1.4 Equipartition Theorem

Equipartition Theorem:

If the dynamics of the system is described by the Hamiltonian:

$$H = A\zeta^2 + H'$$

where ζ is one of the general coordinates $q_1, p_1, \cdots, q_{3N}, p_{3N}$, and H' and A are independent of ζ, then

$$\left\langle A\zeta^2 \right\rangle = \frac{1}{2} k_B T$$

where $\langle\rangle$ is the thermal average, i.e., the average over the Gibbs measure $e^{-\beta H}$.

This result can be easily seen by the following calculation:

$$\begin{aligned} \langle A\zeta \rangle &= \frac{\int A\zeta^2 e^{-\beta H} d^{3N}q d^{3N}p}{\int e^{-\beta H} d^{3N}q d^{3N}p} \\ &= \frac{\int A\zeta^2 e^{-\beta A\zeta^2} d\zeta e^{-\beta H'} [dpdq]}{\int e^{-\beta A\zeta^2} d\zeta e^{-\beta H'} [dpdq]} \\ &= \frac{\int A\zeta^2 e^{-\beta A\zeta^2} d\zeta}{\int e^{-\beta A\zeta^2} d\zeta} \\ &= -\frac{\partial}{\partial \beta} \ln \int e^{-\beta A\zeta^2} d\zeta \\ \left(x = \zeta\sqrt{\beta}\right) \qquad &= -\frac{\partial}{\partial \beta} \ln \left[\beta^{-\frac{1}{2}} \int e^{-Ax^2} dx \right] \\ &= \frac{1}{2\beta} \\ &= \frac{1}{2} k_B T \end{aligned}$$

where $d\zeta\,[dpdq] = d^{3N}q d^{3N}p$, i.e., $[dpdq]$ stands for the phase-space volumn element without $d\zeta$.

Note that if

$$H = \sum A_i p_i^2 + \sum B_i q_i^2$$

where there are total M terms in these sums and A_i and B_i are constant, independent of $\{p_i, q_i\}$, then

$$\langle H \rangle = \left(\frac{1}{2} k_B T \right) M$$

i.e., each quadratic component of the Hamiltonian shares $\frac{1}{2} k_B T$ of the total energy. For example, the Hamiltonian for interacting gas particles is

$$H = \sum_i \frac{p_i^2}{2m} + \sum_{ij} U\left(\mathbf{r}_i - \mathbf{r}_j\right)$$

where $U(\mathbf{r}_i - \mathbf{r}_j)$ is the potential energy between any two particles. The equipartition theorem tells us that the average kinetic energy is $\frac{3}{2}k_B T$ for every particle (since there are three translational degrees of freedom for each particle). Furthermore, for an ideal gas, i.e. gas particles do not interact, we have the average total energy

$$U = \frac{3}{2}k_B T N$$

where N is the total number of particles. Then, the specific heat for this system is

$$\begin{aligned} C_V &\equiv \left(\frac{\partial U}{\partial T}\right)_V \\ &= \frac{\partial}{\partial T}\left(\frac{3}{2}k_B T N\right) \\ &= \frac{3}{2}k_B N \end{aligned}$$

1 The Ising Model

For example, Fe or Ni exhibit macroscopic magnetic field via spontaneous polarization in the same direction for temperatures below the so-called critical temperature T_c, where T_c is referred to as the Curie temperature. For $T > T_c$, the spins are randomly orientated, there is no macroscopic magnetic field.

1.1 Model — Ising spins

The Ising model is a caricature of spin dynamics. It teaches us many interesting aspects of spin dynamics and can be used to contrast real spin systems. Especially, two dimension Ising model is a nontrivial example of phase transitions that can be worked-out exactly.

The model: we consider an n-dimensional lattice (usually with periodic boundary conditions). For two dimensions, for example, the lattice structure can be cubic or hexagonal and it has N sites in total. At each site there is a spin described by the variable s_i , $i = 1, 2, \cdots, N$ with its value:

$$s_i = \begin{cases} +1 & \text{spin up} \\ -1 & \text{spin down} \end{cases}$$

Then, a set of $\{s_i, i = 1, \cdots, N\}$ constitutes a configuration of the system. The energy in a configuration is

$$E\{s_i\} = -\sum_{\langle i,j\rangle} J_{ij} s_i s_j - H \sum_{i=1}^{N} s_i$$

where J is the exchange energy between two spins and H is a constant external magnetic field. $\langle i, i\rangle$ denotes the nearest next neighbor interactions. If the exchange interaction is isotropic, then

$$J_{ij} = J$$

and

$$E\{s_i\} = -J \sum_{\langle i,j\rangle} s_i s_j - H \sum_{i=1}^{N} s_i$$

For $J > 0$, it describes ferromagnetism, in which two neighboring spins like to line up in the same direction. For $J < 0$, it is antiferromagnetism, in which two neighboring spins tend to be in the opposite direction in order to lower the energy of the system. We consider only the case $J > 0$ below.

