Lecture 1: Introduction

Phase transitions, critical phenomena and universality

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To begin with

- Historically, the statistical mechanics was developed by Boltzmann to explain macroscopic phenomena from the 1st principle, i.e., Newton's law (or Schrödinger equation in the later developments).
- However, many cooperative phenomena seem to have good explanation without referring to the 1st principles. In this lecture, we take a look at a few examples.

[1-1] Various Phenomena described by Ising model

- Ferromagnets
- Ferroelectrics
- Binary alloys
- Gas-liquid transition

Ferromagnets

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

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

where $\mathbf{S}_i^\alpha$ 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

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

represents the ferromagnet at least qualitatively.

Real gases

Real gas is described by Schrödinger equation,

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

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

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

Lenard-Jone gas

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

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

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

Lattice gas model

- 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.)

Universality

- The phase diagram one obtains from the LJ model agrees with the phase diagram determined by real experiments. The agreement can be made even quantitatively accurate for noble gases by choosing right values for ϵ and σ.
- This observation shows that the microscopic mechanism and the macroscopic properties are related to each other **only through a few parameters**. We may call this the **universality of statistical mechanical phenomena**.
- 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**.

[1-2] 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**).

Generating function of the bond percolation (1)

- Let us consider the average cluster size defined by

$$\chi \equiv \left\langle \overline{V_c^2} / \overline{V_c} \right\rangle \qquad (7)$$

where V_c is the volume (the number of lattice points) of the connected cluster c.

- The over-line denotes the average over all connected clusters,

$$\overline{Q}_c \equiv \sum_c Q_c / \sum_c 1. \qquad (8)$$

- The angular bracket denotes the statistical average,

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

where the summation runs over all possible connection graphs.

Generating function of the bond percolation (2)

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

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

  where $|G|$ is the number of the connections in G, $N_{\rm B}$ 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,

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

Generating function of the bond percolation (3)

- The generating function of bond-percolation

$$\Xi_{\mathrm{BP}} \equiv \sum_G v^{|G|} \sum_c e^{-hV_c}. \tag{11}$$

- Using $\frac{\partial}{\partial h}\Xi_{\mathrm{BP}}(h)|_{h\to 0} = -N(1-p)^{-N_{\mathrm{B}}}$,

$$\chi = -\left(\frac{\partial^2}{\partial h^2}\Xi_{\mathrm{BP}}\right)_{h\to 0} \Big/ \left(\frac{\partial}{\partial h}\Xi_{\mathrm{BP}}\right)_{h\to 0} \tag{12}$$

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.

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.

Fortuin-Kasteleyn formula (1)

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

$$Z_q \equiv \sum_S e^{-\beta \mathcal{H}_q} = \sum_S \prod_{(ij)} e^{K\delta_{S_i,S_j}} \prod_i e^{h\delta_{S_i,1}} \qquad (13)$$

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

$$e^{K\delta_{S_i,S_j}} = 1 + (e^K - 1)\delta_{S_i,S_j} \equiv \sum_{g_{ij}=0,1} v(g_{ij})\delta(g_{ij}|S_i, S_j) \qquad (14)$$

where

$$v(0) = 1, \quad \text{and} \quad v(1) = e^K - 1. \qquad (15)$$

$$\delta(g_{ij}|S_i, S_j) \equiv \delta_{g_{ij},0} + \delta_{g_{ij},1}\delta_{S_i,S_j} \qquad (16)$$

Fortuin-Kasteleyn formula (2)

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

$$Z_q = \sum_S \prod_{(ij)} \sum_{g_{ij}} v(g_{ij}) \delta(g_{ij}|S_i, S_j) e^{hN_1(S)} \tag{17}$$

- By using a simplifying notation

$$V(G) \equiv \prod_{(ij)} v(g_{ij}) \text{ and } \Delta(G|S) \equiv \prod_{(ij)} \delta(g_{ij}|S_i, S_j) \tag{18}$$

we obtain

$$Z_q = \sum_S \sum_G V(G) \Delta(G|S) e^{hN_1(S)} \tag{19}$$

$$= \sum_G V(G) \sum_S \Delta(G|S) e^{hN_1(S)} \tag{20}$$

Fortuin-Kasteleyn formula (3)

- G is the set of local graph variables, i.e., $G \equiv \{g_{ij}\}$.
- $\Delta(G|S)$ is a binary valued function that represents "matching" of G and S, i.e., if any two variables in S are the same whenever they are connected in G, $\Delta(G|S) = 1$, otherwise $\Delta(G|S) = 0$.
- For each connected cluster in G, let one of local variables S_i $(i \in c)$ represent the cluster degree of freedom and use the symbol S_c for such a representative,

$$\sum_S \Delta(G|S) e^{hN_1(S)} = \sum_{\{S_c\}} e^{h\sum_c V_c \delta_{S_c,1}} = \prod_c (e^{hV_c} + (q-1)). \quad (21)$$

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

$$Z_q = \sum_G v^{|G|} \prod_c (e^{hV_c} + (q-1)). \quad (22)$$

Fortuin-Kasteleyn formula (4)

- When $H = 0$,

$$Z_q = \sum_G v^{|G|} q^{N_c(G)}. \tag{23}$$

- The generating function of the bond-percolation can be derived from Eq.(22) in the limit $\epsilon \equiv q - 1 \to 0$:

$$\begin{aligned} Z_q &= \sum_G v^{|G|} \prod_c (e^{hV_c} + \epsilon) \\ &\approx \epsilon \sum_G v^{|G|} \left(\prod_c e^{hV_c} \right) \sum_c e^{-hV_c} \\ &= \epsilon \sum_G v^{|G|} e^{hN} \sum_c e^{-hV_c} = \epsilon e^{hN} \Xi_{\rm BP}. \end{aligned}$$

[1-3] Summary

- Many cooperative macroscopic phenomena do have good explanation without referring to details of the microscopic mechanisms.
- 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 may be phrased as the *universality of statistical mechanical phenomena*.
- In particular, the universality holds exactly in the critical phenomena. (*universality of critical phenomena*)

Homework

- Following the same type of argument leading to the Fortuin-Kasteleyn formula, show that the susceptibility

$$\chi \equiv \beta \left(\langle M^2 \rangle - \langle M \rangle^2 \right) \quad (24)$$

where

$$M \equiv \sum_i S_i \quad (25)$$

of the Ising model at $H = 0$ is proportional to the average size of the connected clusters.

- Submit your report at the beginning of the next lecture.