Lecture 1: Introduction

Naoki KAWASHIMA

ISSP, U. Tokyo

April 8, 2024

In this lecture, we see ...

- Historically, the statistical mechanics was developed by Boltzmann to explain macroscopic phenomena from the 1st principle, i.e., Newton's law, Schrödinger equation, etc.
- However, many cooperative phenomena seem to have good explanation **without** referring to the 1st principles.
- The essential macroscopic properties can be understood by models in terms of intermediate-scale degrees of freedom.
- Often the same model can describe the essence of multiple phenomena with completely different microscopic origins.
- These observations are reflecting the **universality of many-body systems**.
- In particular, the universality holds exactly in the critical phenomena. (**universality of critical phenomena**)

Very brief review of conventional statistical mechanics

- **Equi-probability principle:** $P(S)$ is constant independent of S.
- **Micro-canonical ensemble:** $P(S|E) = \delta_{E,E(S)}/W(E)$
- **Equilibrium with heat-bath:** (A: the system, B: the heat-bath)

$$P_{AB}((S_A, S_B)|E) = \delta_{E,E_A(S_A)+E_B(S_B)}(W_{AB}(E))^{-1}$$
$$P_A(S_A) = \sum_{S_B} \frac{\delta_{E,E_A+E_B}}{W_{AB}(E))} = \frac{W_B(E - E_A(S_A))}{W_{AB}(E)}$$

- **Entropy and temperature:**

$$S(E) = \log W(E) \text{ (extensive)}, \quad \beta \equiv 1/T \equiv \frac{\partial S}{\partial E} \text{ (intensive)}$$

- **Canonical ensemble:**

$$P_A(S_A) \propto e^{-\beta_B E_A(S_A)}$$

Phenomena described by or related to Ising model

- Ferromagnetism ... exchange coupling
- Ferroelectrics ... optical phonon
- Binary alloys ... change in band structure
- Gases ... van der Waals force
- Voters' decision making model ... human psychology
- Percolation ... trees catching fire
- Potts model ... generalization to higher symmetry

Ferromagnets

For a ferromagnetic insurator, the magnetic contribution to the total energy can be (at least approximately) written as

$$\mathcal{H} = -\sum_{ij} \sum_{\alpha,\beta=x,y,z} J_{\alpha\beta} \boldsymbol{S}_i^\alpha \boldsymbol{S}_j^\beta - D \sum_i (\boldsymbol{S}_i^z)^2 - H \sum_i \boldsymbol{S}_i^z \tag{1}$$

where $\boldsymbol{S}_i^\alpha$ is a generator of SU(2) algebra in some irreducible representation characterized by the magnitude of spin $S = 1/2, 1, 3/2, \cdots$. The coupling constant $J_{\alpha\beta} = J\delta_{\alpha\beta}$ for isotoropic coupling. For some magnets, the anisotropy is easy-axis type and D is positive, in which case, only two states, $S_i^z = \pm S$, are important. As a result of these, in some cases one may consider the Ising model

$$\mathcal{H}_I = -J \sum_{(ij)} S_i S_j - H \sum_i S_i \tag{2}$$

represents the ferromagnet at least qualitatively.

Gases — Real gas

Real gas is described by Schrödinger equation,

$$\mathcal{H}\Psi(\boldsymbol{x}_1, \boldsymbol{x}_2, \cdots, \boldsymbol{x}_N) = E\Psi(\boldsymbol{x}_1, \boldsymbol{x}_2, \cdots, \boldsymbol{x}_N). \tag{3}$$

The Hamiltonian consists of the kinetic energy and the two-body Coulomb interactions among nuclei and electrons.

$$\mathcal{H} \equiv \sum_i \frac{\boldsymbol{p}_i^2}{2m_i} + \sum_{(ij)} V(\boldsymbol{x}_i, \boldsymbol{x}_j). \tag{4}$$

Gases — Lenard-Jones model

- In some circumstances, we can neglect quantum nature of atoms and treat them as classical particle with no internal degree of freedom (e.g., gas-liquid transition at room temperature).
- In such cases, we consider a classical model, such as Lenard-Jones (LJ) model

$$V_{\mathrm{LJ}}(\boldsymbol{x}, \boldsymbol{x}') = 4\epsilon \left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right) \tag{5}$$

where $r \equiv |\boldsymbol{x} - \boldsymbol{x}'|$.

Gases — Lattice gas

- We may simplify the system even further when we focus on the nature of phase transitions.
- For example, by discretizing the space and neglecting the long-range tail of the Lenard-Jones potential, we obtain the lattice gas model

$$\mathcal{H} = -\epsilon \sum_{ij} n_i n_j - \mu \sum_i n_i \tag{6}$$

where $n_i = 0, 1$ represents absense/presense of a particle at the site i. (One can easily verify that this is mathematically equivalent to the Ising model with a uniform magnetic field.)