The partition function for the Ising model is

$$Q(H, T) = \sum_{s_1} \sum_{s_2} \cdots \sum_{s_N} e^{-\beta E\{s_i\}}$$

there are total 2^N terms in the summation and each s_i, ranging over ± 1 is independent from another.

Thermodynamic functions can be obtained via the Helmholtz free energy:

$$A(H,T) = -k_B T \log Q(H,T)$$

For example, the internal energy is

$$u(H,T) = -k_B T^2 \frac{\partial}{\partial T}\left(\frac{A}{k_B T}\right)$$

the heat capacity is

$$c(H,T) = \frac{\partial}{\partial T} u(H,T)$$

and the magnetization is

$$M(H,T) = -\frac{\partial A}{\partial H}$$

It can be easily seen that

$$M(H,T) = \left\langle \sum_{i=1}^{N} s_i \right\rangle$$

where $\langle \cdots \rangle$ is the ensemble average.

The so-called spontaneous magnetization is

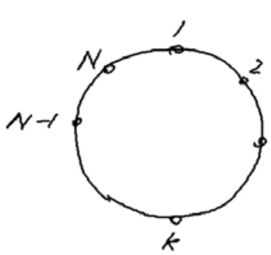
$$M(0,T) \neq 0$$

for the case of $J_{ij} > 0$, i.e., there is a finite magnetization in the absence of the external field.

1.1.1 Transfer-Matrix Method

Here we discuss only the 1D Ising model. The method can be generalized to 2D with considerably difficulty. Consider a chain of N spins, i.e.,

$$s_1 \equiv s_{N+1}$$



For the configuration $\{s_1, \cdots s_N\}$, $s_k = \pm 1$, the energy of the system is

$$E = -J \sum_{k=1}^{N} s_k s_{k+1} - H \sum_{k=1}^{N} s_k$$

and the partition function is

$$Q(H,T) = \sum_{s_1}\sum_{s_2}\cdots\sum_{s_N} e^{\beta\sum_{k=1}^{N}(Js_ks_{k+1}+Hs_k)}$$

Now we can evaluate this explicitly using a matrix formulation. First, using the periodic boundary condition, we rewrite Q in a symmetric form:

$$Q(H,T) = \sum_{s_1}\sum_{s_2}\cdots\sum_{s_N} e^{\beta\sum_{k=1}^{N}\left[Js_ks_{k+1}+\frac{1}{2}H(s_k+s_{k+1})\right]}$$

It turns out that there is a natural matrix formulation underlying this expression. Define a 2×2 matrix P with its elements

$$P_{ss'} = e^{\beta\left[Jss'+\frac{1}{2}H(s+s')\right]}$$

where s, s' takes the value of ± 1 independently. More explicitly, we have

$$\begin{aligned} P_{++} &= e^{\beta(J+H)} \\ P_{+-} &= e^{\beta(J-H)} \\ P_{+-} &= P_{-+} = e^{-\beta J} \end{aligned}$$

i.e.,

$$P = \begin{pmatrix} e^{\beta(J+H)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-H)} \end{pmatrix}$$

Therefore,

$$\begin{aligned} Q(H,T) &= \sum_{s_1}\sum_{s_2}\cdots\sum_{s_N} P_{s_1s_2}P_{s_2s_3}\cdots P_{s_Ns_1} \\ &= \sum_{s_1}\left(P^N\right)_{s_1s_1} \\ &= TrP^N \qquad \text{(a consequence of periodic BCs)} \\ &= \lambda_+^N + \lambda_-^N \end{aligned}$$

where λ_+, λ_- are the eigenvalue of P.

$$\lambda_\pm = e^{\beta J}\left[\cosh(\beta H) \pm \left(\sinh^2(\beta H) + e^{-4\beta J}\right)^{1/2}\right]$$

$\lambda_+ \geq \lambda_-$ for all values of H. P is referred to as the transfer matrix.

As $N \to \infty$, only λ_+ is relevant since

$$\begin{aligned} \frac{1}{N}\log Q(H,T) &= \log\lambda_+ + \log\left(1+\left(\frac{\lambda_+}{\lambda_-}\right)^N\right) \\ &\to \log\lambda_+ \qquad \text{as } N\to\infty \end{aligned}$$

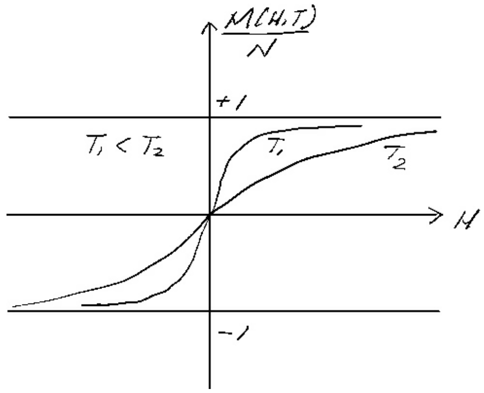
Physical results:

1. The Helmholtz free energy per spin is

$$\frac{1}{N}A(H,T) = -J - k_B T \log\left[\cosh(\beta H) + \left(\sinh^2(\beta H) + e^{-4\beta J}\right)^{1/2}\right]$$

2. The magnetization per spin is

$$\frac{1}{N}M(H,T) = \frac{\sinh(\beta H)}{\left[\sinh^2(\beta H) + e^{-4\beta J}\right]^{1/2}}$$



For $\forall T > 0$,

$$\frac{1}{N}M(H=0,T) = 0$$

therefore is no spontaneous magnetization for 1-D Ising model.

