volume of a shell in $3N$ -dimensional momentum space. The condition $\sum_i \frac{|\vec{p}_i|^2}{2m} = \mathcal{E}$ defines a hypersphere. Let $P_i = \sqrt{2m\mathcal{E}_i}$ be related momenta, then $\sum P_i^2 = 2m\mathcal{E}$. The surface $\sum_{j=1}^{3N} p_j^2 = 2m\mathcal{E}$ corresponds to a sphere of radius $R = \sqrt{2m\mathcal{E}}$ in $3N$ -dimensional momentum space.

The volume of a D -dimensional sphere of radius R is $V_D(R) = C_D R^D$ for some constant C_D . Here $D = 3N$. The volume in momentum space with total energy $\leq \mathcal{E}$ is proportional to $(\sqrt{2m\mathcal{E}})^{3N} \propto \mathcal{E}^{3N/2}$. Let $\text{Vol}_p(\mathcal{E})$ be the volume of momentum space with energy $\leq \mathcal{E}$. $\text{Vol}_p(\mathcal{E}) = K \mathcal{E}^{3N/2}$ for some constant K . The volume of the shell between E and $E + \delta E$ is:

$$\text{Vol}_p(E + \delta E) - \text{Vol}_p(E) \approx \frac{d(\text{Vol}_p)}{dE} \delta E = K \left(\frac{3N}{2} \right) E^{3N/2-1} \delta E$$

So the phase space volume is $\text{Vol}(E, \delta E) \propto V^N E^{3N/2-1} \delta E$.

The number of states is this volume divided by the volume of a single cell (h_0^{3N} or simply h^{3N} if $h_0 = h$):

$$\Omega(E) \propto V^N E^{3N/2-1} \delta E$$

The density of states is:

$$\omega(E) = \frac{\Omega(E)}{\delta E} \propto V^N E^{3N/2-1}$$

For macroscopic systems, $N \sim 10^{23}$ is very large. In this limit $3N/2 - 1 \approx 3N/2$. The notes simplify this to:

$$\Omega(E) \propto V^N E^{3N/2} \delta E \quad (N \gg 1)$$

$$\omega(E) \propto V^N E^{3N/2} \quad (N \gg 1)$$

(Note: This captures the dominant dependence but ignores the -1 in the exponent derived above).

Key takeaway: $\Omega(E)$ (and $\omega(E)$) are extremely rapidly increasing functions of energy E . They also increase exponentially with the number of particles N . This is representative of the general situation for macroscopic systems. In general:

$$\omega(E) \sim E^{Na}$$

where a is a number of order 1 (e.g., $a = 3/2$ for the ideal gas).