Voters' decision making model

- We consider a group of voters behaving in the following way:
  1. Everyone is wondering whether he should vote for Biden or Trump.
  2. Everyone is showing his current preference by wearing a blue cap (for Biden) or a red one (for Trump).
  3. At each time t, everyone is looking around himself, and observe the current average preference $m(t)$ ($-1 \leq m \leq 1$, $m = 1$ for perfect preference for Biden and $m = -1$ for Trump).
  4. Observing $m(t)$ influences him in deciding his next preference: the color of his cap next time is blue with probability $(1 + \tanh(\beta m(t)))/2$ where β is a constant representing vorters' sensitivity to others' opinions.
- Then, we can show that $m(t)$ obeys the following equation of motion:

$$m(t+1) = \tanh(\beta m(t)) \tag{7}$$

  This is exactly identical to the equation of motion of the magnetization of the Ising model.

Universality

- The magnet, the gas, and the voters may behave according to the same model.
- This observation shows that completely different microscopic mechanisms may lead to an identical statistical mechanical model, and the microscopic mechanism influences the macroscopic properties only through a few parameters. This is a manifestation of the **universality**, one of the major subject of the present course.
- Moreover, when we focus on the critical phenomena, one can infer even the **exact** values of real systems from a very simplified model. For example, the value of the critical index β is estimated for the lattice-gas model to be $\beta \approx 0.3272$, and the experimental result can be fit well by assuming this estimate.
- This observation is an example of the **universality of critical phenomena**.

Percolation

- Statistical mechanics applies to phenomena whose microscopic elements are not really microscopic
- Phenomena with completely different microscopic origin can be described by the same (type of) model

Forest fire and percolation

- In a forest fire, a tree catches fire from a burning tree in its neighborhood. An important question is whether there is a big cluster of trees in which they are close to each other.
- Suppose the forest is a square lattice and that a tree is planted with probability p on each lattice point.
- Let us call the two trees are "connected" when they are nearest neighbors to each other.
- How big is the largest cluster of connected trees? (**site-percolation** problem)
- In the **bond-percolation**, every lattice point has a tree, but they are connected only with probability p.
- The largest cluster size is an increasing function of p.
- The function has a singular point at $p = 0.5$. Above this point, the largest cluster is infinity and remains finite below this point. (**percolation transition**).

Average cluster size in percolation

- Let us consider the average cluster size defined by

$$\overline{V_c} \equiv \left\langle \frac{\sum_c V_c^2}{\sum_c V_c} \right\rangle = \frac{1}{N} \left\langle \sum_c V_c^2 \right\rangle, \tag{8}$$

  where V_c is the volume (the number of lattice points) of the connected cluster c in G.
- The angular bracket denotes the statistical average,

$$\langle Q(G) \rangle = \frac{\sum_G W(G) Q(G)}{\sum_G W(G)} \tag{9}$$

  where the summation runs over all possible graphs.

Generating function of bond percolation

- The weight $W(G)$ is expressed formally as

$$W(G) = p^{|G|}(1-p)^{N_\mathrm{B}-|G|} = (\text{const.}) \times v^{|G|} \tag{10}$$

  where $|G|$ is the number of the connections in G, N_B is the total number of the nearest neighbor pairs of sites, and $v \equiv p/(1-p)$.
- To obtain compact expression of the average cluster size,

$$\begin{aligned}
\overline{V_c} &= \frac{1}{N} \left\langle \sum_c V_c^2 \right\rangle = \frac{1}{N} \sum_G p^{|G|}(1-p)^{N_\mathrm{B}-|G|} \sum_c V_c^2 \\
&= \frac{\partial^2}{\partial h^2} (1-p)^{N_\mathrm{B}} \sum_G v^{|G|} \sum_c e^{-hV_c} \bigg|_{h\to 0} \\
&= \frac{1}{N} (1-p)^{N_\mathrm{B}} \frac{\partial^2}{\partial h^2} \Xi_\mathrm{BP} \bigg|_{h\to 0}
\end{aligned}$$

Relation among percolation, Ising and Potts models

- We have seen a few examples in which the statistical mechanics is applied beyond the tight connection to the microscopic mechanisms.
- In the first set of examples, various phenomena was described by the Ising model whereas in the latter the percolation model was essential.
- Now, it may be good to know that these apparently unrelated models can be also related to each other at least in a mathematical level.

q-Potts model

- We first generalize the Ising model to the Potts model. The extension is made by replacing binary variables in the Ising model by q-valued ones.

$$\mathcal{H}_q(S) \equiv -J \sum_{(ij)} \delta_{S_i,S_j} - H \sum_i \delta_{S_i,1}$$

where

$$S \equiv \{S_i\}, \quad \text{and} \quad S_i = 1, 2, \cdots, q$$

- It is easy to verify that the $q = 2$ Potts model is identical to the Ising model after trivial redefinitions of J and H.