1.1.2 Symmetry Breaking

A more general model for spins is, for example, that the energy of the system is

$$E = J\sum_{\langle i,j\rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

where $\mathbf{S}_i$ is a vector with $\mathbf{S}\cdot\mathbf{S} = S^2$, where S is a fixed number. Then the total magnetic moment is determined by

$$\langle M\rangle = \frac{Tr\left(e^{-\beta E}M\right)}{Tr\left(e^{-\beta E}\right)}$$

In general, E is invariant under rotation in the absence of external field. Therefore,

$$\langle M\rangle = 0$$

since M and $-M$ occur with equal probability. A deep question then is how come we have ferromagnetism? This answer lies the fundamental concept of spontaneous symmetry breaking.

Spontaneous Symmetry Breaking Despite the fact that a Hamiltonian is invariant under certain symmetry groups, the ground state of the system does not have to possess the same symmetry of the Hamiltonian. That is, a ground state can be degenerate. For example, a ferromagnet ground state is not rotationally invariant — any one of the degenerate ground state is a physical solution. Once a system magnetizes along a certain direction, it cannot make a transition to another direction (Although, for this transition, there is no energy required, it has almost zero probability since all spins have to rotate simultaneously exactly the same amount).

How can we mathematically capture the spontaneous symmetry breaking? In the case of spontaneous magnetizatoin, we can add an exteranl field H, then let $H \to 0$ in the end:

$$\frac{\langle M \rangle}{V} \equiv \lim_{H\to 0} \lim_{V\to\infty} \frac{1}{V} \frac{Tr\left(Me^{-\beta(E-MH)}\right)}{Tr\left(e^{-\beta(E-MH)}\right)}$$

where it is important to have the correct order of limiting processes, which reflects the underlying thermodynamic limit. If the limit $H \to 0$ is taken before the thermodynamic limit, then we have

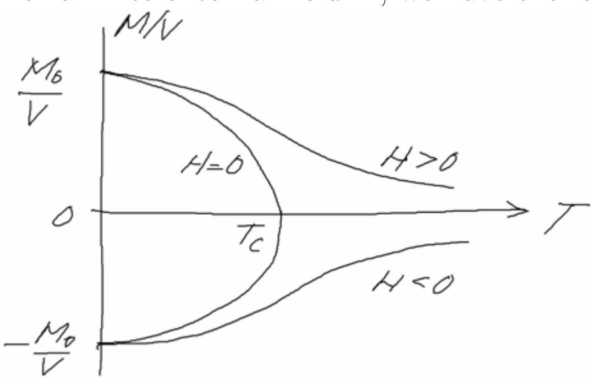
$$\lim_{V\to\infty} \lim_{H\to 0} \frac{1}{V} \frac{Tr\left(Me^{-\beta(E-MH)}\right)}{Tr\left(e^{-\beta(E-MH)}\right)} = 0$$

i.e., there would be no spontaneous magnetization.

For the Ising model, the Hamiltonian is invariant under the discrete, reflectional symmetry:

$$S_i \to -S_i$$

For a finite external field H, we have the following phase diagram:



1.2 Curie-Weiss Model (Mean-field model)

The energy of the Curie-Weiss model is given by

$$E_N\{S_i\} = -\frac{J}{N} \sum_{i,j=1}^{N} S_i S_j - H \sum_{j=1}^{N} S_j$$

which can also be expressed as

$$E_N\{S_i\} = -JN\left(\frac{1}{N}\sum_i^N S_i\right)^2 - H\sum_{j=1}^N S_j$$

or

$$E_N\{S_i\} = -J\sum_i S_i\left(\frac{1}{N}\sum_j^N S_j\right) - H\sum_{j=1}^N S_j \tag{1}$$

where H is the external magnetic field. Note that

1. due to the long-rang nature of the interaction (i.e., everying spin interacts with every other spin with an equal strength of coupling in this model), we can equivallently view the model as a spin interacting with its N neighbors in an N-dimensional lattice.
2. The bracked term in Eq. (1) can be viewed as an effective magnetic field induced by all the spins. The following approximation is based on this observation.

