

1. States of a Model System

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- Mechanics tells us the meaning of work; thermal physics tells us the meaning of heat.
- Three new quantities in thermal physics but do not appear in ordinary mechanics: entropy, temperature, and free energy.
- The **multiplicity** (degeneracy) of an energy level: number of quantum states with very nearly the same energy.
- A quantum state of the system is a state of all particles; quantum states of a one-particle system are called **orbitals**.
- The energy of an orbital of a free particle with 3 positive integral quantum numbers n_x, n_y, n_z :

$$E = \frac{\hbar}{2M} \left(\frac{\pi}{L}\right)^2 (n_x^2 + n_y^2 + n_z^2)$$

- Binary model system: in a distinct site, an elementary magnet either points up or down, corresponding to magnetic moments $\pm m$.
- Listing every distinct state of the system:

$$(\uparrow_1 + \downarrow_1)(\uparrow_2 + \downarrow_2) \cdots (\uparrow_N + \downarrow_N) \quad (1)$$

- Total magnetic moment (M) of N magnets each of magnetic moment m:

$$M = Nm, (N-2)m, (N-4)m, \dots, -Nm$$

- # of states with magnets up: $N_{\uparrow} = \frac{1}{2}N + s$ (s is an integer)
- # of states with magnets down: $N_{\downarrow} = \frac{1}{2}N - s$ (s is an integer)
- **spin excess** (the difference): $N_{\uparrow} - N_{\downarrow} = 2s$
- **multiplicity function**: $g(N, s)$, # of states having $N_{\uparrow} = \frac{1}{2}N + s$ magnets up and $N_{\downarrow} = \frac{1}{2}N - s$ magnets down, for a system of N magnets:

$$g(N, s) = \frac{N!}{(\frac{1}{2}N + s)!(\frac{1}{2}N - s)!} = \frac{N!}{N_{\uparrow}!N_{\downarrow}!} \quad (2)$$

- $g(N, s)$ is the number of states having the same value of s .
- then eq. (1) can be expressed as (similar to binomial expansion):

$$(\uparrow + \downarrow)^N = \sum_{s=-\frac{1}{2}N}^{\frac{1}{2}N} g(N, s) \uparrow^{\frac{1}{2}N+s} \downarrow^{\frac{1}{2}N-s}$$

- The total number of states is given by:

$$\sum_{s=-\frac{1}{2}N}^{\frac{1}{2}N} g(N, s) = 2^N \quad (3)$$

- To work with big N , we use log to simplify calculation. From eq. (2):

$$\log(N, s) = \log N! - \log\left(\frac{1}{2}N + s\right)! - \log\left(\frac{1}{2}N - s\right)! = \log N! - \log N_{\uparrow}! - \log N_{\downarrow}! \quad (4)$$

- Using **Stirling approximation** we can rearrange eq. (4) to evaluate the logarithms (derivation shown in KK p.19). In the limit $s/N \ll 1$, with $N \gg 1$, we have the **Gaussian approximation** as a distribution of values of s :

$$g(N, s) \cong g(N, 0) \exp(-2s^2/N)$$

where

$$g(N, 0) \cong (2/\pi N)^{1/2} 2^N$$

- **average value** of a function $f(s)$ over a probability distribution function $P(s)$:

$$\langle f \rangle = \sum_s f(s) P(s)$$

where distribution function is normalized to unity:

$$\sum_s P(s) = 1$$

- To normalize eq. (2) using its property eq. (3), we define:

$$P(s) = g(N, s)/2^N$$

- Some mean values: $\langle s^2 \rangle = \frac{1}{4}N$, $\langle (2s)^2 \rangle = N$ (mean square spin excess)
- **fractional fluctuation** in $2s$:

$$\mathcal{F} \equiv \frac{\langle (2s)^2 \rangle^{1/2}}{N} = \frac{1}{\sqrt{N}}$$

The fractional fluctuation is smaller as N becomes larger, which means that the central peak of the distribution function becomes relatively more sharply defined as the size of the system increases.