Introducing the bond variables G in Potts model

- By defining $K \equiv \beta J, h \equiv \beta H$, the partition function is

$$Z_q \equiv \sum_S e^{-\beta \mathcal{H}_q} = \sum_S \prod_{(ij)} e^{K\delta_{S_i,S_j}} \prod_i e^{h(\delta_{S_i,1} - q^{-1})} \tag{11}$$

- By introducing a one-bit auxiliary variable $g_{ij} = 0, 1$ for every pair of nearest-neighbor sites:

$$e^{K\delta_{S_i,S_j}} = 1 + (e^K - 1)\delta_{S_i,S_j} \equiv \sum_{g_{ij}=0,1} v(g_{ij})\delta(g_{ij}|S_i, S_j) \tag{12}$$

where

$$v(0) = 1, \quad \text{and} \quad v(1) = e^K - 1. \tag{13}$$

$$\delta(g_{ij}|S_i, S_j) \equiv \delta_{g_{ij},0} + \delta_{g_{ij},1}\delta_{S_i,S_j} \tag{14}$$

Partition function as summation w.r.t. S and G

- With $N_1(S)$ being the number of sites where $S_i = 1$,

$$Z_q = \sum_S \prod_{(ij)} \sum_{g_{ij}} v(g_{ij})\delta(g_{ij}|S_i, S_j) e^{h\sum_i(\delta_{\sigma_i,1} - q^{-1})} \tag{15}$$

- By using a simplifying notation

$$V(G) \equiv \prod_{(ij)} v(g_{ij}) \text{ and } \Delta(G|S) \equiv \prod_{(ij)} \delta(g_{ij}|S_i, S_j) \tag{16}$$

we obtain

$$Z_q = \sum_S \sum_G V(G)\Delta(G|S) e^{h\sum_i(\delta_{\sigma_i,1} - q^{-1})} \tag{17}$$

$$= \sum_G V(G) \sum_S \Delta(G|S) e^{h\sum_i(\delta_{\sigma_i,1} - q^{-1})} \tag{18}$$

Tracing out spin degree of freedom S

- G is the set of local graph variables, i.e., $G \equiv \{g_{ij}\}$.
- $\Delta(G|S) = 0, 1$ represents "mismatching" or "matching" between G and S, respectively.
- For each cluster in G, let S_c be one of local variables S_i $(i \in c)$,

$$\sum_S \Delta(G|S) e^{h \sum_i (\delta_{\sigma_i,1} - q^{-1})} = \sum_{\{S_c\}} e^{h \sum_c V_c (\delta_{S_c,1} - q^{-1})}$$
$$= e^{-hNq^{-1}} \prod_c (e^{hV_c} + (q-1)) \quad (19)$$

- Thus, we have arrived at the **Fortuin-Kasteleyn formula** of the partition functin of the Potts model,

$$Z_q = e^{-hNq^{-1}} \sum_G v^{|G|} \prod_c (e^{hV_c} + (q-1)). \quad (20)$$

Fortuin-Kasteleyn formula reveals Ising/percolation relation

- The generating function of the bond-percolation can be derived from Eq.(20) in the limit $\epsilon \equiv q - 1 \to 0$:

$$Z_{1+\epsilon} = e^{-hNq^{-1}} \sum_G v^{|G|} \prod_c (e^{hV_c} + \epsilon)$$
$$\approx Z_1 + \epsilon e^{-hNq^{-1}} \sum_G v^{|G|} \left(\prod_c e^{hV_c} \right) \sum_c e^{-hV_c}$$
$$= Z_1 + \epsilon \sum_G v^{|G|} \sum_c e^{-hV_c} = \epsilon \, \Xi_{\mathrm{BP}}.$$
$$\Rightarrow \Xi_{\mathrm{BP}} = \lim_{q \to 1+0} \frac{Z_q - Z_1}{q - 1}.$$

q-Potts model and percolation are related.

Exercise 1.1: Following the same type of argument leading to the Fortuin-Kasteleyn formula, show for the Ising model at $H = 0$ that the susceptibility

$$\chi \equiv \beta \left(\langle M^2 \rangle - \langle M \rangle^2 \right) \quad (M \equiv \sum_i S_i),$$

is proportional to the average size of the connected clusters.