The partition function of this system is

$$Q_N(T,H) = \sum_{S_i}\cdots\sum_{S_N}\exp\left(\frac{\beta J}{N}\sum_{i,j=1}^N S_iS_j + \beta H\sum_{i=1}^N S_i\right)$$

We use the mean-field approximation to evaluate this partition as follows. First, we view $\frac{1}{N}\sum_j^N S_j$ as if it were external effective magnetic field, and let

$$m = \frac{1}{N}\sum_j^N S_j$$

then

$$\begin{aligned}
Q_N &= \sum_{S_i}\cdots\sum_{S_N}\exp\left((\beta Jm + \beta H)\sum_{i=1}^N S_i\right)\\
&= \sum_{S_i}\cdots\sum_{S_N}\prod_i^N \exp\left[\beta\left(Jm + H\right)S_i\right]\\
&= \prod_i^N\left(\sum_{S_i}\exp\left[\beta\left(Jm + H\right)S_i\right]\right)\\
&= \prod_i^N\left(e^{\beta(Jm+H)} + e^{-\beta(Jm+H)}\right)\\
&= 2^N\cosh^N\left[\beta\left(Jm + H\right)\right].
\end{aligned}$$

The corresponding Helmholz free energy under this mean-field approximation is

$$\begin{aligned} A_{MF} &= -k_B T \log Q_N \\ &= -k_B T \log \left[2^N \cosh^N \left[\beta \left(Jm + H \right) \right] \right] \end{aligned}$$

in general, the thermal average of $\frac{1}{N}\sum_j^N S_j$ is determined by

$$\left\langle \frac{1}{N} \sum_j^N S_j \right\rangle = -\frac{\partial}{\partial H} \left(\frac{A}{N} \right)$$

a self-consistency requires that

$$m = \left\langle \frac{1}{N} \sum_j^N S_j \right\rangle$$

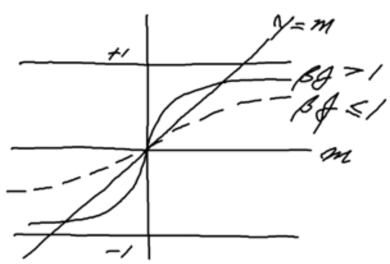
i.e.,

$$\begin{aligned} m &= -\frac{\partial}{\partial H} \left\{ -k_B T \log 2^N \cosh^N \left[\beta \left(Jm + H \right) \right] \right\} \\ &= \tanh \left[\beta \left(Jm + H \right) \right]. \end{aligned}$$

Phase Transition

If $H = 0$, i.e., there is no external field,

$$m = \tanh \beta J m$$



if $\beta J > 1$, i.e.,

$$k_B T < J$$

there are two nonvanishing solutions,

$$m = \pm m \left(\beta \right)$$

in addition to the vanishing solution. If $\beta J \leq 1$, there is a unique solution

$$m = 0.$$

Therefore, the phase transition occurs at the critical temperature

$$T_c = \frac{J}{k_B}.$$

Note that

1. It turns out that this mean-field result is exact. We will demonstrate this later.

2. The Curie-Weiss model has spontaneous magnetization for $T < T_c$.

3. T_c corresponds to the energy scale $k_B T_c \sim J$.

4. Note that $m = \frac{1}{N}\sum_j^N S_j$ should have different values for different configurations. The mean-field approximation assumes that in the large-N limit, the sum converges to a mean-value without fluctuations. Philosophically speaking, there is a law of large number or central-limit theorem lurking behind this mean-field approximation for the contribution from fluctuations to be neglected.

1.2.1 Large Deviation Principle for Curie-Weiss model — the exact result

$\Omega_n = \{-1, +1\}^n$, $\rho = \frac{1}{2}\delta_{-1} + \frac{1}{2}\delta_{+1}$

Let P_n be the product measure on Ω_n with one-dimensional marginals ρ. Clearly, for any $\omega = \{\omega_i, i = 1, \cdots, n\} \in \Omega_n$,

$$P_n\{\omega\} = \left(\frac{1}{2}\right)^n$$

The energy of the system is

$$H_n(\omega) = -\frac{1}{2n}\sum_{i,j=1}^{n}\omega_i\omega_j = -\frac{n}{2}\left(\frac{1}{n}\sum_{j=1}^{n}\omega_i\right)^2$$

The Gibbs measure is

$$P_{n\beta}\{\omega\} = \frac{1}{Z_n(\beta)}e^{-\beta H_n(\omega)}$$

where

$$\begin{aligned} Z_n(\beta) &= \int_{\Omega_n} e^{-\beta H_n(\omega)} P_n(d\omega) \\ &= \sum_{n\in\Omega_n} e^{-\beta H_n(\omega)}\frac{1}{2^n} \end{aligned}$$

