

III Introduction to Statistical Physics

class schedule: March 26, 31

reading assignments: S15A-C,E; R6.2-6.3

examples marked with * are important and should be studied carefully.

III.1 Probabilities and Mean Values

III.1.1 Probability of a System in a Certain Energy State: the Classical Approach

The macroscopic behaviors of thermodynamic systems are determined by properties of the Avogadro number of particles collectively, which can be studied with statistical approaches.

For an isolated system in equilibrium, the probability for the system to stay in any of all accessible micro-states is the same, or an isolated system in equilibrium is equally likely to be found in any accessible micro-states. But when we start to look at a sub-system interacting with the rest of the system, such as a small system in thermal contact with a heat reservoir, or (in a classical approach) a gas particle interacting with the rest of gas particles, there is a probability distribution as a function of the energy state E_r of the small system, which is proportional to the number of micro-states of the rest of the system with energy $E_0 - E_r$.

Example 1: the motion of an individual gas particle in a 1D box is random and irregular, but at a given temperature (i.e., when the gas is in thermal equilibrium), we can study the probability of the single gas particle having a certain kinetic energy (or velocity).

Boltzmann factor and partition function: it can be proved that the probability of a system in a quantum energy state E_r is $P(E_r) \sim e^{-\beta E_r}$, or $P(E_r) = C e^{-\beta E_r}$, where C is a constant, $\beta \equiv 1/(kT)$, and $e^{-\beta E_r}$ is called *Boltzmann factor*. The sum of all probabilities has to be unity, $\sum_r P(E_r) = 1$, yielding $C = (\sum_r e^{-\beta E_r})^{-1}$. Particularly, $Z \equiv \sum_r e^{-\beta E_r}$ is called *partition function*.

In a particle system in equilibrium, the probability P_r of the system at a certain quantum state E_r can be considered to be equivalent to the ratio of the number of particles N_r having energy E_r to the total number of particles N , i.e., $P_r = N_r/N$. Note that this holds when there is no degeneracy.

Example 2: examples of energy distribution functions

III.1.2 Ratio of Probabilities and Mean Values

Given the probability distribution function, the ratio of the probabilities of any two states is given by

$$\frac{P_i}{P_j} = e^{-\frac{(\epsilon_i - \epsilon_j)}{kT}}$$

The mean value of any property y of the system can be calculated as

$$y_{mean} = \frac{\sum_i y_i e^{-\beta \epsilon_i}}{\sum_i e^{-\beta \epsilon_i}}$$

where $\beta = 1/(kT)$.

*Example 3: calculate the probability distribution of a system with quantized energy states $\epsilon = n\epsilon_0$, where $n = 0, 1, 2, \dots$: the probability of the system in the i th state is

$$P_i = \frac{e^{-i\epsilon_0/kT}}{\sum_{i=0}^{\infty} e^{-i\epsilon_0/kT}}$$

And the ratio of the probabilities of the system being in the i th and j th state is

$$\frac{P_i}{P_j} = e^{-(i-j)\epsilon_0/kT}$$

*Example 4: calculate the mean magnetism and magnetic energy of a spin particle system in thermal equilibrium (temperature T) with an external magnetic field B , and qualitatively discuss the mean magnetism and magnetic energy at high and low temperature limits. A spin particle, with the presence of an external magnetic field, can either spin up (with the magnetic moment μ parallel to the external field) or down (with the magnetic moment $-\mu$ anti-parallel to the external field). When spinning up, the magnetic energy is $\epsilon_+ = -\mu B$, and when spinning down, the interaction magnetic energy is $\epsilon_- = -(-\mu)B = \mu B$. Therefore, the probabilities of the particle spinning up or down is $P_+ = Ce^{\mu B/kT}$ and $P_- = Ce^{-\mu B/kT}$, where $C = (e^{\mu B/kT} + e^{-\mu B/kT})^{-1}$.

At very high temperature $kT \gg \mu B$, $P_+ \approx P_-$, and the mean magnetic energy $\bar{\epsilon} = P_+(-\mu B) + P_-\mu B \approx 0$, meaning that the thermal perturbation leads to random alignment of spin particles thus zero net magnetic energy or magnetism. At low temperature $kT \ll \mu B$, $P_+ \gg P_-$, and particles are nearly all aligned along the external field, giving rise to the lowest magnetic energy $\bar{\epsilon} \approx -\mu B$ and maximum magnetization.