We discuss the magnetization

$$\frac{S_n(\omega)}{n} = \frac{1}{n}\sum_{i=1}^{n}\omega_i$$

We are looking for the following property if there is a phase transition as the mean-field approximation indicates:

$$\begin{aligned} \frac{S_n(\omega)}{n} &\to 0 \quad \text{for } \beta \le 1 \\ &\to \pm m(\beta) \quad \text{for } \beta > 1 \end{aligned}$$

where $m(\beta) \in (0,1)$. That is, we want to study the question:

$$P_{n\beta}\left\{\frac{S_n(\omega)}{n} \in dx\right\} = ?$$

i.e., is there a large deviation principle for $\frac{S_n}{n}$ with respect to $P_{n\beta}$? Note that

$$\frac{S_n}{n} \in [-1,+1]$$

In order to demonstrate the equivalence between Laplace principle and the large-deviation principle, we need to find a rate function I_β on $[-1,+1]$ such that for any continuous function $f:[-1,+1] \to \mathbb{R}$,

$$\lim_{n\to\infty} \frac{1}{n} \log \mathbb{E}_{P_{n\beta}}\left\{e^{nf\left(\frac{S_n}{n}\right)}\right\} = \sup_{x\in[-1,+1]}\left\{f(x) - I_\beta(x)\right\}$$

Note that

1.
$$\begin{aligned}\mathbb{E}_{P_{n\beta}}\left\{e^{nf\left(\frac{S_n}{n}\right)}\right\} &= \frac{1}{Z_n(\beta)}\int_{\Omega_n} e^{\left[nf\left(\frac{S_n}{n}\right)+n\frac{\beta}{2}\left(\frac{S_n}{n}\right)^2\right]} P_n(d\omega) \\ &= \frac{1}{Z_n(\beta)}\int_{[-1,+1]} e^{nf(x)+n\frac{\beta}{2}x^2} P_n\left\{\frac{S_n}{n} \in dx\right\} \qquad (2)\end{aligned}$$

   Note that $e^{n\frac{\beta}{2}\left(\frac{S_n}{n}\right)^2}$ is simply $e^{-\beta H_n(\omega)}$.

2.
$$\begin{aligned}Z_n(\beta) &= \int_{\Omega_n} e^{n\frac{\beta}{2}\left(\frac{S_n}{n}\right)^2} P_n(d\omega) \\ &= \int_{[-1,+1]} e^{n\frac{\beta}{2}x^2} P_n\left\{\frac{S_n}{n} \in dx\right\}\end{aligned}$$

3. Cramier Theorem (which is the special case of what we discussed before):

   Let $\Lambda = \{-1,+1\}, \rho = \frac{1}{2}\delta_{-1} + \frac{1}{2}\delta_{+1}$, $\omega \in \Omega_n$, $S_n(\omega) \equiv \sum_{j=1}^n \omega_j$, then $\left\{\frac{S_n(\omega)}{n}, n \in \mathbb{N}\right\}$ satisfies the large-deviation principle on $[-1,+1]$ with rate function:

$$I(x) = \frac{1}{2}(1-x)\log(1-x) + \frac{1}{2}(1+x)\log(1+x)$$

   Proof: For $x \in [-1,+1]$,

$$\frac{S_n(\omega)}{n} \sim x$$

if and only if there are approximately $\frac{n}{2}(1-x)$ components such that $\omega_j = 1$and $\frac{n}{2}(1+x)$ components such that $\omega_j = +1$. Therefore,

$$\begin{aligned} P_n\left\{\frac{S_n(\omega)}{n} \sim x\right\} &\approx P_n\left\{L_n(-1) = \frac{1}{2}(1-x), L_n(+1) = \frac{1}{2}(1+x)\right\} \\ &\approx e^{-nI_\rho\left(\left\{\frac{1}{2}(1-x), \frac{1}{2}(1+x)\right\}\right)} \qquad (\because \text{ Large-deviation principle}) \end{aligned}$$

where $L_n(-1)$ is the empirical frequency of -1 in ω. Note that

$$\begin{aligned} I_\rho\left(\left\{\frac{1}{2}(1-x), \frac{1}{2}(1+x)\right\}\right) &= \frac{1}{2}(1-x)\log\frac{\frac{1}{2}(1-x)}{\frac{1}{2}} + \frac{1}{2}(1+x)\log\frac{\frac{1}{2}(1+x)}{\frac{1}{2}} \\ &= I(x) \end{aligned}$$

$\mathbb{QED}$

Applying Cramier theorem to the denominator and numerator of Eq. (2), we obtain

1.
$$\lim_{n\to\infty}\frac{1}{n}\log Z_n(\beta) = \sup_{x\in[-1,+1]}\left\{\frac{\beta}{2}x^2 - I(x)\right\}$$

2.
$$\lim_{n\to\infty}\frac{1}{n}\log\int_{[-1,+1]} e^{nf(x)+n\frac{\beta}{2}x^2} P_n\left\{\frac{S_n}{n}\in dx\right\} = \sup_{x\in[-1,+1]}\left\{f(x) + \frac{\beta}{2}x^2 - I(x)\right\}$$

with

$$I(x) = \frac{1}{2}(1-x)\log(1-x) + \frac{1}{2}(1+x)\log(1+x)$$

Now define

$$I_\beta(x) \equiv I(x) - \frac{\beta}{2}x^2 - \inf_{y\in[-1,+1]}\left\{I(y) - \frac{\beta}{2}y^2\right\}$$

therefore

$$\lim_{n\to\infty}\frac{1}{n}\log\mathbb{E}_{P_{n\beta}}\left\{e^{nf\left(\frac{S_n}{n}\right)}\right\} = \sup_{x\in[-1,+1]}\{f(x) - I_\beta(x)\}$$

that is $\frac{S_n}{n}$ satisfies the Laplace principle on $[-1,+1]$, therefore, $\frac{S_n}{n}$ satisfies large-deviation principle with the rate function $I_\beta(x)$, i.e.,

$$P_{n\beta}\left\{\frac{S_n(\omega)}{n}\in dx\right\} \sim e^{-nI_\beta(x)}$$

In the limit of $n\to\infty$, only those minima x^* of $I_\beta(x)$ such that

$$I_\beta(x^*) = 0$$

will have a nonvanishing contribution. Obviously, x^* satisfies

$$I'_\beta(x^*) = 0$$

i.e.,

$$I'(x^*) = \beta x^* \quad \text{or} \quad x^* = (I')^{-1}(\beta x^*)$$

Note that $I(x) = \frac{1}{2}(1-x)\log(1-x) + \frac{1}{2}(1+x)\log(1+x)$, It is easy to verifty that

$$x^* = \tanh \beta x^*$$

Therefore, we have three solutions: $0, \pm m(\beta)$, i.e.,

$$P_{n\beta}\left\{\frac{\sum_j \omega_j}{n} \in dx\right\} \overset{W.}{\Longrightarrow} \begin{cases} \delta_0 & \text{for } 0 \leq \beta \leq 1 \\ \frac{1}{2}\delta_{m(\beta)} + \frac{1}{2}\delta_{-m(\beta)} & \text{for } \beta > 1 \end{cases}$$

i.e., the set

$$\varepsilon_\beta = \{x \in [-1,+1], \quad I_\beta(x) = 0\}$$

is the support of $P_{n\beta}\left\{\frac{S_n(\omega)}{n} \in dx\right\}$. Note that $x^* \in \varepsilon_\beta$.

We can also compute the free energy, which is simply

$$\lim_{n\to\infty} \frac{1}{n} \log Z_n(\beta) = \sup_{x\in[-1,+1]} \left\{\frac{\beta}{2}x^2 - I(x)\right\}$$

Clearly, maximizing $\frac{\beta}{2}x^2 - I(x)$ leads to the solution x^*.

1.3 Renormalization Groups/Phase Transitions

Critical properties reflect the nature of long wavelength fluctuation, not of short-distance details. An effective and efficient way of understanding their underlying dynamics is by coarse-graining out the irrelevant scales all the way up to the correlation length.

1.3.1 Block-spin Transformation

The concept of the block spins captures the "average" spin within a block materials near the critical point, where the notion of average depends on a particular coarse-graining procedure in use and it accentuates the fact that the fluctuations with the block are not relevant. We illustrate this notion using the one-dimensional Ising model. Although we have already learnt that it has no phase transition at finite (i.e., $T \neq 0$) temperatures, it is nevertheless an instructive example in which the coarse-graining (block-spin transformation) procedure can be carried out exactly. The Ising model is

$$E = -J\sum_{i}^{N} s_i s_{i+1} - H\sum_{i=1}^{N} s_i$$

or

$$\beta E = -j\sum_{i}^{N} s_i s_{i+1} - h\sum_{i=1}^{N} s_i$$

where $j = \beta J,\ h = \beta H$. The corresponding transfer matrix is

$$\begin{aligned} P &= \begin{pmatrix} e^{j+h} & e^{-j} \\ e^{-j} & e^{j-h} \end{pmatrix} \\ &\equiv \begin{pmatrix} \frac{1}{\mu\nu} & \mu \\ \mu & \frac{\nu}{\mu} \end{pmatrix} \end{aligned}$$

where $\mu = e^{-\beta J}$, and $\nu = e^{-\beta H}$. For ferromagnetic $J > 0$, without loss of generality, we can assume $h \geq 0$, then, $\mu, v \in [0,1]$. Recall that the partition function is

$$Q_N = TrP^N.$$

Now consider the block which consists of every two nearest next neighbors and rewrite this Q_N as if the site were block spins, i.e.,

$$Q_N = Tr\left(P^2\right)^{N/2}$$

where $P_2 \equiv P^2$ would be the transfer matrix for the chain of spins which are block type. Obviously,

$$P_2 = P^2 = \begin{pmatrix} \mu^2 + \frac{1}{\mu^2\nu^2} & \nu + \frac{1}{\nu} \\ \nu + \frac{1}{\nu} & \mu^2 + \frac{\nu^2}{\mu^2} \end{pmatrix}$$

If the block spin can be viewed as effective spins, P_2 should be expressed in the form:

$$P_2 = c\begin{pmatrix} \frac{1}{\mu'\nu'} & \mu' \\ \mu' & \frac{\nu'}{\mu'} \end{pmatrix}$$

Note that the over-all constant c is needed for finding such a form — the diagonal and off-diagonal terms in the matrix gives rise to three equations. Now we have three unknowns, μ', ν', and c. i.e.,

$$\begin{aligned} \frac{c}{\mu'\nu'} &= \mu^2 + \frac{1}{\mu^2\nu^2} \\ \frac{c\nu'}{\mu'} &= \mu^2 + \frac{\nu^2}{\mu^2} \\ c\mu' &= \nu + \frac{1}{\nu} \end{aligned}$$

which have the following solutions:

$$
\begin{aligned}
\mu' &= \left(\nu + \frac{1}{\nu}\right)^{\frac{1}{2}} \left(\mu^4 + \frac{1}{\mu^4} + \nu^2 + \frac{1}{\nu^2}\right)^{-\frac{1}{4}} \\
\nu' &= \left(\mu^4 + \nu^2\right)^{\frac{1}{2}} \left(\mu^4 + \nu^2\right)^{-\frac{1}{2}} \\
c &= \left(\nu + \frac{1}{\nu}\right)^{\frac{1}{2}} \left(\mu^4 + \frac{1}{\mu^4} + \nu^2 + \frac{1}{\nu^2}\right)^{-\frac{1}{4}}
\end{aligned}
$$

Therefore, P_2 can be written as

$$
P_2 = \begin{pmatrix} e^{j'+h'+c'} & e^{-j'+c'} \\ e^{-j'+c'} & e^{j'-h'+c'} \end{pmatrix}
$$

where $c \equiv \exp(c')$. To carry out the coarse-graining procedure, we now ask the following question: Is there an Ising model which has exactly the same transfer matrix as P_2? Clearly, the answer is affermative and the corresponding Hamiltonian is

$$
\beta E' = -\sum_{i'} \left(j' S_{i'} S_{i'+1} + h' S_{i'} + c'\right).
$$

where $i' = 1, 2, \cdots, N/2$.The last term only gives rise to a shift in the total energy and is independent of the spin configuration $\{S_{i'}\}$. Hence, no effect on thermodynamics.

The computation above has a simple block spin coarse-graining interpretation: If we group spin s_i and spin s_{i+1} to form a block with the rule that the value of s_i is used to represent the effective spin of the block, we perform the sum over all possible configuration of s_{i+1} to obtain a new Hamiltonian of block spins. Mathematically,

$$\begin{aligned}
Q_N &= \sum_{s_1}\sum_{s_2}\cdots\sum_{s_N} e^{j'\sum_{i=1}^N s_i s_{i+1} + h'\sum_{i=1}^N s_i} \\
&= \sum_{s_1}\sum_{s_2}\cdots\sum_{s_N} e^{\sum_{i=1}^N j' s_i s_{i+1} + \frac{h'}{2}(s_i + s_{i+1})} \\
&= \sum_{s_1}\sum_{s_2}\cdots\sum_{s_N}\prod_{i=1}^N e^{j' s_i s_{i+1} + \frac{h'}{2}(s_i + s_{i+1})} \\
&= \sum_{s_1}\sum_{s_2}\cdots\sum_{s_N} P_{s_1 s_2} P_{s_2 s_3}\cdots P_{s_{N-1} s_N} \\
&= \sum_{s_1}\sum_{s_3}\cdots\sum_{s_{2i-1}}\cdots\sum_{s_{N-1}}\sum_{s_N}\left(\sum_{s_2} P_{s_1 s_2} P_{s_2 s_3}\right)\left(\sum_{s_4} P_{s_3 s_4} P_{s_4 s_5}\right)\cdots \\
&\quad \times\cdots\left(\sum_{s_{2i}} P_{s_{2i-1} s_{2i}} P_{s_{2i} s_{2i+1}}\right)\cdots\left(\sum_{s_{N-1}} P_{s_{N-2} s_{N-1}} P_{s_{N-1} s_N}\right) \\
&= \sum_{s_1}\sum_{s_3}\cdots\sum_{s_{2i-1}}\cdots\sum_{s_{N-2}}\sum_{s_N} \left(P^2\right)_{s_1 s_3}\left(P^2\right)_{s_3 s_5}\cdots\left(P^2\right)_{s_{N-2} s_N} \\
&= \sum_{s_1}\sum_{s_3}\cdots\sum_{s_{2i-1}}\cdots\sum_{s_{N-2}}\sum_{s_N} e^{\sum_{i'}\left(j' s_{2i-1} s_{2i+1} + \frac{h'}{2}(s_{2i-1} + s_{2i+1}) + c'\right)} \\
&= C\sum_{s_1}\sum_{s_3}\cdots\sum_{s_{2i-1}}\cdots\sum_{s_{N-2}}\sum_{s_N} e^{-\beta E'}
\end{aligned}$$

which involves only effective spins of blocks. This illustrates that the corase-graining procedure is realized using partial sums.

In the case of the Ising model, the renormalization group constitutes the follwoing two steps:

1. Coarse-graining via the block-spin transformation:

$$(j, h) \to (j', h')$$

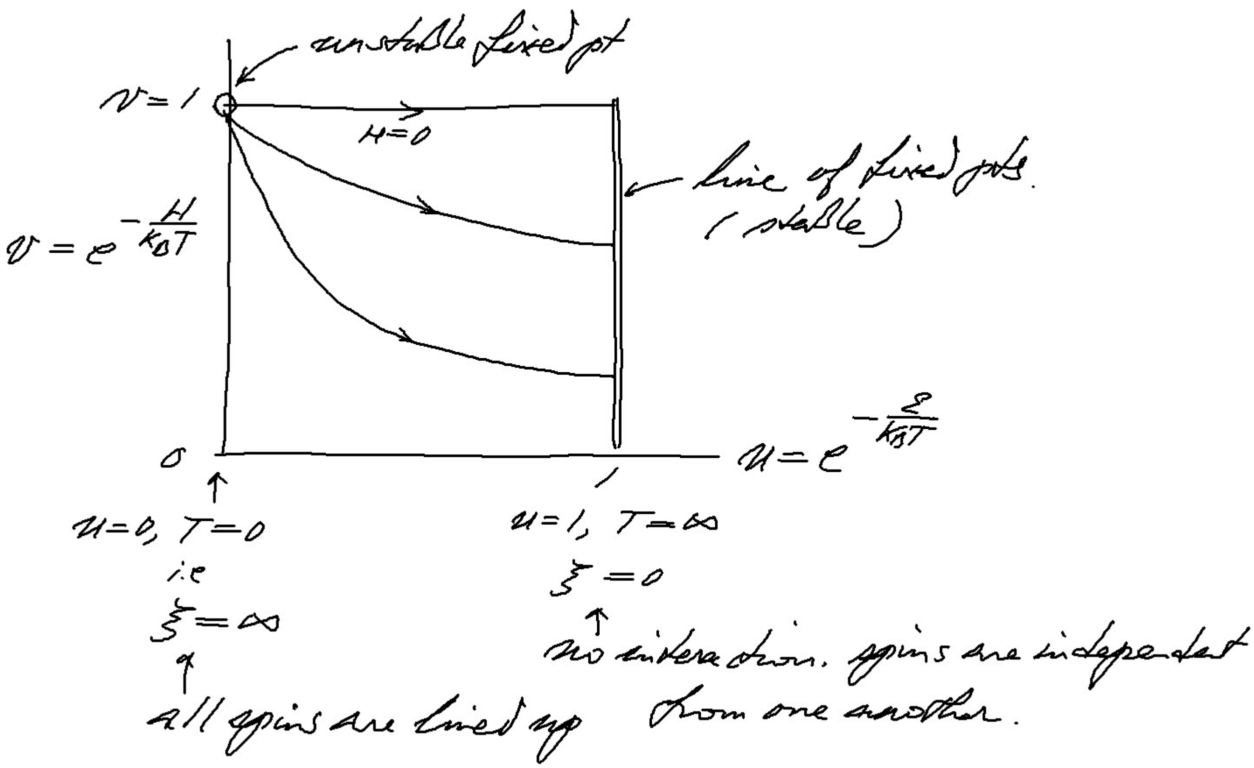
   with the length-scale change from 2 to 1 (since every two spins form a single new, effective block spin). After the block-spin transformation, we have regained the form of the Hamiltonian exactly modullo an unimporant constant. This transformation forms a semi-group map.

2. Seek fixed points of this semi-group map. Physically, some of these fixed points correspond to critical points of phase transitions. This is determined by the fact that the only relevant length scale is the longwave for critical phenomena. The relevant scale is measured by the correlation length ξ. Therefore, at a critical point $\xi \to \infty$ in the thermodynamic limit $N \to \infty$.

For the one dimensional Ising model, the fix points of the block-spin transformation is

$$\begin{cases} u = 0, \\ v = 1 \end{cases} \quad \text{and} \quad \begin{cases} u = 1, \\ v \text{ is any positive value} \end{cases}$$

$u = 0$ corresponds to $j = \infty$, the effective exchange energy diverges, or $T \to 0$.; $v = 1$ corresponds to zero external field. It can be easily shown that $(u, v) = (0, 1)$ is an unstable fixed point under block-transformation. The second fixed point corresponds to the effective $j = 0$, (i.e., no interaction or $T \to \infty$) with an arbitrary field. This is a stable fixed point under the block transformation. Note that since spins do not interact or $T \to \infty$ at this fixed point, then all spins are independent from one another and they have equal probability of lining up or down.



the invariant length scale under the semi-group map is

$$\xi = 0 \quad \text{or} \quad \xi = \infty$$

the latter of which correspond to a phase transtion at $T = 0$. For the one-dimensional Ising spins, there is no $T \neq 0$ fixxed point for $\xi = \infty$, therefore, there is no phase transition at finite temperature — this is what we already learned in previous lectures.

1.4 Momentum-Space Renormalization

Contrast between coarse-graining in real space and coarse-graining in momenum space: