Statistical Mechanics

Advanced Topics and Applications

Prof. Youjin Deng, my undergraduate Advanced Statistic Physics Teacher, has signed us eight modern statistical mechanics topics for survey and investigation purposes. These topics, showing in the text, is quite challenging to a student with limited knowledge of this vast area.

Li, Zimeng 3/17/2012 Revised Version



Topics overview

- 1. A brief survey of percolation. Please include the definition of the percolation model, its applications, exact solution on Cayley tree, and exact solution of the percolation threshold on the square lattice.
- 2. Exact solution of the mean-field Blume-Capel model.

$$H = -\frac{K}{N} \sum_{i \neq j=1}^{N} s_i s_j + D \sum_{k=1}^{N} s_i^2 \quad (s = 0, \pm 1)$$

Please locate the line of the phase transitions, which is consisted of a line of critical point, a tricritical point, and a segment of 1st order transition. Summarize the behavior of the energy density, the specific heat, the magnetization density, the susceptibility, the vacancy density, the compressibility near the transition line, and as a function of temperature 1/K. Derive critical exponents.

- 3. Ising model is an amazingly beautiful toy model in statistical mechanics. Please describe the exact solution of the Ising model in 1D (including partition sum and all observable quantities), the exact solution of the critical point on the square lattice. Summarize theoretical exponent for d>1. Summarize its generalization to the Potts model (ordinary and chiral). Can you locate the critical point of the ordinary Potts model on the square lattice (using the duality relation)?
- 4. 4, Quantum Ising model plays an important role in quantum statistics. Its Hamiltonian is

$$H = -t \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z - \sum_k \sigma_k^x$$

where sigma is the Pauli matrix. Please describe its phase transition. Using the path-integral language (Suzuki-Trotter formula), a d-dimensional quantum Ising model can be mapped onto a (d+1) dimensional quantum Ising model. Please derive this mapping.

- 5. The classical XY model is frequently used to describe the universal behavior in the phase transition between Mott-insulator and superfluidity (or superconductivity). Please give reasoning why this is possible. Summarize the phase transition of the classical XY model in 1D, 2D, 3D, and more. Give the reasoning why the 2D XY model does not have long-ranged ordering at non-zero temperature (as rigorously as possible)—Mermin-Wagner theorem.
- 6. In real worlds, we have bosons and fermions. By interchanging two of such particles, the phase of the wave function accumulates 0 and PI, respectively, for

bosons and fermions. Their statistical behavior obeys the Bose-Einstein and the Fermi-Dirac statistics, respectively. Please derive them. In some 2D systems with strong interactions, however, the excitons—psedo-particles—do not obey either of the statistics. Interchanging two excitons can lead to a phase change of any value between 0 and 2 Pi. Such pseudo-particles are named "anyons". They are used explain the quantum Hall effects as well as the recently discovered quantum Spin-Hall effects, and are found to have profound implication in quantum computation. Two beautiful models for anyons are the Kitaev model and the Wen model. Please give a survey of anyons and these two models.

- 7. Define the renormalization group (RG) in the language of the Ginzburg-Landau model. Explain the universality by RG. Derive the Gaussian the fixed point and the associated critical
- 8. Monte Carlo method is an important tool in researches, engineering, as well as in industries. In particular, Markovian-chain Monte Carlo (MCMC) method is found extensive applications in statistical physics. Please give a survey of MCMC. Design your own for the 2D Ising model; calculate energy, density, specific heat, magnetization density, and susceptibility. Locate the critical point, and calculate the associated critical exponents.

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Class Homework 2

Percolation Edited by Li,Zimeng

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The phase transition of Percolation is a typical Non-Hamiltonian System phase transition. It shows us property of continuous phase transition, and to some extent, in deep contact with the q-state Potts Model. This article would showcase a brief survey of a Percolation Model and its applications.

1.Definition

Suppose there is a hypercubic lattice G, with sites and bonds combining the nearest sites. Two models of Percolation can be divided here –

[1] Bond Percolation

The probability is p for a bond to be occupied, thus 1-p for those unoccupied.

[2] Lattice Percolation

The probability is p for a site to be occupied, thus 1-p for those unoccupied.

In both models above, **clusters** are formed when nearest occupied bonds or sites are joined together. We define P(p) as the probability that an infinitely large cluster is formed. It is easy to see and also by computer simulation, that P(p) = 0 when $p < p_{c'}$ and p significantly increases when it passes $p_{c'}$ later reaches 1 when p = 1. We call pc **percolation threshold**. It transpires that P(p) can be seen as the analogue of the order parameter of magnetic systems, which I will not proved here, q-states Potts Model.

2.Application

[1]Forest Fires

Percolation can be used to predict how long it takes a fire to penetrate the forest or to be extinguished.

[2]Oil Fields

Percolation can be used as an idealized simple model for the distribution of oil or gas

inside porous rocks in oil reservoirs.

[3]Diffusion in Disordered Media

Hydrogen atoms are known to diffuse through many solids, an effect which might become important for energy storage. A particularly simple disordered medium is our percolation lattice.

[4]Gelation

3.Exact Solution on Cayley Tree

Cayley Tree

Bethe lattice, or Cayley tree, have every of its sites connected with z neighbours, but none of them form loops. See Fig 3.1



Cayley Tree

As can be seen above, there is an origin site in the center, and around each site is its neighbours. Branches are all sites besides the origin site, and subbranches can also be defined similarly, but in the branch region.

Since there is no close loop in Cayley Tree, each bond is in different directions. It's therefore no wonder Cayley Tree is infinite dimension.

To get the percolation threshold of Cayley Tree, we start from the center, following the

path outward, to see if an infinitely large cluster is formed. We find z-1 new bonds emanating from every new site. So the probability that these new neighbours are occupied is p(z-1). If p(z-1)<1, we cannot find an infinitely large cluster which extend to the infinity, therefore the probability of an infinitely large cluster is formed, or P, is determined by p(z-1)=1, thus we get

$$p_c = \frac{1}{z - 1}$$

4.Exact Solution on Square Lattice

[1]Site Percolation

Currently, only numerical value of percolation threshold is done for site percolation in square lattice, and Pc here is 0.5927

[2]Bond Percolation

Bond Percolation can be exactly solved by using RG (Renormalized Group) method and the percolation threshold is 0.5

Coarse Grain Transformation

Suppose the lattice constant of square lattice is a. We pick out a cell (length=2a) and the probability that its bond is occupied is p'.

We can thus define the RG as
$$p' = \sum_{K, a} A_{K}(a) p^{K} (1-p)^{5-K}$$

where $A_{K}(a) = \begin{cases} 1 & \text{if the occupied bond is a percolate state} \\ 0 & \text{other} \end{cases}$

Here the total lattice bonds we need to consider is 5, which is easily seen in the following figure.



Fig 4.1

It's easily seen that $p'=2p^2(1-p)^3+8p^3(1-p)^2+5p^4(1-p)+p^5(4.1)$ Taking $8p^3(1-p)^2$ as an example, referring to the blue line in Fig 4.1, if all the up bonds are occupied, we have $C_3^1p^3(1-p)^2$

It the same when down bonds are all occupied. The third case is the case in Fig 4.1 where the marked (with p) bond is occupied, and the case of its counterpart. Therefore we totally have $2C_3^1p^3(1-p)^2 + 2p^3(1-p)^2 = 8p^3(1-p)^2$ We now search for the fixed point in (4.1)

 $p = 2 p^{2} \cdot (1-p)^{3} + 8 p^{3} \cdot (1-p)^{2} + 5 p^{4} \cdot (1-p) + p^{5} \xrightarrow{\text{solutions for } p} 0, 1, \frac{1}{2}, \frac{1}{2} + \frac{1}{2} \sqrt{5}, \frac{1}{2} - \frac{1}{2} \sqrt{5}$

Because 0<p<1, so only 0, 1, $\frac{1}{2}$ is applicable. 2 $p^2 \cdot (1-p)^3 + 8 p^3 \cdot (1-p)^2 + 5 p^4 \cdot (1-p) + p^5 \rightarrow$



It's easily seen that $\frac{1}{2}$ is a unstable fixed point and so is the critical point. Therefore $\frac{1}{2}$ is the percolation threshold on square lattice.

Reference

1.Introduction to Percolation Theory 2nd ed - D. Stauffer, A. Aharony (T&F, 2003) WW 2.Yang, Z. R. (2007). "Quantum Statistic Physics." High Education Press: 421.

Mean-Field Blume Capel Model

Edited by Li, Zimeng

Contents:

1. Definition

- 1.1 Tricritical Ising Model
- 1.2 Blume, Emery and Griffiths (BEG) Model

2. Phase Transition Diagram

3. Mean Field Solution of the Blume-Capel model

- 3.1 One Dimension Case
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- 3.3 Observable and Critical Exponents

1. Definition

In order to introduce in the Blume Capel Model, we would like to take a review of the tricritical Ising model and the Blume, Emery and Griffiths (BEG) Model.

1.1 Tricritical Ising Model

The first generalization of Ising criticality is obtained when considering an Ising antiferromagnet with Hamiltonian

$$\mathcal{H} = +J\sum_{\langle i,i'\rangle}\sigma_i\sigma_{i'} - B\sum_{s}\sigma_i - B\sum_{s}\sum_{s}(-1)^i\sigma_{i'}$$
 where B_s is called the staggered magnetic

field.

It is easily drawn that the tricritical Ising model falls to normal Ising Model when B and B_s =0. When considering the Hamiltonian above fully, we can draw the phase diagram of the tricritical Ising model.See Fig 1.1.1





In the above diagram, the (broken) first-order line and the (full) line of Ising critical points (second-order) meet at the tricritical point (Bt,Tt)shown as black dot.

Phase diagram of above has been realized in 3D metamagnetic systems such as Ising model with annealed vacancies, modeled by a vacancy variable $v_i = 0, 1$

and the Hamiltonian
$$\mathcal{H} = -J \sum_{\langle i, i' \rangle} \sigma_i \sigma_{i'} v_{i' j'} - \mu \sum v_i^2 - B \sum \sigma_{i' j} v_{j'} v_{j'}$$

If we define $s_i = \sigma_i v_i$, which takes the value $s_i = -1$, 0, 1, then we obtain the Blume Capel model with Hamiltonian

$$\mathcal{H} = -J \sum_{\langle i, i' \rangle} s_i s'_i - B \sum_{i} s_i - \mu \sum_{j} s_i^2 (1.1.1)$$

1.2 Blume, Emery and Griffiths (BEG) Model

Historically, the Blume-Capel model is a simplification of the BEG model. The spin-1 model

 $\mathcal{H} = -J \sum_{\langle i, i' \rangle} s_i s_{i'} (1 + as_i s_{i'}) + \Delta \sum s_i^2$ was introduced by Blume, Emery and Griffiths. Here

J is the usual Ising coupling, a is the constant of biquadratic exchange and the parameter

 Δ stand for the interaction of the spins with the crystal field at each site i. If we set a=0, it becomes the Blume-Capel model (1.1.1) with B=0. Here $s_i = 0, \pm 1. s_i = \pm 1$ is well known for the normal Ising model, while $s_i = 0$ can be viewed as Ising model with vacancies, or zero occupation, or the site with spin annealed.(see Sec. 1.1)

2. Phase Transition Diagram

Considering $\mathcal{H} = -J \sum_{\langle i, i' \rangle} s_i s'_i - B \sum_{i} s_i - \mu \sum_{j} s_i^2$ with B=0. It is easily drawn that when $\mu \to -\infty$, and $s_i = 0$, the model returns to normal Ising model because μs_i is limited value, thus the Hamiltonian is rewritten as Ising Hamiltonian:

$$\mathcal{H} = -J \sum_{\langle i, i' \rangle} s_{i'} s_{j'} - \sum_{\mu's_{i'}} where \mu' = \mu s_{i'}$$

Replace μ with Δ (see Sec. 1.2), we rewrite the Hamiltonian of the simplified Blume-Capel model as:

$$\mathcal{H} = -J \sum_{\langle i, i' \rangle} s_i s_{i'} + \Delta \sum s_i^2$$

The ordered states with $s_i = \pm 1$ have energy per site $\Delta - J$, while the state with $s_i = 0$ has zero energy. The ground state of an ordered state must thus guarantee the condition that $\Delta > J$, and we therefore conclude that there is a zero-temperature transition from the state with $s_i = 0$ to ordered state with $s_i = \pm 1$ at $\Delta = J$. This is a first order transition, in the sense that there are discontinuities in the magnetization and the derivative of the energy with respect to Δ . Also the correlation length is zero at this point, since there are no fluctuations. The first order transition must persist for some length since there is a convergent radius for the perturbation. Therefore, along the boundary of the ordered state and the disordered state, there is a change from the first order transition to the second order transition. And the transition point is called the tricritical point. The figure is shown below: (We can compare it to the tricritical Ising model Fig 1.1.1)



Fig 2.1

3. Mean Field Solution of the Blume-Capel model

Considering simplified Blume-Capel model Hamiltonian $\mathcal{H} = -\frac{J}{2} \sum_{\langle i, i' \rangle} s_i s_{i'} + \Delta \sum s_i^2$, where

 $\frac{1}{2}$ is a factor when the sum of different sites is repeated twice.

3.1 One Dimension Case

The central idea of mean field theory is to approximate the interacting case $-\frac{J}{2}\sum_{\langle i,i'\rangle}s_is_{i'i'}$

by a simpler noninteracting partition function.

We first rewrite

$$s_{i}s_{i'} = (M + s_{i} - M)(M + s_{i'} - M) = M^{2} + M \cdot (s_{i} - M) + M \cdot (s_{i'} - M) + o(\delta^{2}s_{i}) \text{ where}$$

 $\delta s_i = s_i - M$

Therefore the partition function can be written as

$$Z = Tre^{\int \frac{J}{2}\beta \sum_{\langle i, i' \rangle} \left(M \cdot \left(s_{i} + s_{i'} \right) - m^{2} \right) - \beta \Delta \sum s_{i}^{2}} = Tre^{-\frac{NJ}{2}\beta M^{2} + \beta JM \sum s_{i} - \beta \Delta \sum s_{i}^{2}}$$
$$= Tre^{-\frac{NJ}{2}\beta M^{2} - \beta \Delta N'} (2 \cosh \beta JM)^{N'}$$

, where N' is the number of sites which either spin 1 or spin -1 occupies.

The above derivation of the last equation can be found at Homework 1.[2] in the Email package.

We have free energy
$$f = -\frac{k_B^T}{N} lnZ = \frac{1}{2} JM^2 + \frac{\Delta \cdot N'}{N} - \frac{N'k_B^T}{N} ln(2 \cosh \beta JM)$$

We can derive the critical point at which the free energy of the system is minimized, when we set to zero of the derivative of the free energy with respect to M. So we have

$$M = \frac{N'}{N} \tanh(\beta IM)$$
 (3.1)

The solution of M can be obtained through graphical method. See Fig 3.1





Alternatively, we can also draw the picture of f with respect to M to catch the critical point.

[1] Ising Model with $S_i = \pm 1, 0$

When $\Delta = 0$, the Blume-Capel model just corresponds to Ising model without outfield $f \approx \frac{1}{2}J\left(1 - \frac{N'}{N}\beta J\right)M^2 + const + o\left(M^4\right)$ (through Taylor expansion at M when $\Delta=0$) Since $\ln(1 + \cosh(x) - 1) \xrightarrow{\text{series in } x} \frac{1}{2} x^2 - \frac{1}{12} x^4 + o(x^6)$, we notice that the coefficient of M^4 in the free energy is positive. If $1 > \frac{N'}{N}\beta J$, the only minimum of free energy is at M=0, this corresponds to paramagnetic phase.

If $1 < \frac{N'}{N}\beta$, the minimum can be found in two places, M_0 and $-M_0$, which means the

symmetry $s \rightarrow -s$ is spontaneously broken. This corresponds to ordered states. See Figure below:



Which states $(M_0 \text{ or } - M_0)$ is chosen depends on how the limit of $\Delta \rightarrow 0$ is taken, since the applied field Δ will give rise to some non-zero magnetization. In the ferromagnetic phase this non-zero magnetization will survive even in the limit of $\Delta \rightarrow 0$. Therefore when $\Delta \neq 0$, the figure is different:





We thus conclude there will be a first order phase transition at the point when M^2 is

vanished at
$$1 = \frac{N'}{N}\beta J$$
 or $T_c = \frac{N'J}{Nk_B}$

[2] Blume-Capel Model

The Blume-Capel model is different from [1] in its additional term $\Delta \sum s_i^2$, which allows

the coefficient of M^4 in the free energy to change sign. Therefore the coefficient of M^4 may happen to be negative, and so the above diversity of free energy with respect to M can be interpreted in the following figure:





Here T_c , similar to T_c in [1], is also the first order phase transition critical point. (When M^2 in the free energy vanishes)

From Sec. 2 we know there is a tricritical point where the first order phase transition turns into the second order phase transition. The tricritical point can be obtained when both M^2 and M^4 vanishes.

3.2 Two Dimension Case

We give the result here without proof. On a square lattice, the Blume-Capel model

exhibits two equivalent, ferromagnetic ground states A and B, $s_i = \pm 1$, for $\frac{\Delta}{J} < 2$; and

one ground state, $s_i = 0$, for $\frac{\Delta}{J} > 2$. At $T_c(D/J)$ (with $T_c(2) = 0$) the ferromagnetic phases A

and B undergo an order-disorder transition which is second-order for $0 \le \frac{D}{I} < 1.945$,

tricritical for D/J \approx 1.945 and first order for 1.945 < $\frac{D}{J} \leq$ 2 (d=2).

3.3 Observable and Critical Exponents

Energy Density ϵ

$$InZ = -\frac{NJ}{2}\beta M^{2} - \beta \Delta N' + N' ln(2 \cosh \beta JM)$$
$$E = -\frac{\partial}{\partial \beta} InZ = \frac{NJ}{2}M^{2} - N' JM tanh(\beta JM)$$
$$\epsilon = \frac{E}{N} = \frac{J}{2}M^{2} - \frac{N'}{N} JM tanh(\beta JM)$$

Specific Heat C

$$C = \frac{\partial}{\partial T} E = \frac{N' J^2 M^2}{k_B T^2} \operatorname{coth}(\beta J M)$$

Magnetization Density

 $M = \frac{N'}{N} \operatorname{tanh}(\beta JM)$ (see 3.1), we can only solve it by using graphical method.

Susceptibility

To be implemented.

Critical Exponents

The numerical results for the tricritical point are for the Blume-Capel quantum spin model with

 γ = 0, α = 0.910207, β = 0.415685, ζ = 0.56557

Reference

1.Cardy J. Scaling and Renormalization in Statistical Physics (CUP, 1996)(T)(252s)
2.Uzunov D.I. Introduction to theory of critical phenomena (WS)(KA)(T)(461s)
3.Henkel M. Conformal invariance and critical phenomena (Springer, 1999)(ISBN 354065321X)(K)(T)(434s)

4.Yang, Z. R. (2007). "Quantum Statistic Physics." High Education Press: 421. 5.Domb C., Lebowitz J.L. (eds.) Phase Transitions and Critical Phenomena v.12 (Academic

Press, 1988)(ISBN 0122203127)(T)(K)(498s)

Ising Model

Edited by Li, Zimeng

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- 1. Describe the exact solution of Ising model is 1D
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- 1.2 Considering Outfield
- 2. The exact solution of the critical point on the square lattice
- 3. Summarize the critical exponent for d>2

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4.3 Use duality relation to locate the critical point of the ordinary Potts model on square lattice

1. Describe the exact solution of Ising model is 1D

1.1 Taking no regard of outfield

$$H = -J \sum_{i} s_{ij}^{N}$$

$$Z = e^{\beta J \sum_{i} s_{ij}^{N}}$$
[1]Taking free border condition
Define $\eta_i = s_{ij}^{N}$ then $\eta_i = \begin{cases} -1 \quad S_i = -S_{i+1} \\ 1 \quad S_i = S_{i+1} \end{cases}$
So, $Z = \sum_{\{\eta_i\}} e^{\beta J \sum_{i} \eta_i} = 2[2 \cosh(K)]^{N-1}$, $K = \beta J$
Correlation Function:G[N]=<
 $S_{ij}^{N} > = \frac{1}{Z} \sum_{i} \eta_i e^{K \sum_{i} \eta_i} = \frac{\partial^N}{\partial K^N} Z = (\tanh(K))^N = e^{-N/n(\coth(K))} = e^{-N\xi}$
 $\xi = \frac{1}{\ln(\coth(K))}$ is correlation length,
Thus, we can plot the relation of correlation function and r or N



We will derive observables below:

1. Energy

$$Z := \beta \rightarrow 2 \left(2 \cosh(\beta \cdot J) \right)^{N-1}$$

$$Z := \beta \rightarrow 2 \left(2 \cosh(\beta \cdot J) \right)^{N-1}$$

$$Z := \beta \rightarrow -\frac{\partial}{\partial \beta} \ln(Z(\beta))$$
(1)

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(5)

(8)

$$-\frac{9 \sinh\left(\frac{1}{K T}\right)}{\cosh\left(\frac{1}{K T}\right)}$$

 $\int diff((5), T)$

$$\frac{9}{\kappa T^{2}} - \frac{9 \sinh\left(\frac{1}{\kappa T}\right)^{2}}{\cosh\left(\frac{1}{\kappa T}\right)^{2} \kappa T^{2}}$$
(6)

>
$$eval\left((6), \left[T = \frac{1}{K \cdot \beta}\right] \right)$$

9 $K \beta^{2} - \frac{9 \sinh(\beta)^{2} K \beta^{2}}{\cosh(\beta)^{2}}$
(7)
=> $eval((7), [K=1])$

9
$$\beta^2 - \frac{9 \sinh(\beta)^2 \beta^2}{\cosh(\beta)^2}$$

> smartplot(**(8)**)







So, 1 D Ising has no phase change at none-zero temperature, or 1 D Ising model has no phase change;

4. Partition Function

$$Z = 2 \left(2 \cosh(K) \right)^{N-1} \xrightarrow{\text{evaluate at point}} Z = 1024 \cosh(K)^9 \rightarrow$$



- 5. Magnetism Intensity =0
- 6. Magnetism susceptibility =0

1.2 Considering Outfield

1. Magnetization

First we should derive the partition function by using the matrix method - Taking the periodic border condition,

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

$$Z = \sum_{s_{1}} \sum_{s_{2}} \dots \sum_{s_{N}} e^{-\beta \left(-J \sum_{i=1}^{N} s_{i+1} - W \sum_{i=1}^{N} s_{i} \right)} = \sum_{s_{1}} \sum_{s_{2}} \dots \sum_{s_{N}} \Pi e^{\beta J s_{i+1} + \frac{\beta W}{2} \left(s_{i} + s_{i+1} \right)}$$

Define matrix
$$\langle s_{j}^{J} P | s_{i+1} \rangle = e^{\beta J s_{j+1}^{c} + \frac{\beta W}{2} (s_{i}^{c} + s_{i+1})}$$

Then Z=tr(P^{N}), $W = \mu B$
and $P = \begin{bmatrix} e^{\beta J + \beta \cdot \mu \cdot B} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J - \beta \cdot \mu \cdot B} \end{bmatrix} \xrightarrow{\text{eigenvalues}}$
 $\left[\left[\frac{1}{2} e^{\beta J - \beta \mu \cdot B} + \frac{1}{2} e^{\beta J + \beta \cdot \mu \cdot B} + \frac{1}{2} e^{\beta J - \beta \cdot \mu \cdot B} e^{\beta J + \beta \cdot \mu \cdot B} + (e^{\beta J + \beta \cdot \mu \cdot B})^{2} + 4 (e^{-\beta J})^{2} \right] \right]$
 $\left[\frac{1}{2} e^{\beta J - \beta \cdot \mu \cdot B} + \frac{1}{2} e^{\beta J + \beta \cdot \mu \cdot B} e^{\beta J + \beta \cdot \mu \cdot B} + (e^{\beta J + \beta \cdot \mu \cdot B})^{2} + 4 (e^{-\beta J})^{2} \right] \right]$
 $\left[\frac{1}{2} e^{\beta J - \beta \cdot \mu \cdot B} + \frac{1}{2} e^{\beta J - \beta \cdot \mu \cdot B} e^{\beta J + \beta \cdot \mu \cdot B} + (e^{\beta J + \beta \cdot \mu \cdot B})^{2} + 4 (e^{-\beta J})^{2} \right] \right]$
 $\lambda_{1} := \frac{1}{2} e^{\beta J - \beta \cdot \mu \cdot B} + \frac{1}{2} e^{\beta J + \beta \cdot \mu \cdot B} e^{\beta J + \beta \cdot \mu \cdot B} + (e^{\beta J + \beta \cdot \mu \cdot B})^{2} + 4 (e^{-\beta J})^{2}$
 $\frac{1}{2} e^{\beta J - \beta \cdot \mu \cdot B} + \frac{1}{2} e^{\beta J + \beta \cdot \mu \cdot B} e^{\beta J - \beta \cdot \mu \cdot B} e^{\beta J + \beta \cdot \mu \cdot B} + (e^{\beta J + \beta \cdot \mu \cdot B})^{2} + 4 (e^{-\beta J})^{2}$
(14)

$$+ \frac{1}{2} \sqrt{\left(e^{\beta J - \beta \mu B}\right)^{2} - 2 e^{\beta J - \beta \mu B} e^{\beta J + \beta \mu B} + \left(e^{\beta J + \beta \mu B}\right)^{2} + 4 \left(e^{-\beta J}\right)^{2}} \lambda_{2} := \frac{1}{2} e^{\beta J - \beta \mu B} + \frac{1}{2} e^{\beta J + \beta \mu B} - \frac{1}{2} \sqrt{\left(e^{\beta J - \beta \mu B}\right)^{2} - 2 e^{\beta J - \beta \mu B} e^{\beta J + \beta \mu B} + \left(e^{\beta J + \beta \mu B}\right)^{2} + 4 \left(e^{-\beta J}\right)^{2}} \frac{1}{2} e^{\beta J - \beta \mu B} + \frac{1}{2} e^{\beta J + \beta \mu B}$$
(15)

$$-\frac{1}{2}$$

$$\sqrt{\left(e^{\beta J-\beta \mu \cdot \theta}\right)^{2}-2 e^{\beta J-\beta \mu \cdot \theta} e^{\beta J+\beta \mu \cdot \theta}+\left(e^{\beta J+\beta \cdot \mu \cdot \theta}\right)^{2}+4 \left(e^{-\beta J}\right)^{2}}$$

$$F=-KTln\left(\lambda_{1}^{N}+\lambda_{2}^{N}\right)$$

$$M=-\frac{\partial}{\partial B}F=\frac{NKT\left(\lambda_{1}^{N-1}-\frac{\partial}{\partial B}\lambda_{1}+\lambda_{2}^{N-1}-\frac{\partial}{\partial B}\lambda_{2}\right)}{\lambda_{1}^{N}+\lambda_{2}^{N}}$$

$$\frac{\partial}{\partial B}\lambda_{1,2}=\beta \mu \left(e^{\beta J}\sinh(\beta \mu \cdot \theta)\pm\frac{e^{2\beta J}\sinh(\beta \mu \cdot \theta)\cosh(\beta \mu \cdot \theta)}{\left(e^{-2\beta J}+e^{2\beta J}\sinh^{2}(\beta \cdot \theta)\right)^{\frac{1}{2}}}\right)=$$

$$\pm\frac{\beta \mu e^{\beta J}\sinh(\beta \mu \cdot \theta)\lambda_{1,2}}{\left(e^{-2\beta J}+e^{2\beta J}\sinh^{2}(\beta \mu \cdot \theta)\right)^{\frac{1}{2}}}$$

$$(1)J=0$$

$$M:=\frac{N\cdot\mu\cdot\sinh(\beta\cdot\mu\cdot \theta)\left(\lambda_{1}^{N}-\lambda_{2}^{N}\right)}{\left(e^{4\beta \cdot J}+\left(\sinh(\beta\cdot\mu\cdot \theta)\right)^{2}\right)^{\frac{1}{2}}\left(\lambda_{1}^{N}+\lambda_{2}^{N}\right)}}$$

$$\left(100 \sinh(\beta \cdot \theta)\left(\left(\frac{1}{2}e^{-\beta \cdot \theta}+\frac{1}{2}e^{\beta \cdot \theta}+\left(e^{\beta \cdot \theta}\right)^{2}+4\right)^{100}-\left(\frac{1}{2}e^{-\beta \cdot \theta}+\frac{1}{2}e^{\beta \cdot \theta}+\frac{1}{2}\sqrt{\left(e^{-\beta \cdot \theta}\right)^{2}-2e^{-\beta \cdot \theta}e^{\beta \cdot \theta}+\left(e^{\beta \cdot \theta}\right)^{2}+4}\right)^{100}\right)\right)\right)/\left(1$$



$$M := \frac{N \cdot \mu \cdot \sinh(\beta \cdot \mu \cdot \beta) \left(\lambda_{1}^{N} - \lambda_{2}^{N}\right)}{\left(e^{4\beta \cdot J} + (\sinh(\beta \cdot \mu \cdot \beta))^{2}\right)^{\frac{1}{2}} \left(\lambda_{1}^{N} + \lambda_{2}^{N}\right)}}{\left(100 \sinh(\beta) \left(\left(\frac{1}{2} + \frac{1}{2} e^{2\beta} + \frac{1}{2} \sqrt{1 - 2 e^{2\beta} + (e^{2\beta})^{2} + 4 (e^{-\beta})^{2}}\right)^{100}\right)\right) / \left(e^{4\beta} \left(\left(\frac{1}{2} + \frac{1}{2} e^{2\beta} - \frac{1}{2} \sqrt{1 - 2 e^{2\beta} + (e^{2\beta})^{2} + 4 (e^{-\beta})^{2}}\right)^{100}\right)\right) / \left(e^{4\beta} \left(\left(\frac{1}{2} + \frac{1}{2} e^{2\beta} + \frac{1}{2} \sqrt{1 - 2 e^{2\beta} + (e^{2\beta})^{2} + 4 (e^{-\beta})^{2}}\right)^{100}\right) + \left(\frac{1}{2} + \frac{1}{2} e^{2\beta} - \frac{1}{2} \sqrt{1 - 2 e^{2\beta} + (e^{2\beta})^{2} + 4 (e^{-\beta})^{2}}\right)^{100}\right) + \sinh(\beta) \left(\left(\frac{1}{2} + \frac{1}{2} e^{2\beta} + \frac{1}{2} \sqrt{1 - 2 e^{2\beta} + (e^{2\beta})^{2} + 4 (e^{-\beta})^{2}}\right)^{100}\right) + \left(\frac{1}{2} + \frac{1}{2} e^{2\beta} - \frac{1}{2} \sqrt{1 - 2 e^{2\beta} + (e^{2\beta})^{2} + 4 (e^{-\beta})^{2}}\right)^{100}\right) + \left(\frac{1}{2} + \frac{1}{2} e^{2\beta} - \frac{1}{2} \sqrt{1 - 2 e^{2\beta} + (e^{2\beta})^{2} + 4 (e^{-\beta})^{2}}\right)^{100}\right) + \left(\frac{1}{2} + \frac{1}{2} e^{2\beta} - \frac{1}{2} \sqrt{1 - 2 e^{2\beta} + (e^{2\beta})^{2} + 4 (e^{-\beta})^{2}}\right)^{100}\right) + \left(\frac{1}{2} + \frac{1}{2} e^{2\beta} - \frac{1}{2} \sqrt{1 - 2 e^{2\beta} + (e^{2\beta})^{2} + 4 (e^{-\beta})^{2}}\right)^{100}\right) + \left(\frac{1}{2} + \frac{1}{2} e^{2\beta} - \frac{1}{2} \sqrt{1 - 2 e^{2\beta} + (e^{2\beta})^{2} + 4 (e^{-\beta})^{2}}\right)^{100}\right) + \left(\frac{1}{2} + \frac{1}{2} e^{2\beta} - \frac{1}{2} \sqrt{1 - 2 e^{2\beta} + (e^{2\beta})^{2} + 4 (e^{-\beta})^{2}}\right)^{100}\right) + \left(\frac{1}{2} + \frac{1}{2} e^{2\beta} - \frac{1}{2} \sqrt{1 - 2 e^{2\beta} + (e^{2\beta})^{2} + 4 (e^{-\beta})^{2}}\right)^{100}\right) + \left(\frac{1}{2} + \frac{1}{2} e^{2\beta} - \frac{1}{2} \sqrt{1 - 2 e^{2\beta} + (e^{2\beta})^{2} + 4 (e^{-\beta})^{2}}\right)^{100}\right) + \frac{1}{2} + \frac{1}{2} e^{2\beta} + \frac{1}{2} \sqrt{1 - 2 e^{2\beta} + (e^{2\beta})^{2} + 4 (e^{-\beta})^{2}}}\right)^{100}$$



2. Magnetism susceptibility

$$M := \frac{N \cdot \mu \cdot \sinh(\beta \cdot \mu \cdot B) \left(\lambda_{1}^{N} - \lambda_{2}^{N}\right)}{\left(e^{4\beta \cdot J} + \left(\sinh(\beta \cdot \mu \cdot B)\right)^{2}\right)^{\frac{1}{2}} \left(\lambda_{1}^{N} + \lambda_{2}^{N}\right)}$$
2 Energy

$$Z := \lambda_1^N + \lambda_2^N$$

$$\left(\frac{1}{2} e^{\beta J - \beta \mu B} + \frac{1}{2} e^{\beta J + \beta \mu B}\right)$$
(17)

$$+ \frac{1}{2} \\ \sqrt{\left(e^{\beta J - \beta \mu B}\right)^{2} - 2 e^{\beta J - \beta \mu B} e^{\beta J + \beta \mu B} + \left(e^{\beta J + \beta \mu B}\right)^{2} + 4 \left(e^{-\beta J}\right)^{2}} \right)} \\ + \left(\frac{1}{2} e^{\beta J - \beta \mu B} + \frac{1}{2} e^{\beta J + \beta \mu B} - \frac{1}{2} \right) \\ - \frac{1}{2} \\ \sqrt{\left(e^{\beta J - \beta \mu B}\right)^{2} - 2 e^{\beta J - \beta \mu B} e^{\beta J + \beta \mu B} + \left(e^{\beta J + \beta \mu B}\right)^{2} + 4 \left(e^{-\beta J}\right)^{2}} \right)} \\ N$$

$$E := -\frac{\partial}{\partial\beta} \ln(Z)$$

$$\xrightarrow{evaluate at point B = 1, \mu = 1, l = 1, J = 1, N = 100}$$

$$-\left(100 \left(\frac{1}{2} + \frac{1}{2} e^{2\beta} + \frac{1}{2} \sqrt{1 - 2 e^{2\beta} + (e^{2\beta})^{2} + 4 (e^{-\beta})^{2}}\right)^{99} \left(e^{2\beta} + \frac{1}{4} \frac{-4 e^{2\beta} + 4 (e^{2\beta})^{2} - 8 (e^{-\beta})^{2}}{\sqrt{1 - 2 e^{2\beta} + (e^{2\beta})^{2} + 4 (e^{-\beta})^{2}}}\right) + 100 \left(\frac{1}{2} + \frac{1}{2} e^{2\beta} - \frac{1}{2} \sqrt{1 - 2 e^{2\beta} + (e^{2\beta})^{2} + 4 (e^{-\beta})^{2}}\right)^{99} \left(e^{2\beta} - \frac{1}{4} \frac{-4 e^{2\beta} + 4 (e^{2\beta})^{2} - 8 (e^{-\beta})^{2}}{\sqrt{1 - 2 e^{2\beta} + (e^{2\beta})^{2} + 4 (e^{-\beta})^{2}}}\right) \right) / \left(\left(\frac{1}{2} + \frac{1}{2} e^{2\beta} + \frac{1}{2} \sqrt{1 - 2 e^{2\beta} + (e^{2\beta})^{2} + 4 (e^{-\beta})^{2}}\right)\right) - \frac{1}{2} \sqrt{1 - 2 e^{2\beta} + (e^{2\beta})^{2} + 4 (e^{-\beta})^{2}} \right) + \frac{1}{2} \sqrt{1 - 2 e^{2\beta} + (e^{2\beta})^{2} + 4 (e^{-\beta})^{2}} + \frac{1}{2} e^{2\beta} + \frac{1}{2} \sqrt{1 - 2 e^{2\beta} + (e^{2\beta})^{2} + 4 (e^{-\beta})^{2}} + \frac{1}{2} e^{2\beta} + \frac{1}{2} \sqrt{1 - 2 e^{2\beta} + (e^{2\beta})^{2} + 4 (e^{-\beta})^{2}} + \frac{1}{2} e^{2\beta} + \frac{1}{2} e$$






5.Correlation function G

$$G = \langle s_{ij} \rangle = \frac{\left(k \cdot T\right)^2}{Z} \frac{\partial}{\partial B} \frac{\partial}{\partial B} Z \xrightarrow{evaluate at point B = 1, \mu = 1, l = 1, J = 1, N = 100}$$







Fig 12

2. The exact solution of the critical point on the square lattice

We define our effective Hamiltonian as $-\beta H = K \sum_{i \in A} s_i s_i + h \sum_{i \in A} s_i$ We introduce in the following variables: N $_+$: the number of spin - ups N : the number of spin – downs N $_{++}$: the number of spin - ups in nearest neighbours $N_{_}$: the number of spin – downs in nearest neighbours N $_{+-}$: the number of one spin – down and one spin – up in nearest neighbours We have $(Z_a is the coordinate number)$ $N_+ + N_- = N$ $Z_{a}N_{+} = 2N_{++} + N_{+-}$ $Z_{a}N_{-}=2N_{-}+N_{+-}$ Therefore $\sum_{\langle i,j \rangle} s_{ij} = N_{++} + N_{--} - N_{+-} = 4N_{++} - 2Z_{g}N_{+} + \frac{Z_{g}N_{+}}{2}$ $\sum_{i} s_{i} = N_{+} - N_{-} = 2N_{+} - N$ So $-\beta H = K \left(4N_{++} - 2Z_{g}N_{+} + \left(\frac{ZN}{2} \right) \right) + h(2N_{+} - N)$ We here introduce in the Bragg-Williams method We define $\frac{N_{+}}{N_{+}} = \frac{1}{2}(l+1)$ and $\frac{N_{-}}{N_{+}} = \frac{1}{2}(-l+1)$ We therefore rewrite the effective Hamiltonian as $-\beta H = \frac{N}{2} Z_{g} K \left(\frac{4N_{++}}{ZN_{-}} - 2I - 1 \right) + hNI$ We suppose $\frac{N_{++}}{\frac{Z}N} \approx \left(\frac{N_{+}}{N}\right)^2$

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We get
$$-\beta H = \frac{N}{2} Z_g K I^2 + h N I$$

Partition function Z=
$$\sum g(I)e^{-\beta H} = \sum \frac{N!}{\left(\frac{1}{2}N(1+I)\right)!\left(\frac{1}{2}N(1-I)\right)!}e^{\frac{N}{2}Z_{g}KI^{2} + hNI}e^{\frac{N}{2}Z_{g}KI^{2} + hNI}e$$

When $N \rightarrow \infty$, we replace InZ with its largest term. We use Sterlin formula and get $\frac{1}{N}InZ = \frac{1}{2}Z_gKI^2 + hI - \frac{1+I}{2}\ln\left(\frac{1+I}{2}\right) - \frac{1-I}{2}\ln\left(\frac{1-I}{2}\right)$ We can find when will the above equation gets its largest term by deriving it with

We can find when will the above equation gets its largest term by deriving it with respect to I and set it to zero, and we get

$$\ln\left(\frac{1+I}{1-I}\right) = 2h + 2Z_g K I \rightarrow I = \tanh\left(\frac{B}{k_B T} + \frac{ZJ}{k_B T}I\right) \rightarrow I = \tanh\left(\frac{ZJ}{k_B T}I\right) \text{ when } B = 0 \text{ (2.1)}$$

We find I happens to connect with M by $M = N_{+} - N_{-} = NI_{-}$

We can solve (2.1) by diagram method. See figure below





Here we define $\frac{Z_{g}}{k_{B}T} = \frac{T_{c}}{T}$

We have the solution through diagram method:

$$I=0 \left(\frac{\frac{Z}{g}}{k_{B}T} < 1\right)$$
$$I=\begin{cases} \pm I_{0} & \frac{Z}{g} \\ 0 & \frac{g}{k_{B}T} > 1 \end{cases}$$

It is easily seen that I=0 means there is no self-magnetization, which corresponds to high-temperature limit. I= $\pm I_0$ shows there are two ordered states or ferromagnetic

states in low temperature. Thus we obtain the critical temperature at

 $\frac{ZJ}{k_BT} = 1 \text{ or } T_c = \frac{ZJ}{k_B}$

3. Summarize the critical exponent for d>2

We will use d=2 for an example here. We simplify $I = \tanh\left(\frac{Z}{g} \frac{J}{k_B}I\right)$ as $L := \tanh\left(\frac{T}{T} \cdot L\right)$

[1] β

We need to solve a transcendental equation when trying to obtain L(definition see below)

Especially when there is no outfield, we have

$$L := \tanh\left(\frac{T}{T} \cdot L\right), L \text{ satisfies } \frac{1}{2}(L+1) = \frac{N_{+}}{N}, \text{ where } N_{+} \text{ is the total number of spin}$$
$$-up \text{ particles}$$
$$\xrightarrow{\text{evaluate at point}}$$

tanh(0.75 *L*)

evaluate at point

 $tanh(1.5 L) \rightarrow$





Partition Function has the following expression:

 $\frac{\ln Z}{N} = \beta \left(\frac{1}{2} \gamma L^2 + WL\right) - \frac{1+L}{2} \ln \frac{1+L}{2} - \frac{(1-L)}{2} \ln \left(\frac{1-L}{2}\right), \text{ where} \gamma \text{ is the coordination}$ number,W is magnetism energy and J is the energy of spin interaction. $T > T_{c, L} = 0; T < T_{c, L} = L_0$

٢

$$U = -\frac{\partial}{\partial \beta} \ln Z = \begin{cases} 0 & T > T_{c} \\ -\frac{1}{2} N \gamma L_{0}^{2} & T < T_{c} \end{cases}$$
$$C = \frac{d}{d T} U = \begin{cases} 0 & T > T_{c} \\ -\frac{1}{2} N \gamma \frac{d}{d T} L_{0}^{2} & T < T_{c} \end{cases}$$

Therefore, heat capacity experience mutation at T_{a}

[3]γ

When there exists outfield, the transcendental equation is L=tanh $\begin{pmatrix} T \\ -\frac{c}{T}L + \frac{B}{k_B T} \end{pmatrix}$ $T > T_{c,}B \rightarrow 0$, we have $I \ll 1$ (the trend can also draw from fig 1),

thus we can replace tank with x, so
$$L = \frac{B}{k_B(T - T_c)}$$

 $M = N\mu L \approx \frac{N\mu B}{k_B(T - T_c)}$, therefore $\chi = \left(\frac{\partial M}{\partial B}\right)_T = \frac{N}{k_B(T - T_c)} \sim (T - T_c)^{-1}$
Therefore $\gamma = -1$

[4]
$$\delta$$

 $T = T_{C,}$ we have $L = \tanh\left(\frac{B}{k_B T} + L\right) \sim B + L - \frac{1}{3}(B + L)^3 \Rightarrow B \sim L^3 \Rightarrow M \sim L \sim B^{\frac{1}{3}}$
Therefore, $\delta = \frac{1}{3}$

4. Summarize the generalization of Ising model to Potts model

4.1 Ordinary Potts model

The difference of q-states Potts model to Ising model is that it allow to take q different values on each site

$$\mathcal{H} = -J \sum_{\langle i, i' \rangle} \delta(\theta_i - \theta_{i'}) \text{ where } \theta = 0, 1, ..., q-1$$

The Ising model is recovered if q=2. Defining $\sigma = 2\left(\theta - \frac{1}{2}\right)$, we have

 $\delta(\theta_i - \theta_{i'}) = \frac{(\sigma_i \sigma_{i'} + 1)}{2}$ and, up to a multiplicative factor in the coupling J and a trivial

additive constant, the Ising Hamiltonian $\mathcal{H} = -J \sum_{\langle i, i' \rangle} \sigma_i \sigma_{i'}$ recovers.

4.2 Chiral Potts model

A variant of q-states model is the clock model, but which is equivalent to the q-state Potts model only for q=2,3. The clock model is defined as

$$\mathcal{H} = -J \sum_{\langle i, i' \rangle} \cos\left(\theta_{i} - \theta_{i'}\right) \text{ where } \theta = \frac{2 \pi r}{q}, r = 0, 1, ..., q - 1$$

An variant of the clock model is the chiral Potts model, which sometimes is referred to as asymmetric clock model. The Hamiltonian is given as

$$\mathcal{H} = \mathcal{H} = -J_{z} \sum_{\langle i, i' \rangle} \cos(\theta_{i+1, i'} - \theta_{i, i'} - \delta_{x}) - J_{y} \sum_{\langle i, i' \rangle} \cos(\theta_{i+1, i'} - \theta_{i, i'} - \delta_{y})$$

where (i,i')labels the points on the square lattice and $\delta_{\!\chi}^{}, \delta_{\!\chi}^{}$ are free parameters.

4.3 Use duality relation to locate the critical point of the ordinary Potts model on square lattice

In q-states model, there is a disordered high-temperature phase and an ordered lowtemperature phase. They are related through a duality transformation. The partition function can be written as

$$Z = \sum_{\langle \theta \rangle} e^{\frac{\kappa \sum_{\langle i, i' \rangle} \delta(\theta_{i} - \theta_{i'})}{\langle i, i' \rangle}} = \sum_{i, i'} \prod_{i' \in I} e^{\kappa \delta(\theta_{i} - \theta_{i'})} = \sum_{i, i'} \prod_{i' \in I} \left(1 + \nu \delta(\theta_{i} - \theta_{i'})\right) \text{ where } \kappa = -\beta J, \nu = e^{\kappa \delta(\theta_{i'} - \theta_{i'})}$$

Considering a square lattice with N sites, we can calculate the contribution of individual spin configuration in (4.3.1) in a graphical way. We draw a bond between nearest sites i and i' if each of them is occupied with a variable θ_i and $\theta_i = \theta_i$. We define the above configuration as graph G, and define b(G) as the number of bonds in G. We therefore have the contribution to the partition function as $v^{b(G)}$

The sum over all configurations can be rewritten as $\sum_{\langle \theta \rangle} = \sum_{G} \sum_{values}$, where the second sum refers to possible values of θ_i in a given cluster of G. We define n(G) as the number of disconnected nearest neighbours in the graph G, and so the second sum simply produce

a factor $q^{n(G)}$

Therefore Z=
$$\sum_{G} q^{n(G)} v^{b(G)}$$

Now we introduce in a dual lattice and dual bonds. See figure below.





The black dots are normal sites and the open dots are dual sites. Full lines make up graph G, and broken lines make up dual graph D. Note that the dual bond does not intersect with a bond of G.We define c(G) the number of loops in graph G and it's easily seen that each such loop would encircle a dual site. Each dual loop also encircles a normal site. We thus have

$$n(D) = c(G) + 1$$
$$n(G) = c(D) + 1$$

The Euler relation says that for any graph c(G) = b(G) + n(G) - N, where N is the number of sites in graph G

We define the total number of bonds is B=b(G)+b(D), and N^{\uparrow} as the number of sites in graph D

Therefore the partition function can be written in the language of dual graphs

$$Z = \sum_{D} v^{B-b(D)} q^{c(D)+1} = v^{B} \sum_{D} v^{-b(D)} q^{b(D)+n(D)-N^{*}+1} = v^{B} q^{1-N^{*}} \sum_{D} \left(\frac{q}{v}\right)^{b(D)} q^{n(D)}$$

At the limit of $N \rightarrow \infty$, we have B=2N, N=N^{*}, therefore we have $Z^* = v^2 n q^{1-N}$

$$\sum_{D} (v^*)^N q^{n(D)} \left(we define the dual coupling K^* = \frac{J^*}{T} through \frac{q}{v} = v^* = e^{K^*} - 1 \right)$$

Thus we can proof the self-duality relation

$${}_{N}\lim_{\to\infty}\left(\frac{1}{N}\ln Z\right) = {}_{N}\lim_{\to\infty}\left(\frac{1}{N}\ln Z^{*}\right) + \ln\left(\frac{e^{K}-1}{e^{K}-1}\right) \text{ where}$$
$$vv^{*} = \left(e^{K}-1\right) \cdot \left(e^{K}-1\right) = \frac{q}{v}v = q \text{ (4.3.2)}$$

Any singularity occurring in a thermodynamic quantity at a critical point $K = K_c$ is mapped through the duality transformation to another coupling $K = K_c^*$. And the critical point must be at the fixed point of the duality transformation. We thus solve the fixed point of

(4.3.2) and get
$$(e^{K} - 1)^{2} = q \rightarrow K_{c} = \ln(\sqrt{q} + 1) = \frac{J}{T_{c}} \rightarrow T_{c} = \frac{J}{\ln(\sqrt{q} + 1)}$$

The critical point is thus at $T_c = \frac{J}{\ln(\sqrt{q} + 1)}$

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Quantum Ising Model

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3.Suzuki-Trotter Formula

1. Describe the phase transition in Quantum Ising model

1.1 Introduction to Quantum Ising model

Quantum Ising model is the extension of Ising model to quantum situations, also a member of quantum spin model family.

1D quantum Ising model is also called quantum Ising chain. Instead of single spin direction in normal Ising model, the quantum Ising model uses three Pauli Matrixes to replace spin s (± 1).Similar to Ising model, we can define the Hamiltonian in Quantum Ising model:

$$\mathcal{H} = -J \sum \sigma_j^z \sigma_{j+1}^z - gJ \sum \sigma_j^x$$

where J>0 and $g \ge 0$ is a dimensionless coupling constant.

1.2 Phase Transition in Quantum Ising model

It can be shown through RG method that for non-zero temperatures, the critical behavior of the quantum Ising model reduces to the classical Ising Hamiltonian. For T = 0, however, quantum effects do become important and must be included in the analysis. We are not going to describe the finite-temperature phase transition here, but rather describe second-order phase transition at absolute zero temperature, where we can catch how a strong quantum effect modulates the phase transition.

In the thermodynamic limit $N \to \infty$, the ground state of \mathcal{H} exhibits a second order phase transition as g cross over a critical value g_{c} , we will illustrate below how to get the critical point of the phase transition.

First, consider the ground state for $g \ll 1$, when g=0, we have two degenerate ferromagnetic state.

$$\left| \Uparrow > = \sum \right| \uparrow >_{j}, \ \left| \Downarrow > = \sum \right| \downarrow >_{j}$$

We define the ferromagnetic moment $N_0 = \langle \uparrow | \sigma_j^z | \uparrow \rangle = -\langle \downarrow | \sigma_j^z | \downarrow \rangle$ At g=0 we have $N_0 = 1$, and even in the thermodynamic limit, this ground state still survives for a small range of g ($g < g_c$), but with $0 < N_0 < 1$. This can be proved by perturbation theory, and is also similar to the extension of first order line in the tricritical Ising model. (see Homework Blume-Capel Model Sec.2) Therefore the two ferromagnetic ground state remains and are still 2-fold degenerate. We notice that the symmetry is broken as the state is divided into two independent state $|\downarrow\rangle$ and $|\uparrow\rangle$.

Now consider the ground state for $g \gg 1$,when $g=\infty$, we have a single nondegenerate ground state which mix $|\downarrow \rangle$ and $|\uparrow \rangle$ (thus preserving all symmetries), the state is written as

 $\left| \Rightarrow > = 2^{-\frac{N}{2}} \prod \left(\left| \uparrow >_{j} + \right| \downarrow >_{j} \right) \text{ where } 2^{-\frac{N}{2}} \text{ is used for unity and } N \text{ is the number of sites} \right.$

We can verify that this state has no ferromagnetic moment (which is in z direction): $N_0 = \langle \leftarrow |\sigma_j^z| \Rightarrow \rangle = 0$ Similar to the case of $a \ll 1$ the ground state is preserved for a finite range of large

Similar to the case of $g \ll 1$, the ground state is preserved for a finite range of large g (g $> g_c$), we can view this ground state as a result of strong quantum fluctuations, as the mixed state shows quantum tunneling between spin up and spin down.

Therefore, the very different ground states of $g \ll 1$ and $g \gg 1$ indicates that the ground state cannot evolve smoothly as a function of g. There must be singularity at some point as a function of g for the quantum Hamiltonian, and g=1 is the nonanlytical point.

We thereby conclude the critical point for the second order quantum phase transition at $g=g_c = 1$

2.Derive the mapping: a d dimensional quantum Ising model can be mapped onto a d+1 dimensional classical Ising model.

The mapping is a bridge between quantum field theory and classical statistic physics.We shall see below how quantum quantities is connected with statistic quantities.

Considering a quantum mechanical d dimensional system, we define the time-evolution

operator $U(t', t) = e^{-\frac{l}{\hbar}H(t'-t)}$

Now take the time difference between t' and t to be infinitesimal, and we can write the transition amplitude \mathcal{Z} between $\begin{pmatrix} t \\ a \end{pmatrix}$ and $\begin{pmatrix} t \\ b \end{pmatrix}$ via the Feynman path integral

$$\mathcal{Z} = \int \prod_{i} U(t_{i+1}, t_{i}) dx_{i} = \int e^{-\frac{i}{\hbar}S} Dx \quad (2.1) \qquad \text{where } Dx = \prod x_{i} U(t_{i+1}, t_{i})$$
$$= e^{-\frac{i}{\hbar}S(t_{i+1}, t_{i})}, S(t_{1}, t_{2}) = \int_{t_{1}}^{t_{2}} \mathcal{L} dt \text{ is the action}$$

The above path integral language is based on the Suzuki-Trotter formula (see Sec.3). We can use it in quantum field theory to solve quantum Ising chain problems. A most common method is the Landao Ginzburg Wilson method or LGW method. In Sec. 1.2, we have given a simple description of states when $g \ll g_c$ and $g \gg g_c$. In order to discuss phenomena around the critical point, we have to turn to region of $g \approx g_c$.

Following the LGW strategy, we have to first identify an order parameter, which distinguishes the two very different ground phases described in Sec.1.2. This order parameter is just ferromagnetic moment N_0 (see Sec.1.2). Using coarse grain strategies in RG method, we coarse-grain these moments over some finite averaging region, and at long wavelengths this yields a real order parameter field φ , a measure of the local average of N_0 as defined in Sec.1.2.

The second step of LGW method is to write down a general field theory for the order parameter. As we are dealing with a quantum transition, the field theory has to extend over spacetime, with the temporal fluctuations representing the sum over histories in the Feynman path-integral approach. Thus we will write down (2.1) as the needed field theory, with the Hamiltonian replaced by the Landao Ginzburg Wilson Hamiltonian. We shall note that the integration above is d+1 spacetime (+1 is the time dimension) dimensional where Ising model corresponds to d=1 case, although it is a d dimensional quantum model.

We will now show how the above functional integral is connected with analogous expressions in the language of statistic mechanics.

We consider a statistical system on a d+1 dimensions hypercubic lattice, and define one of its dimension as time and the other d dimensions as space.

Consider two times τ_1 , τ_2 and their time-dependent Ising spins, the transfer matrix \mathcal{T} links the two configurations and has the elements:

$$\langle \{\sigma\}(\tau_1) | \mathcal{T} | \{\sigma\}(\tau_2) \rangle = e^{-\beta (\mathcal{H})} \text{ where } \mathcal{H} = \sum \mathcal{H}(\tau_1, \mathcal{H})$$

 $\tau_2 \rightarrow \tau_2$ is the classical Hamiltonian of the spin system and

 $\mathcal H$ include the sum over interaction pairs in the space direction. The partition function Z can thus be written:

$$\sum_{\{\sigma\}} e^{-\beta \mathcal{H}} = \sum_{\sigma} \langle \{\sigma\}(\tau_{\sigma}) | \mathcal{T} | \{\sigma\}(\tau_{1}) \rangle \langle \{\sigma\}(\tau_{1}) | \mathcal{T} | \{\sigma\}(\tau_{2}) \rangle \dots \langle \{\sigma\}(\tau_{\tau}) | \mathcal{T} | \{\sigma\}(\tau_{b}) \rangle$$
$$= tr \mathcal{T}^{M}$$

where M is the number of sites in time direction and periodic boundary condition $| \{\sigma\}(\tau_a) \ge |\{\sigma\}(\tau_b) > \text{ is assumed.}$

Compare the transition amplitude in (2.1) and the partition function in (2.2), we can write the correspondence between statistic physics and quantum mechanics.

$$\mathcal{T}^{M} \to e^{-\frac{i}{\hbar}S} \Rightarrow \mathcal{T} \to e^{-\frac{i}{\hbar}S\binom{t}{i+1}, t} \to U(t_{i+1}, t_{i}) \to e^{-\frac{i}{\hbar}H\binom{t}{i+1}, t} \to e^{-\frac{i}{\hbar}H\binom{t}{i+1}, t} \to e^{-\frac{i}{\hbar}H}$$

We have $\mathcal{T} = e^{-\frac{i}{\hbar}H}$ which the quantum Hamiltonian is defined.

Therefore we obtain a map of a d+1 dimensional problem with classical variables onto a d dimensional problem with quantum variables.

3.Suzuki-Trotter Formula

In the derivation of (2.1), we have used the Suzuki-Trotter Formula, which we will illustrate below:

The path integral arises from the fact that $e^{A} = \left(e^{\frac{A}{N}}\right)^{N}$ (3.1)

 $\frac{H(t-t_0)}{\hbar}$ and we

The propaganda operator is the Green function $G(t, t_0) = \Theta(t - t_0)e^{-\frac{iH(t - t_0)}{\hbar}}$ use (3.1) to rewrite it as

$$G(x, t; y) = \left\langle x \middle| e^{-\frac{\lambda(T+V)}{N}} e^{-\frac{\lambda(T+V)}{N}} \dots e^{-\frac{\lambda(T+V)}{N}} \middle| Y \right\rangle (3.2)$$

We can prove that
$$G(x, t; y) = \lim_{N \to \infty} \langle x | \left(e^{-\frac{\lambda(T)}{N}} e^{-\frac{\lambda(V)}{N}} \right)^{N} | Y \rangle$$
 (3.3)

The correspondence between (3.2) and (3.3) is just one example of Suzuki-Trotter Formula.We are not going to derive (3.3) from (3.2) here, as we have learned it in the Advanced Quantum Mechanics Course.However I would like to give the definition of general Suzuki-Trotter Formula below:

THEOREM: (Suzuki-Trotter Formula) Let A and be linear operators on a Banach space X such that , and A+B are the infinitesimal

generators of the contraction semigroups P^{t} , Q^{t} , and R^{t} respectively. Then for all

$$\varphi \in X$$
, we have $R^t \varphi = \lim_{N \to \infty} \left(P^{\frac{t}{n}} Q^{\frac{t}{n}} \right)'' \varphi$

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XY Model

Edited by Li,Zimeng

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1.Definition

XY Model is a continuous spin system with its spin s=(sx,sy), so it is a two-dimensional spin system with its two order parameters (n=2). This type of system (d=2, n=2) is called KT phase transition.

First we define $s_i = e^{i\theta_i}$, and here θ is the phase angle. Thus we can conclude the Hamiltonian for XY Model:

$$H = \sum_{ij} J_{ij} s_{ij} s_{j} = \sum_{ij} J_{ij} e^{i\theta_{ij} - i\theta_{j}} = \sum_{ij} J_{ij} cos(\theta_{ij} - \theta_{j})$$
(1.1)

Here the sum is counted so that i,j is not repeated, otherwise we have to multiply a $\frac{1}{2}$ factor ahead of (1.1)

Because the sum is calculated within the nearest neighbours, therefore we can expand

$$\cos\left(\theta_{i}-\theta_{j}\right) = 1 - \frac{1}{2!}\left(\theta_{i}-\theta_{j}\right)^{2} + \dots$$

and so H=
$$\sum J_{ij} \left(1 - \frac{1}{2!} \left(\theta_i - \theta_j \right)^2 \right)$$
 (1.2)

There are two parts in the above equation, the first part is irrelevant to spin, and we will omit it later. The second part can be transformed into continuous form by the following steps:

Define
$$k = i - j$$
, $\left(\theta_{i} - \theta_{j}\right)^{2} = \left(\frac{\partial}{\partial i}\theta_{i}\right)^{2} (i - j)^{2} = \left(\frac{\partial}{\partial i}\theta_{i}\right)^{2} (k)^{2}$,
therefore, $H = \sum_{ij} J_{ij} \left(\frac{1}{2!} \left(\theta_{i} - \theta_{j}\right)^{2}\right) = \iint_{k} J_{k} \left(\frac{1}{2!} \left(\frac{\partial}{\partial i}\theta_{i}\right)^{2} (k)^{2}\right) di dk$

2.XY Model is frequently used to describe the universal behavior of Mott-insulator and superfluidity phase transition. Why it is possible?

2.1 Mott-insulator

The first successful theory to describe the metals, insulators and transition between them is the noninteracting electron theory. This theory, or band theory, says that insulators have their highest filling band fully filled, and metals are just partially filled. But this theory failed to describe some metals and insulators that contradict the stated band filling. And later we found that electron-electron correlation, or the strong Coulomb repulsion of the filling electrons cannot be ignored, which leads to Mott's theory and the word - Mott insulator - to describe strong Coulomb repulsion state. The transition between metals and insulators is called MIT or Metal Insulator Transition.

In Mott's opinion, a large Coulomb repulsion would split the band in two. The lower band consists of electrons that occupy empty sites with each site one electron, while the upper band consists of sites fully filled by electrons. Thus the lower band would be full and leads to an insulator.

2.2 Hubbard Model

A prototype of theoretical understanding of MIT is the Hubbard model, which simplifies that electrons are only in a single band. Two most important parameters in Hubbard model is the correlation length U/t and the filling n, see Fig 2.2.1 below





There are two modes of the transition, the first one is filling-control MIT, or FC-MIT; And the second one, BC-MIT or band-control MIT is another case. We are not going to dip into the transitions here, but will take a look at how XY Model connects with the Mott insulator. U and t in the above figure will be defined below.

The Hamiltonian of the Hubbard Model in the second-quantized form is given by (where we define two wave operators - $\phi_{i\sigma}$ on site i and $\phi_{j\sigma}$ on site j)

$$\begin{aligned} \mathcal{H}_{H} &= \mathcal{H}_{t} + \mathcal{H}_{U} - \mu N \\ \mathcal{H}_{t} &= -t \sum_{\langle ij \rangle} \left(c_{i\sigma j\sigma}^{\dagger} c_{j\sigma} + H.c. \right), t = \int \phi_{i\sigma}^{*} \left(\frac{1}{2m} \right) \nabla^{2} \phi_{j\sigma} dx \text{ (2.2.1)} \\ \mathcal{H}_{U} &= U \sum_{i} \left(n_{i\uparrow} - \frac{1}{2} \right) \left(n_{i\downarrow} - \frac{1}{2} \right) \\ N &= \sum_{i\sigma} n_{i\sigma}, n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma} \\ U &= \iint dx dx' \left(\phi_{i\sigma}^{*}(x) \phi_{i\sigma}(x) \left(\frac{e^{2}}{|x - x'|} \right) \phi_{i-\sigma}^{*}(x') \phi_{i-\sigma}(x') \right) \end{aligned}$$

So \mathcal{H}_t is the kinetic part and U is the Coulomb potential. From the above Hamiltonian,

we can see Hubbard Model takes tremendous simplifications. It only takes into interacting of the nearest neighbours, and neglects multiband effect. However, it still works fine with MIT transitions and the Mott insulating phase. As we have stated before (see Sec. 2.1), the Mott insulating phase appears only at half filling sites. For the nearest-neighbour Hubbard model on a hypercubic lattice, the band structure of the noninteracting part is described as (see to (2.2.1))

$$\mathcal{H}_{t} = -t \sum_{\langle ij \rangle} \left(c_{i\sigma j\sigma}^{\dagger} c_{j\sigma} \right) = -2 t \sum_{k\sigma} \left(\sum_{v = x, y, \dots} cosk_{v} \right) c_{k\sigma k\sigma}^{\dagger} c_{k\sigma} = \sum_{k\sigma} \epsilon_{o}(k) \left(c_{k\sigma k\sigma}^{\dagger} c_{\sigma} \right), \text{ and } \epsilon_{o}(k) = -2 t \sum_{v = x, y, \dots} cosk_{v}$$
(2.2.2)

We have used Fourier transform in the above derivation. $c_{k\sigma}^{\dagger} = \sum_{i} e^{ik \cdot r_{i\sigma}^{\dagger}} c_{i\sigma}^{\dagger}$

Therefore, the parameters in the Hamiltonian depend on the direction of **i-j**. We compare (1.1) with (2.2.2), and thus we conclude that Mott-insulator can be described by XY model.

Note the Hubbard Model here has ignored degeneracy of both obitals' and spins'.It comes into degenerating Hubbard Model when introducing in obital and spin freedoms. To introduce in the spin interaction, we just need to multiply the original Hubbard

Hamiltonian with $\sum_{i,j} s_{i,j}$. It should be noted here that XY type or Ising type anisotropy for the spin exchange also easily occurs.

2.3 Superfluid-insulator transition

The situation for bosonic superfluid-insulator transition is simpler than the fermionic Mott-insulator transition, similar to the Hubbard Model, we can write the Hamiltonian for the interacting bosons as follows (with boson operators b_i^{\dagger} and b_i this time)

$$\mathcal{H} = \mathcal{H}_{0} + \mathcal{H}_{1}$$
$$\mathcal{H}_{0} = -\sum_{\langle ij \rangle} t_{ij} \left(b_{i}^{\dagger} b_{j} + H.c \right)$$
$$\mathcal{H}_{1} = U \sum_{i} n_{i}^{2} - \mu \sum_{i} n_{i} n_{i} = b_{i}^{\dagger} b_{i}$$

Similar to Fig 2.2.1, the system undergoes bandwidth-control phase transition from Mott insulator to superfluid when U/t is changed. Also, when U is large, the Mott

insulating phase appears similarly to the fermionic case.

We can use path integral method to solve the criticality. First we write down the action $S = \int L dt = \int (2T + \mathcal{H}) dt = \int (b_i^{\dagger} \partial_t b_i + \mathcal{H}) dt$

Similar to the derivation of Hubbard model, the above action can be mapped into d+1 dimensional XY model. So the universality of superfluid-insulator transition can also be described by XY model.

3.Mermin-Wagner theorem - 2D XY Model has no long-ranged ordering at non-zero temperature

3.1 Spin Correlation

To demonstrate the above theorem, we first look at the correlation of the spins between two sites:

 $\langle ss \atop ij \rangle = \operatorname{Re} \langle e^{i\left(\theta_{i} - \theta_{j}\right)} \rangle$, and we can demonstrate that this equals to $e^{-\left\langle \theta_{i}^{2} \right\rangle + \left\langle \theta_{i}\theta_{j} \right\rangle}$

Proof:
$$\langle ss_{ij} \rangle = \operatorname{Re} \langle e^{i\left(\theta_{i} - \theta_{j}\right)} \rangle = e^{-\langle \theta_{i}^{2} \rangle + \langle \theta_{ij} \rangle}$$

In order to demonstrate it, first we can draw from the second part of equ (1.2) that $(\theta_i - \theta_j)^2 \stackrel{\text{expand}}{=} \theta_i^2 - 2 \theta_i \theta_j + \theta_j^2$

So the Hamiltonian would have the common form of binomial $-\frac{1}{2}\sum_{i}\theta_{j}\theta_{i}$

We introduce a generate function
$$e^{i\sum_{i}\theta_{i}A_{i}}$$
, and
 $\left\langle e^{i\sum_{i}\theta_{i}A_{i}}\right\rangle = e^{i\mathbf{A}\cdot\langle\mathbf{\theta}\rangle - \frac{1}{2}\sum_{i}A_{j}J_{ij}^{-1}A_{i}} = e^{-\frac{1}{2}\sum_{i}A_{j}J_{ij}^{-1}A_{i}} = e^{i\mathbf{A}\cdot\langle\mathbf{\theta}\rangle - \frac{1}{2}\sum_{i}A_{i}J_{ij}^{-1}A_{i}} = e^{i\mathbf{A}\cdot\langle\mathbf{\theta}\rangle} = e^{i\mathbf{A}\cdot\langle\mathbf{\theta}\rangle - \frac{1}{2}\sum_{i}A_{i}J_{ij}^{-1}A_{i}} = e^{i\mathbf{A}\cdot\langle\mathbf{\theta}\rangle} = e^{i\mathbf{A}\cdot\langle\mathbf{\theta}\rangle}$

Here $\langle \mathbf{0} \rangle = 0$ can be easily drawn, so when we derivate A_i and A_j from the above equation, and set A_i and $A_j = 0$, we get,

$$\begin{pmatrix} \theta_{i}\theta_{j} \\ \theta_{j} \end{pmatrix} = J_{ij}^{-1}, \text{ and so } e^{-\frac{1}{2}\sum_{ij}A_{j}^{j-1}A_{j}} = e^{-\frac{1}{2}\left(A_{i} < \theta_{i}^{2} > + A_{j} < \theta_{j}^{2} > + A_{i} < \theta_{i}\theta_{j} > A_{j}\right)} = e^{-\left\langle\theta_{i}^{2}\right\rangle + \left\langle\theta_{i}\theta_{j}\right\rangle},$$

the above equation has set $A_{j} = 1$ and $A_{j} = -1$,

Proof done

Once we have solved $\langle \theta_i \theta_j \rangle$, we solve $\langle ss_i \rangle$, we use Fourier Transformation or FT method to solve $\langle \theta_i \theta_j \rangle$.

3.2 Solving $\left\langle \boldsymbol{\theta}_{i} \boldsymbol{\theta}_{j} \right\rangle$

We define correlation function $g_{ij} = \langle \theta_i \theta_j \rangle = \frac{1}{(2\pi)^d} \int g_{kk'} e^{i\mathbf{k}\cdot\mathbf{i}} e^{i\mathbf{k}\cdot\mathbf{j}} d^d k d^d k'$

and its counterpart in momentum space

$$g_{kk'} = \left\langle \theta_{k} \theta_{k'} \right\rangle = \frac{1}{\left(2\pi\right)^{d}} \int g_{ij} e^{i\mathbf{k}\cdot\mathbf{i}} e^{i\mathbf{k}'\cdot\mathbf{j}} d^{d}id^{d}j = g_{kk'} \delta_{k,-k} = \left\langle \left|\theta_{k}\right|^{2} \right\rangle, \text{ where } \mathbf{k}' = -\mathbf{k}$$

Because $\theta_{i} = \frac{1}{\left(2\pi\right)^{d}} \int \theta_{k} e^{i\mathbf{k}\cdot\mathbf{i}} d^{d}k = \sum \theta_{k} e^{i\mathbf{k}\cdot\mathbf{i}}$

Therefore

$$-\beta H = -\beta \sum_{ij} J_{ij} \left(\frac{1}{2!} \left(\theta_{i} - \theta_{j} \right)^{2} \right) = -\beta \int_{k} J_{k} \left(\frac{1}{2!} \left(\frac{\partial}{\partial i} \theta_{i} \right)^{2} \left(k \right)^{2} \right) di dk = -\kappa \int_{k} \left(\frac{\partial}{\partial i} \theta_{i} \right)^{2} di = -\kappa$$

$$\sum_{k} k^{2} |\theta_{k}|^{2}$$
(3.2.0)
where $\kappa = \frac{1}{2} \beta \int_{k} J_{k} k^{2} dk$,
so $g_{k} = g_{kk} = g_{kk}^{2} = \langle |\theta_{k}|^{2} \rangle = \frac{\int_{k} |\theta_{k}|^{2} e^{-\beta H} d\theta_{k}}{\int_{k} e^{-\beta H} d\theta_{k}} = \frac{2}{\kappa k^{2}}$

The above derivation used Gauss Integration, $\int x^2 e^{-ax^2} dx = \frac{\sqrt{\pi}}{2a^{\frac{3}{2}}}$, and $\int e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}$

When d=2, we get

$$=\frac{1}{\left(2\pi\right)^{2}}\int_{0}^{\infty}\frac{2}{\kappa}\,\mathrm{d}k_{r}\int_{0}^{2\pi}\frac{e^{ik\,r\cos\left(\theta\right)}}{k_{r}}\,\mathrm{d}\theta$$

Here r=i-j, k'=-k (see previous proof), and the last part has changed rectangular coordinates to polar coordinates,

saying $(k,k') \rightarrow (k_r, \theta)$, and k_r is just the momentum part of the lattice constant a, and

therefore we can approximate
$$\int_{0}^{\infty} dk_{r} = \int_{0}^{\frac{1}{a}} dk_{r}$$

Noticing $e^{ik_{r}cos(\theta)} = J_{0}(k_{r}) + 2\sum_{i} i^{n}J_{n}(k_{r})cos(n\theta)$, where J_{n} is Bessel function
We integrate the above equation by θ , and the second part $\int_{0}^{2\pi} cos(n\theta) d\theta = 0$,
Therefore, $g_{ij}(r) = \frac{1}{(2\pi)^{2}} \int_{0}^{\frac{1}{a}} \frac{2}{k} dk_{r} \int_{0}^{2\pi} J_{0}(k_{r}) d\theta = \frac{1}{\pi K} \int_{0}^{\frac{1}{a}} \frac{J_{0}(k_{r})}{k_{r}} dk_{r}$
 $g_{ij}(0) = \frac{1}{\pi K} \int_{0}^{\frac{1}{a}} \frac{1}{k} dk_{r} (3.2.1)$
as $J_{0}(0) = 1$, so $g_{ij}(r) - g_{ij}(0) = -\frac{1}{\pi K} \int_{0}^{\frac{1}{a}} \frac{1 - J_{0}(k_{r})}{k_{r}} dk_{r} (3.2.2)$,
as $|J_{0}(z)| \leq 1$ when z is real, therefore the largest part of equ (3.2.2) is $g_{ij}(0)$, and we can
approximate the lower limit of (3.2.1) by $\frac{1}{r} \to 0$

when $r \rightarrow \infty$ so $g_{ij}(r)$

$$-g_{ij}(0) = -\left\langle \theta_{i}^{2} \right\rangle + \left\langle \theta_{i}^{0} \right\rangle = -\frac{1}{\pi K} \int_{0}^{\frac{1}{a}} \frac{1 - J_{0}\left(\frac{k r}{r}\right)}{k_{r}} dk_{r} = -\frac{1}{\pi K} \int_{\frac{1}{r}}^{\frac{1}{a}} \frac{1}{k_{r}} dk_{r} + \dots = -\frac{1}{\pi K} \ln\left(\frac{r}{a}\right) (when r)$$

and there goes

$$\langle s_{ij} \rangle = \operatorname{Re} < e^{i\left(\theta_{i} - \theta_{j}\right)} > = e^{-\left\langle\theta_{i}^{2}\right\rangle + \left\langle\theta_{ij}^{0}\right\rangle} = e^{-g_{ij}(0) + g_{ij}(r)} = \left(\frac{r}{a}\right)^{-\frac{1}{\pi\kappa}} (3.2.4)$$

The long-range correlation is thus power-law decreasing (see (3.2.4)), and from (3.2.3) the angle deviation is increasing with r increased.

Therefore there couldn't be long-ranged correlation in 2D XY model.

4.Summarize the phase transition of Classical XY Model in 1D,2D,3D and more

4.1 1D Ising Model

The phase transition of Ising Model is done on another article - Ising Model (Homework 3)

4.2 2D XY Model - KT phase transition

The derivation in Section 3 is based on a continuous function of θ , and so inconsistent with situations when vortice state occur. The spin experience $2\pi q$ mutation in a loop and so we divide the loop into two parts, one is θ_{s} (describing vortice state) and the other is

 θ_{i} (describing spin state).

 $\theta = \theta_1 + \theta_2$, and $\oint \nabla \theta_1 \cdot ds = 2 \pi q$ and $\oint \nabla \theta_2 \cdot ds = 0$, we define $\theta_1 = q \theta_2$ Here q is the vortice quantum number, s is the arc length and ds=rd φ , *r is the* polar *coordinate*.

It can be easily drawn that $\nabla \theta = \frac{q}{r}$

Thus (3.2.0) can be rewritten as

$$-\beta H = -\kappa \int \left(\frac{\partial}{\partial i}\theta_{i}\right)^{2} di = -\kappa \int_{a}^{L} \left(\frac{q}{r}\right)^{2} r \, dr d \, \varphi = -2 \, \pi q^{2} \, \kappa \ln \left(\frac{L}{a}\right)$$

$$E = 2 \pi q^2 K' \ln\left(\frac{L}{a}\right)$$
, with $K' = \frac{K}{\beta}$

Here L is the length of lattice and a is lattice constant.

Whether the vortice state is stable can be decided by whether it can minimize the free energy at some conditions. We write down the free energy:

$$F = E - TS = 2 \pi q^{2} \mathcal{K}' \ln\left(\frac{L}{a}\right) - 2 k_{B} T \ln\left(\frac{L}{a}\right)^{2} = 2\left(\pi q^{2} \mathcal{K}' - 2 k_{B} T\right) \ln\left(\frac{L}{a}\right)$$
When $q = \pm 1$, we have $F = \begin{cases} Negative \ T > -\frac{\pi \mathcal{K}'}{2 k_{B}} \\ Positive \ T < -\frac{\pi \mathcal{K}'}{2 k_{B}} \end{cases}$, and $T = -\frac{\pi \mathcal{K}'}{2 k_{B}}$ is the transition

temperature when vortice state become stable or unstable.

And this $T = -\frac{\pi K'}{2 k_B}$ is thus called KT critical temperature T_{KT}

4.3 3D - Heisenberg Model

To be implemented

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Anyons Edited by Li, Zimeng

Contents:

1. Fractional Statistics

2. Kitaev model

3. Wen model

1. Fractional Statistics

Particles in 3D are either bosons and fermions. In 2D, however, particles can obey fractional statistics(anyons).

We use $e^{i\phi}$ of the wavefunction to identify the phase change and the statistics of identical particles. If the Hamiltonian doesn't contain long range interactions, but only two nearest neighbours, we have the two particle configuration doubly connected and a double interchange must give back the original wavefunction in 3D or higher dimensions, leading to even (bosons) or odd (fermions) wavefunction.

This effect makes φ accumulates 0 (bosons) and π (fermions) only, saying $\Psi \to e^{i\,\varphi}\Psi$, Φ

is 0 for bosons and 1 for fermions. While in 2D, the configuration space is infintely connected and φ is arbitrary(anyons). Anyons are particles which satisfy fractional

statistics. The case which $\frac{\Phi}{\pi}$ is $\frac{1}{2}$ corresponds to Quasiparticles half way between bosons and fermions, namely semions.

2. Kitaev model

See Ref.3 and 4

3. Wen model

See Ref.3 and 4

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Renormalization Group

Edited by Li, Zimeng

Contents:

1. Gauss Model

- 1.1 Introduction
- 1.2 Momentum Space Gauss Model
- 1.3 Renormalization Group in Momentum Space
- 1.4 Derive the Gaussian fix points and Critical exponents

2. Define RG in the language of Ginzburg-Landau model

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- 3. Derive the new fixed point in d=4- ϵ dimensions and the associated critical exponents
- 4. Explain the Universality by RG

1.Gauss Model

1.1 Introduction

Gauss model is a generalization of Ising model. We extend the domain of s, in Ising

model to infinity, and introduce in weighing function $W(\{s_i\}) = \prod_{i=1}^{N} \delta(s_i^2 - 1)$

Therefore the partition function changes to $Z = \int_{-\infty}^{\infty} \prod_{i=1}^{N} \delta(s_i^2 - 1) e^{K \sum_{j=1}^{N} s_j s_j} ds_1 ds_2 \dots ds_{N'}$

where $K = \frac{J}{k_B T}$

Actually, Z does not vanish only when $s_i = \pm 1$, which corresponds to Ising model.

In Gauss model we change the weighing function to the form $W = \prod_{i=1}^{N} e^{-\frac{b}{2}s_i^2}$ to ensure convergence since the domain has been extended to infinity.

Therefore the partition function
$$Z = \int_{-\infty}^{\infty} e^{\kappa \sum_{\langle i,j \rangle}^{N} s_{ij} - \frac{b}{2} \sum_{j} s_{i}^{2}} ds_{1} ds_{2} \dots ds_{N}$$
 with

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$$-\beta H = K \sum_{\langle i,j \rangle}^{N} s_{ij} - \frac{b}{2} \sum s_{i}^{2} (1.1.1)$$

Adding outfield, we have the effective Hamiltonian $-\beta H = K \sum_{\langle i,j \rangle}^{N} s_{ij} - \frac{b}{2} \sum s_{ij}^{2} + h \sum s_{ij}$

1.2 Momentum Space Gauss Model

Changing it to momentum space by FT method, we have

$$s_{i} = \frac{1}{V} \sum s(k) e^{ikr} = \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{1}{(2\pi)^{d}} s(k) e^{ikr} d^{d}k \text{ and } s(k) = a^{d} \sum_{i=1}^{N} e^{-ikr} s_{i}, \text{ where the range (}$$

 $-\frac{\pi}{a}, \frac{\pi}{a}$) is the first Brillouin zone and a is the lattice constant. a^d is the volume of primitive cell and we have $V = Na^d$

The first term of (1.1.1) is rewritten as

$$\begin{split} \kappa \sum_{\langle i,j \rangle}^{N} s_{j} &= \\ \frac{\kappa}{2 \sqrt{2}} \sum_{\langle i,j \rangle} \sum_{k',k} s(k) e^{ikr_{j}} s(k') e^{ikr_{j}} &= \frac{\kappa}{2 \sqrt{Na^{d}}} \sum_{\langle i,j \rangle} \sum_{k',k} s(k) e^{ik \binom{r_{i}-r_{j}}{2}} s(k') e^{i(k+k')r_{j}} \\ &= \frac{\kappa}{2 \sqrt{Na^{d}}} \sum_{k',k} s(k) s(k') \sum_{i-j} e^{ik \binom{r_{i}-r_{j}}{2}} \sum_{j} e^{i(k+k')r_{j}} \\ &= \frac{\kappa}{2 \sqrt{a^{d}}} \sum_{k',k} B(k) \delta(k'+k) s(k) s(k') \\ &= \frac{\kappa}{2 \sqrt{a^{d}}} \sum_{k',k} B(k) s^{2}(k) \end{split}$$

where B(k)=K

$$\sum_{i=j}^{ik \binom{r_i - r_j}{l}} = \kappa \left(e^{ik_1 a} + e^{-ik_1 a} + e^{ik_2 a} + e^{-ik_2 a} + \dots \right) = 2 \kappa \left(\cos k_1 a + \cos k_2 a + \dots + \cos k_a a \right) (1.2.1)$$

and $\frac{1}{N} \sum_{i}^{i(k+k')r_j} = \delta(k'+k)$

Note that when calculating B(k) only nearest neighbours are considered.

The second term of (1.1.1) is rewritten as
$$-\frac{b}{2}\sum_{i}s_{i}^{2}=-\frac{b}{2}\frac{1}{Va^{d}}\sum_{k}s^{2}(k)$$

Therefore Z can be rewritten as

$$Z = \int_{-\infty}^{\infty} e^{-\frac{1}{2} \frac{1}{Va^d} \sum_{k} (b - B(k)) s^2(k)} ds_1 ds_2 \dots ds_N = \prod_{k} \left(2 \pi \frac{Va^d}{b - B(k)} \right)^{\frac{1}{2}}$$

The free energy is $F = -k_B T \ln Z = \frac{1}{2} k_B T \sum \ln(b - B(k)) - \frac{1}{2} k_B T \sum \ln(2 \pi V a^d)$ Because $b \ge B(k)$ and $B(k) \le B(0) = 2 K d$ (see (1.2.1))

Therefore the singularity can only occur when b=B(0)=2Kd=-2d $\frac{J}{k_B T_c}$, which can be used to identify critical temperature T_c

Since only k=0 has a significant impact on the free energy, we thus expand the cosine in (1.1.2) at k=0 to k^2 , thus

$$B(k) = 2 K \left(d - \frac{1}{2} k^2 a^2 \right)$$

If outfield is added, an additional term $h\sum_{i} s_{i}$ in effective Hamiltonian is calculated as

$$h\sum_{i} s_{i} = \frac{h}{Na^{d}} \sum_{k} \sum_{i} e^{ikr_{i}} s(k) = h\sum_{k} \frac{1}{a^{d}} s(k) \delta(k) = \frac{h}{a^{d}} s(k=0) = \frac{h}{a^{d}} s_{0}$$

The effective Hamiltonian is thus $-\beta H = \frac{1}{2} \frac{1}{Va^{d}} \sum_{k} (-b+2 Kd - Kk^{2}a^{2}) s^{2}(k) + \frac{h}{a^{d}} s_{0}$

We change the sum to integration and get $-\beta H = -\frac{1}{2} \frac{1}{(2\pi)^d} \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} d^d k (k^2 + r) \sigma^2(k) + h' \sigma_0$

(1.2.2) where $r = \left(\frac{b}{K} - 2d\right)a^{-2}$, $h' = \frac{h}{a^d \sqrt{ka^{2-d}}}$, $\sigma(k) = \sqrt{ka^{2-d}}s(k)$

1.3 Renormalization Group in Momentum Space

Two steps in RG method: Coarse Grain Transformation and Rescaling process. [1]Coarse Grain Transformation

In the coarse grain transformation, the real length is increased to b times large, which corresponds to a b times decrease in momentum space. So we need to integrate out the

momentum length which is larger than
$$\frac{\Lambda}{b}$$
, or the short wave section (since k= $\frac{2\pi}{\lambda}$),

where $\Lambda = \frac{1}{a}$ is the lattice constant in momentum space.

We divide k into two parts: (define I as the length of spin block or coarse grain, I is just the rescale factor b above)

Long wave part $0 \le |k| \le \frac{\pi}{la}$

Short wave part $\frac{\pi}{la} \leq |k| \leq \frac{\pi}{a}$

We also divide spin into two parts: $\sigma(k) = \sigma_L(k) + \sigma_S(k)$, L means long wave and S means short wave, thus σ_0 in (1.2.2) is σ_{LO}

Therefore (1.2.2) can be rewritten as
$$-\beta H = -\frac{1}{2} \frac{1}{(2\pi)^d} \int_{-\frac{\pi}{la}}^{\frac{\pi}{la}} d^d k (k^2 + r) \sigma_L^2(k) + -\frac{\pi}{la}$$

$$h' \sigma_{L0} - \frac{1}{2} \frac{1}{\left(2\pi\right)^d} \int_{\substack{\frac{\pi}{|a|} \le |k| \le \frac{\pi}{a}}} d^d k \left(k^2 + r\right) \sigma_S^2(k) = -\beta H_L - \beta H_S$$

And Z=

$$\int_{-\infty}^{\infty} \frac{-\frac{1}{2} \frac{1}{(2\pi)^d} \int_{-\frac{\pi}{la}}^{\frac{\pi}{la}} d^d k (k^2 + r) \sigma_L^2(k) + h' \sigma_{L0}}{-\frac{\pi}{la}}$$

$$\int_{-\infty}^{\infty} \frac{-\frac{1}{2} \frac{1}{(2\pi)^d} \int_{\frac{\pi}{la} \le |k| \le \frac{\pi}{a}} d^d k (k^2 + r) \sigma_S^2(k)}{\prod_k d\sigma_S(k) e} = Z_L Z_S$$

So free energy is $f = -k_B T ln Z_L + f_S$

Since the singularity of f occurs at k=0 in the long wave section, therefore the second part of f has nothing to do with critical phenomena (which is singular). We will thus omit short wave part in H and f. We have

$$-\beta H' = -\beta H_{L} = -\frac{1}{2} \frac{1}{(2\pi)^{d}} \int_{-\frac{\pi}{la}}^{\frac{\pi}{la}} d^{d}k (k^{2} + r) \sigma_{L}^{2}(k) + h' \sigma_{L0} (1.3.1)$$

This is the coarse grain transformation.

π

[2]Rescaling

We need to rescale in order to remove the difference between (1.2.2) and (1.3.1)

We introduce in lk=k' and $\sigma_L(k) = \sigma_L\left(\frac{k'}{l}\right) = \theta(l)\sigma_L(k')$ where $\theta(l)$ is the rescaling of spin

$$-\beta H' = -\frac{1}{2} \frac{\theta^{2}(I)}{(2\pi)^{d} I^{2+d}} \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} d^{d} k' (k'^{2} + I^{2}r) \sigma_{L}^{2}(k') + h' \theta(I) \sigma_{L0}$$

$$-\frac{\pi}{a}$$

Define r'=I^{2}r and h''=h' \theta(I)
We have $-\beta H' = -\frac{1}{2} \frac{\theta^{2}(I)}{(2\pi)^{d} I^{2+d}} \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} d^{d} k' (k'^{2} + r') \sigma_{L}^{2}(k') + h'' \sigma_{L0}$

have
$$-\beta H' = -\frac{1}{2} \frac{\theta(I)}{(2\pi)^{d} I^{2+d}} \int_{-\frac{\pi}{a}} d^{d}k' (k'^{2} + r') \sigma_{L}^{2}(k') + h'$$

$$\frac{2+a}{2}$$

Compare (1.2.2) with above, we conclude $\theta(I) = I^{-2}$ and we return to (1.2.2) and get the following RG recurrence relation or RG transformation:

(1.3.2)
$$\begin{cases} r' = l^{2}r \\ \frac{2+d}{2} \\ h'' = h'l^{2} \end{cases}$$

1.4 Derive the Gaussian fix points and Critical exponents

We obviously get one unstable fix point (0,0) in the RG recurrence relation (1.3.2) above

Referring to Appendix 1, we have
$$y_t = \frac{\ln(\Lambda_T)}{\ln(I)} = \frac{\ln(l^2)}{\ln(I)} = 2$$
, $y_h = \frac{\ln(\Lambda_H)}{\ln(I)} = \frac{\ln(\frac{2+d}{2})}{\ln(I)} = 2 + d$

where Λ_{τ} and Λ_{μ} are eigenvalue of RG transformation (1.3.2) With the following known relation:

$$\alpha = 2 - \frac{d}{y_t}, \beta = \frac{d - y_h}{y_t}, \gamma = \frac{2y_h - d}{y_t}, \delta = \frac{y_h}{d - y_h}, \nu = \frac{1}{y_t}, \eta = 2(1 - y_h) + d$$

We conclude

$$\alpha = 2 - \frac{d}{2}, \beta = \frac{d-2}{d+2}, \gamma = 1, \delta = \frac{d+2}{d-2}, v = \frac{1}{2}, \eta = 0$$

2.Define RG in the language of Ginzburg-Landau model

2.1 Introduction to Ginzburg-Landau Model

In Ginzburg Landau model we change the weighing function to the form

 $W = \prod_{i=1}^{N} e^{-\frac{b}{2}s_i^2 - us_i^4}$ to ensure convergence since the domain has been extended to

infinity. (see Sec. 1.1)

We thus get the known φ^4 model (or s^4 model), which Z is rewritten as

$$Z = \int_{-\infty}^{\infty} e^{K \sum_{\langle i,j \rangle}^{N} s_{ij} - \frac{b}{2} s_i^2 - us_i^4} ds_1 ds_2 \dots ds_N$$

because its Hamiltonian is $-\beta H = K \sum_{\langle i,j \rangle}^{N} s_{ij} - \frac{b}{2} s_{i}^{2} - u s_{i}^{4}$ with s^{4} contained. We'll return to

Gauss Model if we set u=0.

We set the coordinate in the above equation to a continuous state, where we would set $\nabla s = s_i - s_j$ and the coefficient unity.

So we get
$$-\beta H = \int d^d r \left(-\frac{1}{2} \left(\nabla s \right)^2 - \frac{r_0}{2} s_i^2 - \frac{u_0}{4} s_i^4 + h_0 s \right)$$
, here the field term $h_0 s$ is added.

Changing it to momentum space by FT method, with previous work done on Gauss

model (see (1.2.2)), we only have to deal with the term $\frac{u_0}{\lambda}s_i^4$

$$\int s^{4} d^{d} r = \int d^{d} r \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{\prod_{i=1}^{4} d^{d} k_{i}}{(2\pi)^{4d} \prod_{i} s(k_{i}) e^{i\left(\sum_{i=1}^{4} k_{i}\right) \cdot r}} = \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{\prod_{i=1}^{4} d^{d} k_{i}}{(2\pi)^{4d} \prod_{i} s(k_{i}) (2\pi)^{d} \delta\left(\sum_{i=1}^{4} k_{i}\right)} -\frac{\pi}{a}$$

Therefore effective Hamiltonian without outfield in momentum space is (see (1.2.2))

$$-\beta H = -\frac{1}{2} \frac{1}{(2\pi)^{d}} \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} d^{d}k (k^{2} + r) s^{2}(k) - \frac{1}{4} u_{0} \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{\prod_{i=1}^{4} d^{d}k_{i}}{(2\pi)^{4d}} \prod_{i} s(k_{i}) (2\pi)^{d} \delta\left(\sum_{i=1}^{4} k_{i}\right) = -\frac{1}{2} \frac{u_{2}}{(2\pi)^{d}} \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} d^{d}k s^{2}(k) - \frac{1}{4} u_{0} \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{\prod_{i=1}^{4} d^{d}k_{i}}{(2\pi)^{4d}} \prod_{i} s(k_{i}) (2\pi)^{d} \delta\left(\sum_{i=1}^{4} k_{i}\right) (2.1.1)$$

where $u_2 = k^2 + r$
2.2 RG solution on G-L model

[1] Coarse Grain Transformation

Similar to section 1.3, we will divide k and s into short wave (subscript S) and long wave (subscript L) parts. Therefore (2.1.1) can be rewritten as

 $-\beta H = H_L(\sigma_L) + H_S(\sigma_S) + V(\sigma_L, \sigma_S) \text{ where } s(k) = \sigma_L + \sigma_S$ Here $H_L(\sigma_L) + H_S(\sigma_S)$ stands for the first term in (2.1.1) and $V(\sigma_L, \sigma_S)$ stands for the second term in (2.1.1)

Because the first term can be divided independently while the second term has couplings.

$$Z = \int_{-\infty}^{\infty} \prod_{k} d\sigma_{L}(k) \int_{-\infty}^{\infty} \prod_{k} d\sigma_{S}(k) e^{H_{L}(\sigma_{L}) + H_{S}(\sigma_{S}) + V(\sigma_{L'},\sigma_{S})} = \int_{-\infty}^{\infty} \prod_{k} d\sigma_{L}(k) e^{H_{L}(\sigma_{L})} e^{g}$$
$$< e^{V} >_{0}$$
$$\text{where } e^{g} = \int_{-\infty}^{\infty} \prod_{k} d\sigma_{S}(k) e^{H_{S}(\sigma_{S})} = const \text{ and } < e^{V} >_{0} = \frac{\int_{-\infty}^{\infty} \prod_{k} d\sigma_{S}(k) e^{H_{S}(\sigma_{S}) + V}}{\int_{-\infty}^{\infty} \prod_{k} d\sigma_{S}(k) e^{H_{S}(\sigma_{S})}}$$

 e^{g} corresponds to the short wave part, which has no singularity (See Sec. 1.3.[1]) and we can thus take it as constant and omit it.

Note that e^{H_s} is a Gauss function and there is a mathematic theorem for the Gauss distribution:

$$iq < x > -\frac{q^{2}}{2\sigma^{2}}$$

$$\left\langle e^{iqx} \right\rangle = e$$
Therefore, $\left\langle e^{V} \right\rangle_{0} = e^{\left\langle V \right\rangle_{0} + \frac{1}{2} \left(\left\langle V^{2} \right\rangle_{0} - \left\langle V \right\rangle_{0}^{2} \right)}$

$$So Z = \int_{-\frac{\pi}{lg}}^{\frac{\pi}{la}} \prod_{k} d\sigma_{L}(k) e^{H_{L}(\sigma_{L})} e^{\left\langle V \right\rangle_{0} + \frac{1}{2} \left(\left\langle V^{2} \right\rangle_{0} - \left\langle V \right\rangle_{0}^{2} \right)} (2.2.0)$$

The above equation has the short wave part e^{g} integrated out and so the integration

range is the long wave part (- $\frac{\pi}{la}$, $\frac{\pi}{la}$)

[2] Rescale

We introduce in the following transformation (see Sec. 1.3.[2] and (1.3.2))

(2.2.1)
$$\begin{cases} -lk = k' \\ \sigma_{L}(k) = \Theta(l)s(k') = l^{\frac{2+d}{2}}s(k') \end{cases}$$

And we replace the corresponding items in (2.2.0), which needs the calculation of $< e^V >_{0}$, and get

$$-\beta H = -\frac{1}{2} \frac{u'_{2}}{(2\pi)^{d}} \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} d^{d}k's^{2}(k') - \frac{1}{4}u'_{4} \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{\prod_{i=1}^{4} d^{d}k'_{i}}{(2\pi)^{4d}} \prod_{i} s(k'_{i}) (2\pi)^{d} \delta\left(\sum_{i=1}^{4} k'_{i}\right) (2.2.2)$$

Compare (2.2.2) and (2.1.1) we derive the RG transformation (the expression of u'_{2} and u'_{4}), which is calculated in detail below. The demonstration of (2.2.1) is also done below.

[3]Calculation of $\langle e^{V} \rangle_{0}$

$$< e^{V} >_{0} = e^{\langle V \rangle_{0} + \frac{1}{2} \left(\langle v^{2} \rangle_{0} - \langle V \rangle_{0}^{2} \right)}$$

There are two parts in the above equation, and we now calculate the first part.

$$V = -\frac{1}{4}u_{0}\int_{-\frac{\pi}{q}}^{\frac{\pi}{q}} \frac{\prod_{i=1}^{4} d^{d}k_{i}}{(2\pi)^{4d}} \prod_{i=1}^{4} s(k_{i})(2\pi)^{d} \delta\left(\sum_{i=1}^{4} k_{i}\right) \text{ and } s(k) = \sigma_{L} + \sigma_{S}$$

We need to calculate

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$$\prod_{i}^{4} s(k_{i}) \text{ by means of } \sigma_{L} \text{ and } \sigma_{S}$$

$$\prod_{i}^{4} s(k_{i}) = \prod_{i}^{4} (\sigma_{L} + \sigma_{S}) = \sigma_{L} \sigma_{L} \sigma_{L} \sigma_{L} + \sigma_{S} \sigma_{S} \sigma_{S} \sigma_{S} + 4 \sigma_{S} \sigma_{S} \sigma_{S} \sigma_{L} + 4 \sigma_{L} \sigma_{L} \sigma_{L} \sigma_{S} + 6 \sigma_{S} \sigma_{S} \sigma_{L} \sigma_$$

Put (2.2.3) into the above equation we get five parts, which are shown separately below.

The first term

$$< V(\sigma_{L}\sigma_{L}\sigma_{L}\sigma_{L}) >_{0} = -\frac{1}{4}u_{0} \int_{-\frac{\pi}{la}}^{\frac{\pi}{la}} \frac{\prod_{i=1}^{4} d^{d}k_{i}}{(2\pi)^{4d}} < \sigma_{L}(k_{1})\sigma_{L}(k_{2})\sigma_{L}(k_{3})\sigma_{L}(k_{4})$$

$$> \int_{0}^{-\frac{\pi}{la}} (2\pi)^{d}\delta\left(\sum_{i=1}^{4}k_{i}\right) = -\frac{1}{4}u_{0}\int_{-\frac{\pi}{la}}^{\frac{\pi}{la}} \frac{\prod_{i=1}^{4} d^{d}k_{i}}{(2\pi)^{4d}\sigma_{L}(k_{1})\sigma_{L}(k_{2})\sigma_{L}(k_{3})\sigma_{L}(k_{4})(2\pi)^{d}\delta\left(\sum_{i=1}^{4}k_{i}\right) = -\frac{1}{4}u_{0}\int_{-\frac{\pi}{la}}^{-\frac{\pi}{la}} (1+\frac{\pi}{la})^{4} + \frac{\pi}{la}$$



We have used (2.2.2) in the above derivation.

The Second term

 $\sigma_{s}\sigma_{s}\sigma_{s}\sigma_{s}\sigma_{s}$ contains no σ_{L} , so it contains no singularity and $so < V(\sigma_{s}\sigma_{s}\sigma_{s}\sigma_{s}\sigma_{s}) >_{0} = const$ (see 1.3.[1])

The third and forth term

Because $\langle V \rangle_0$ is a Gauss integration, so odd number of σ_L or σ_S will make the integration zero.

The fifth term

$$< V(\sigma_{L}\sigma_{L}\sigma_{S}\sigma_{S}\sigma_{S}) >_{0} = -\frac{6}{4}u_{0} \int_{0}^{\frac{\pi}{la}} \int_{\frac{\pi}{la}}^{\frac{\pi}{a}} \frac{\prod_{i=1}^{4} d^{d}k_{i}}{(2\pi)^{4d}} \sigma_{L}(k_{1})\sigma_{L}(k_{2}) < \sigma_{S}(k_{3})\sigma_{S}(k_{4})$$
$$> (2\pi)^{d}\delta\left(\sum_{i=1}^{4}k_{i}\right)$$

We need to calculate $< \sigma_{s}(k_{3})\sigma_{s}(k_{4}) > 0$ here and the integration is Gauss type with

exponent H_S

$$H_{S} =$$

$$-\frac{1}{2} \frac{u_{2}}{(2\pi)^{d}} \int_{\frac{\pi}{l_{d}}}^{\frac{\pi}{d}} d^{d}k \sigma_{s}^{2}(k) = -\frac{1}{2} \frac{1}{(2\pi)^{d}} \int_{\frac{\pi}{l_{d}}}^{\frac{\pi}{d}} (k^{2}+r) d^{d}k \sigma_{s}^{2}(k) = -\frac{1}{2(2\pi)^{d}} \sum_{\frac{\pi}{l_{d}} < k < \frac{\pi}{d}} (k^{2}+r) \sigma_{s}^{2}(k)$$
(see (2.1.1))
Therefore
$$< \sigma_{s}(k_{3}) \sigma_{s}(k_{4}) > \int_{0}^{\infty} \prod_{k} d\sigma_{s}(k) e^{H_{s}(\sigma_{s})} \sigma_{s}(k_{3}) \sigma_{s}(k_{4}) = \frac{(2\pi)^{d}}{k^{2}+r} \delta(k_{3}+k_{4}) (2.2.4)$$
Here we have used relation
$$\int_{-\infty}^{\infty} e^{-ax^{2}} dx = \sqrt{\frac{\pi}{a}} \text{ and } \int_{-\infty}^{\infty} x^{2} e^{-ax^{2}} dx = \frac{\sqrt{\frac{\pi}{a}}}{2a^{\frac{3}{2}}} \text{ and } \int_{-\infty}^{\infty} xe^{-ax^{2}} dx = 0 \text{ and } \sigma_{s}(k) = \sigma_{s}^{*}(-k) \text{ and } \sigma_{s}^{2}(k) = \sigma_{s}(k)\sigma_{s}^{*}(k)$$

Therefore we have

$$< V(\sigma_{L}\sigma_{L}\sigma_{S}\sigma_{S}\sigma_{S}) >_{0} = -\frac{6}{4}u_{0}\int_{0}^{\frac{\pi}{la}}\int_{\frac{\pi}{la}}^{\frac{\pi}{a}}\frac{\prod_{j=1}^{4}d^{d}k_{j}}{(2\pi)^{4d}}\sigma_{L}(k_{1})\sigma_{L}(k_{2}) < \sigma_{S}(k_{3})\sigma_{S}(k_{4})$$



In the last equation above (rescaling process), we have first, only rescaled $\sigma_L(k_1)\sigma_L(k_2)$, and second, the term $\delta\left(\sum_{i=1}^4 k_i\right) = \delta(k_1 + k_2)$ since $k_3 = -k_4$ (see 2.2.4)

Therefore, the approximate form of Hamiltonian in (2.2.0) is (only the first part of $< e^{V} >_{0}$ is considered.

$$H_{L} + < V >_{0} = -\frac{1}{2} \frac{1}{(2\pi)^{d}} \int_{0}^{\frac{\pi}{la}} (k^{2} + r) d^{d}k \sigma_{L}^{2}(k) - \frac{6}{4} u_{0} l^{-2d} l^{d} \left(l^{\frac{2+d}{2}}\right)^{2} \int_{0}^{\frac{\pi}{a}} \frac{d^{d}k'}{(2\pi)^{d}} s(k') s(-k) d^{d}k \sigma_{L}^{2}(k) - \frac{6}{4} u_{0} l^{-2d} l^{d} \left(l^{\frac{2+d}{2}}\right)^{2} \int_{0}^{\frac{\pi}{a}} \frac{d^{d}k'}{(2\pi)^{d}} s(k') s(-k) d^{d}k \sigma_{L}^{2}(k) - \frac{6}{4} u_{0} l^{-2d} l^{d} \left(l^{\frac{2+d}{2}}\right)^{2} \int_{0}^{\frac{\pi}{a}} \frac{d^{d}k'}{(2\pi)^{d}} s(k') s(-k) d^{d}k \sigma_{L}^{2}(k) - \frac{6}{4} u_{0} l^{-2d} l^{d} \left(l^{\frac{2+d}{2}}\right)^{2} \int_{0}^{\frac{\pi}{a}} \frac{d^{d}k'}{(2\pi)^{d}} s(k') s(-k) d^{d}k \sigma_{L}^{2}(k) - \frac{6}{4} u_{0} l^{-2d} l^{d} \left(l^{\frac{2+d}{2}}\right)^{2} \int_{0}^{\frac{\pi}{a}} \frac{d^{d}k'}{(2\pi)^{d}} s(k') s(-k) d^{d}k \sigma_{L}^{2}(k) - \frac{6}{4} u_{0} l^{-2d} l^{d} \left(l^{\frac{2+d}{2}}\right)^{2} \int_{0}^{\frac{\pi}{a}} \frac{d^{d}k'}{(2\pi)^{d}} s(k') s(-k) d^{d}k \sigma_{L}^{2}(k) - \frac{6}{4} u_{0} l^{-2d} l^{d} \left(l^{\frac{2+d}{2}}\right)^{2} \int_{0}^{\frac{\pi}{a}} \frac{d^{d}k'}{(2\pi)^{d}} s(k') s(-k) d^{d}k \sigma_{L}^{2}(k) - \frac{6}{4} u_{0} l^{-2d} l^{d} \left(l^{\frac{2+d}{2}}\right)^{2} \int_{0}^{\frac{\pi}{a}} \frac{d^{d}k'}{(2\pi)^{d}} s(k') s(-k) d^{d}k \sigma_{L}^{2}(k) - \frac{6}{4} u_{0} l^{-2d} l^{d} \left(l^{\frac{2+d}{2}}\right)^{2} \int_{0}^{\frac{\pi}{a}} \frac{d^{d}k'}{(2\pi)^{d}} s(k') s(-k) d^{d}k \sigma_{L}^{2}(k) - \frac{6}{4} u_{0} l^{-2d} l^{d} \left(l^{\frac{2+d}{2}}\right)^{2} \int_{0}^{\frac{\pi}{a}} \frac{d^{d}k'}{(2\pi)^{d}} s(k') s(-k) d^{d}k \sigma_{L}^{2}(k) - \frac{6}{4} u_{0} l^{-2} \left(l^{\frac{2+d}{2}}\right)^{2} \int_{0}^{\frac{\pi}{a}} \frac{d^{d}k'}{(2\pi)^{d}} s(k') s(-k) d^{d}k \sigma_{L}^{2}(k) - \frac{6}{4} u_{0} l^{-2} \left(l^{\frac{2+d}{2}}\right)^{2} \int_{0}^{\frac{\pi}{a}} \frac{d^{d}k'}{(2\pi)^{d}} s(k') s(-k) d^{d}k \sigma_{L}^{2}(k) d^{d}k \sigma_{L}^{2}(k) - \frac{6}{4} u_{0} l^{-2} \left(l^{\frac{2+d}{2}}\right)^{2} \int_{0}^{\frac{\pi}{a}} \frac{d^{d}k'}{(2\pi)^{d}} s(k') d^{d}k \sigma_{L}^{2}(k) d^{d}$$

$$\left(\int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{d^{d}k}{\left(2\pi\right)^{d}\left(k^{2}+r\right)} - \frac{1}{4}u'_{4} \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{\prod_{i=1}^{4} d^{d}k'_{i}}{\left(2\pi\right)^{4d}} \prod_{i} s\left(k'_{i}\right) \left(2\pi\right)^{d} \delta\left(\sum_{i=1}^{4}k'_{i}\right) - \frac{\pi}{a} \right) \right)$$



where we have concluded the following RG transformation

$$\left\{ u'_{2} = l^{2} \left(\frac{k'^{2}}{l^{2}} + r + 3 u_{0} \int_{\frac{\pi}{la}}^{\frac{\pi}{a}} \frac{d^{d}k}{(2\pi)^{d}(k^{2} + r)} \right) \\ u'_{4} = u_{0} l^{4-d} \right\}$$

If the second part of $\langle e^{V} \rangle_{0'}$, saying, $\langle V^{2} \rangle_{0} - \langle V \rangle_{0'}^{2}$, is also considered, we would have to use Feynman diagram to solve the quadratic term.

We will not draw the full Feynman diagram solution here, but will give the result:

(2.2.5)
$$\begin{cases} r' = l^{2} (r + 3 u_{01}) \\ u' = u_{0} l^{\epsilon} (1 - 9 u_{02}) & where \epsilon = 4 - d \end{cases}$$

where

$$\begin{cases} I_{1} = \int_{-\frac{\pi}{la}}^{\frac{\pi}{a}} \frac{d^{d}k}{(2\pi)^{d}(k^{2} + r)} \\ I_{2} = \int_{-\frac{\pi}{la}}^{\frac{\pi}{a}} \frac{d^{d}k}{(2\pi)^{d}(k^{2} + r)^{2}} \end{cases}$$

(2.2.5) is just the RG transformation of Ginzburg-Landau model.

3.Derive the new fixed point in d=4- ϵ **dimensions and the associated critical exponents** Refer to (2.2.5), we have defined d=4- ϵ , here we would not limit d to integer, therefore if d is near 4, we can expand the I at d=4 in (2.2.5) with respect to a small ϵ .

$$I(\epsilon) = I(d=4) + \epsilon I'(\epsilon) + o(\epsilon^2)$$

Generally, we can solve the following integration if it has spherical symmetry,

$$I = \int \frac{d^{d}k}{(2\pi)^{d}} f(q^{2}) = S_{d} \int \frac{q^{d-1}d^{d}k}{(2\pi)^{d}} f(q^{2}) \text{ where } S_{d}$$
$$= \frac{2\pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}\right)} \text{ is d dimensional sphere surface area}$$

Therefore we have



$$\frac{u'}{4} = l^{\epsilon} \left(\frac{u_0}{4} - \frac{9}{(2\pi)^2} \left(\frac{u_0}{4} \right)^2 \ln(l) \right) = \frac{u_0}{4} + \frac{u_0}{4} \left(\epsilon - \frac{9}{(2\pi)^2} \left(\frac{u_0}{4} \right) \right) \ln(l) \quad \text{where } \epsilon = 4 - d$$

We have expanded $l^{\epsilon} = e^{\epsilon lnl} = 1 + \epsilon lnl + ...$ in the above derivation

There're two fixed points in the RG relation above. The first is Gauss fixed point (0,0) The second is called WF fixed point showing below

$$u'=u_0=u^*=\frac{8\pi^2}{9}\epsilon$$
$$r'=r_0=r^*=-\frac{\epsilon}{6}\left(\frac{\pi}{a}\right)^2$$

In order to solve associated critical exponents, we have to solve the eigenvalue of (3.1)

$$\begin{vmatrix} \frac{\partial}{\partial r} \mathbf{r}' & \frac{\partial}{\partial u_0} \mathbf{r}' \\ \frac{\partial}{\partial r} \mathbf{u}' & \frac{\partial}{\partial u_0} \mathbf{u}' \\ \frac{\partial}{\partial r} \mathbf{u}' & \frac{\partial}{\partial u_0} \mathbf{u}' \\ 1 \end{vmatrix} |_{(0,0)} = \begin{bmatrix} r^2 & \frac{3\Delta^2(r^2 - 1)}{4\pi^2} \\ 0 & r^{\epsilon} \end{bmatrix} \text{Here } \Delta = \frac{\pi}{a}$$

$$\begin{bmatrix} r^2 & \frac{3\Delta^2(r^2 - 1)}{4\pi^2} \\ 0 & r^{\epsilon} \end{bmatrix} \xrightarrow{\text{eigenvalues}} \begin{bmatrix} r^2 \\ r^{\epsilon} \end{bmatrix} \rightarrow y_t = \frac{\ln(\Lambda_T^G)}{\ln(r)} = \frac{\ln(r^2)}{\ln(r)} = 2, y_h = \frac{\ln(\Lambda_2^G)}{\ln(r)} = \frac{\ln(r^{\epsilon})}{\ln(r)} = \epsilon$$

And

$$\begin{bmatrix} \frac{\partial}{\partial r} \mathbf{r}' & \frac{\partial}{\partial u_0} \mathbf{r}' \\ \frac{\partial}{\partial r} \mathbf{u}' & \frac{\partial}{\partial u_0} \mathbf{u}' \\ \frac{\partial}{\partial r} \mathbf{u}' & \frac{\partial}{\partial u_0} \mathbf{u}' \\ \end{bmatrix} \begin{bmatrix} \frac{8\pi^2}{9} \epsilon_r - \frac{\epsilon}{6} \left(\frac{\pi}{a}\right)^2 \right]^2 = \begin{bmatrix} 2 - \frac{\epsilon}{3} & \frac{3\Delta^2(l^2 - 1)}{4\pi^2} \\ 0 & l^{-\epsilon} \end{bmatrix}$$
$$\begin{bmatrix} 2 - \frac{\epsilon}{3} & \frac{3\Delta^2(l^2 - 1)}{4\pi^2} \\ 4\pi^2 & \frac{1}{4\pi^2} \\ 0 & l^{-\epsilon} \end{bmatrix} \xrightarrow{\text{eigenvalues}} \begin{bmatrix} 2 - \frac{1}{3} \epsilon \\ l & \frac{1}{3} \epsilon \\ l^{-\epsilon} & \frac{1}{3} \epsilon \end{bmatrix}$$
$$\xrightarrow{\mathbf{v}_t} = \frac{\ln\left(\frac{\Lambda_T^{WF}}{1}\right)}{\ln(l)} = \frac{\ln\left(\frac{2 - \frac{1}{3} \epsilon}{1} \epsilon\right)}{\ln(l)} = 2 - \frac{1}{3} \epsilon_r \mathbf{v}_h = \frac{\ln\left(\frac{\Lambda_2^{WF}}{1}\right)}{\ln(l)} = \frac{\ln(l^{-\epsilon})}{\ln(l)} = -\epsilon$$

Their eigenvectors are the same:

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$$e_{t} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, e_{2} = \begin{bmatrix} -\frac{3\Delta^{2}}{4\pi^{2}} \\ 4\pi^{2} \end{bmatrix}$$

The following discussion is based on a small ϵ or d ≈ 4 When d>4 or $\epsilon < 0_{,,} \Lambda_{T}^{G} > 1, \Lambda_{2}^{G} < 1$, so the Gauss fixed point is unstable at e_{t} , but stable at e_{2} , so the Gaussian fixed point is a critical point and e_{2} is the critical surface. On the other hand, $\Lambda_{T}^{WF} > 1, \Lambda_{2}^{WF} > 1$, so the WF fixed point is unstable and not a critical point.

The Critical Exponent can be drawn from

$$\alpha = 2 - \frac{d}{y_t}, \beta = \frac{d - y_h}{y_t}, \gamma = \frac{2y_h - d}{y_t}, \delta = \frac{y_h}{d - y_h}, \nu = \frac{1}{y_t}, \eta = 2(1 - y_h) + d$$

We thus get

$$\alpha = 2 - \frac{d}{2}, \beta = \frac{d - \epsilon}{2}, \gamma = \frac{2\epsilon - d}{2}, \delta = \frac{\epsilon}{d - \epsilon}, \nu = \frac{1}{2}, \eta = 2(1 - \epsilon) + d$$

When d<4 or $\epsilon > 0$, $\Lambda_{\tau}^{G} > 1$, $\Lambda_{2}^{G} > 1$, $\Lambda_{\tau}^{WF} > 1$, $\Lambda_{2}^{WF} < 1$, the Gaussian fixed point is unstable and the WF fixed point is stable at e_2 . We draw the critical exponent of WF fixed point:

$$\alpha = 2 - \frac{3d}{6-\epsilon}, \beta = 3\frac{d+\epsilon}{6-\epsilon}, \gamma = 3\frac{-2\epsilon-d}{6-\epsilon}, \delta = \frac{-\epsilon}{d+\epsilon}, \nu = \frac{3}{6-\epsilon}, \eta = 2(1+\epsilon) + d$$

4. Explain the Universality by RG

The RG transformation relation is

δК'= МδК

where M is the RG transformation Matrix and K can be seen as the interaction in Ising model $K \sum_{i,j} s_{i,j}$

$$M_{s}e^{\sigma} = \Lambda_{s}e^{\sigma}$$

where e^{σ} is the eigenvector of M_s and Λ_s is the eigenvalue of M_s

Because M is not usually symmetric, the left eigenvector and the right eigenvector may not be the same, and thus we get

$$M_{s}M_{s'} = M_{ss'}$$
 (This is the property of RG) and we get $\Lambda_{s}\Lambda_{s'} = \Lambda_{ss'}$ (4.1)
We conclude $\Lambda_{s} = s^{\phi}$ if it satisfies (4.1)

Therefore, $\delta K' = M \delta K = M \sum_{\sigma} a^{\sigma} e^{\sigma} = \Lambda_s \sum_{\sigma} a^{\sigma} e^{\sigma} = s^{\sigma} \sum_{\sigma} a^{\sigma} e^{\sigma}$

Thus we can divide the following situations:

y >0, δK will become larger and larger, thus unstable σ <0, δK will become zero in the end, thus stable σ =0, δK won't change σ We define the eigenvector of M in the case x < 0 the critical su

We define the eigenvector of M in the case y < 0 the critical surface, and all the points on

the surface would go towards to the fixed point after the RG transformation. If the Hamiltonian of a system happens to be on the critical surface, then the critical behavior of this system will be the same as that of the fixed point. Therefore, all systems which lay on the same critical surface belongs to the same university, although their Hamiltonian may be totally different. The following fig would help explain the universality. The systems, A,B,C, all belongs to a same universality since they all fall on the same critical surface.



Fig 4.1

Reference

1.Yang, Z. R. (2007). "Quantum Statistic Physics." High Education Press: 421.

Markovian-chain Monte Carlo Edited by Li, Zimeng

Contents:

1.Introduction
1.1 Simple Sampling
1.2 Importance Sampling
2.Markov Process
3.MCMC application on 2D Ising model

First, we have learned the MCMC method in Computational Physics, therefore I would only give a brief review of the method and, second, an extension to the 2D Ising model.

1.Introduction

Partition functions and functional integrals (path integrals) reduce many-body problems to complicated multidimensional integrals or sums.

The Monte Carlo technique has its origins in the numerical evaluation of integrals. The technique was later generalized to calculate the partition function and the mean value of observables in classical systems.

The key of numerical integration is sampling. There are many sampling methods in Monte-Carlo method. We will only introduce two of them here.

1.1 Simple Sampling

We first generate random numbers x_i uniformly distributed in [a,b], and get the probability density of these points:

$$P = \begin{cases} \frac{1}{b-a} & x \in [a, b] \\ 0 & x \notin [a, b] \end{cases}$$

We can calculate the expectation value of a function f with respect to the distribution P:

$$E(f(x)) = \int_{a}^{b} f(x) P(x) dx = \frac{1}{b-a} \int_{a}^{b} f dx = \frac{1}{b-a}$$

In order to calculate the above integration I in a numerical way, we define the Monte-Carlo Integral I_{MC}

where
$$I_{MC} = (b - a) \sum_{i=1}^{n} \frac{f(x = x_i)}{n}$$
 (1.1.1)

Due to the Central Limit Theorem, we have $E[I_{MC}] = I$ when $N \rightarrow \infty$ Therefore we can use (1.1.1) to calculate the Integral

1.2 Importance Sampling

In order to dismiss the dramatic change in functions which might lead to great error in the numerical integration in the simple sampling method, we introduce in important sampling to select points according to the trend of function, and this selection is previously set.

Referring to (1.1.1), we change it to

$$I_{MC} = (b-a) \sum_{i=1}^{n} \frac{f(x=x_i)}{n} = I_{MC} = \sum_{i=1}^{n} \frac{f(x=x_i)}{n \cdot P} \text{ where } P = \frac{1}{b-a}$$

In importance sampling, P is relevant with x_i , and therefore we have $I_{sel} = \sum_{i=1}^{n} \frac{f(x = x_i)}{n \cdot P(x_i)}$

We can also demonstrate that $E[I_{sel}]$ =I in the sense of central limit theorem.

An application of importance sampling will be illustrated here. In statistic physics, an observable is calculated in the following means:

$$\langle B \rangle = \frac{1}{Z} \int B e^{-\beta H} dx$$

This is easily done by simple sampling method, but the exponent function is such a dramatic function that we would use important sampling instead to increase efficiency. Therefore we write:

$$\langle B \rangle \approx \sum_{i=1}^{n} \frac{B(x_i)e^{-\beta H(x_i)}P^{-1}(x_i)}{e^{-\beta H(x_i)}P^{-1}(x_i)}, (1.2.1)$$

if $P(x_i)$ is carefully selected so that it is proportional to the distribution $e^{-\beta H(x_i)}$, we will get instantly that

$$\langle B \rangle \approx \sum_{i=1}^{n} \frac{B(x_i)}{n}$$

However, $P(x_i)$ cannot not be easily solved on many conditions. We would use Markov Process instead to solve this problem.

2.Markov Process

Markov process is an example of 'random walk' through phase space in a series of $\{x_i\}$.

We would first give the three properties of Markov chain below:

 $[1]w(x \to x') \ge 0$ $[2]\sum_{x'}w(x \to x') = 1$ $[3]f(x)w(x \to x') = f(x')w(x' \to x)$

 $w(x \rightarrow x')$ means the probability that a point transfer from site x to site x'. [1] is obvious. [2] says the random walk is not restrict to history, the sites can be visited many times, and we will finally reach to the border or equilibrium state. We call this "ergodicity hypothesis". [3] is just the learned "detailed balance" where the equilibrium distribution f(x) is reached.

How to efficiently converge in the Marcov Chain depends on the selection of $w(x \rightarrow x')$, which has a large freedom to choose. A simple choice is seen below, also known as the **Metropolis method**.

How to pursue the random walk? We use (1.2.1) as an example and use Metropolis method. We define the transition probability as

$$\frac{f(x')}{f(x)} = \frac{w(x \to x')}{w(x' \to x)} = e^{-\beta(E(s') - E(s))}, \text{ where } f(x) = e^{-\beta E(s)} \text{ is just } P(x_i) \text{ defined in Sec. 1.2}$$

Following Metropolis, we choose another transition probability p, which reads

$$p = \begin{cases} e^{-\beta(E(s') - E(s))} & E(s') > E(s) \\ 1 & E(s') < E(s) \end{cases}$$

or
$$p = \min\left[1, \frac{f(x')}{f(x)}\right]$$

Then follow the following steps:

[1] Select a site i, and its first random step to the nearest neighbour i'

- [2] Compute E(s') E(s)
- [3] Calculate $\frac{f(x')}{f(x)}$, if $\frac{f(x')}{f(x)} > 1$, then p=1, accept the spin value of this site; otherwise,

go to [4]

[4] Generate a random number r in the range [0,1].

[5] If $r < \frac{f(x')}{f(x)}$, flip the spin, saying, $s_i \to -s_i$, otherwise leave on the site i and go to [1] again.

3.MCMC application on 2D Ising model

The known 2D Ising model without outfield is $H = \sum_{\langle i,j \rangle} J_{ij} ss_{ij}$

The calculation of observables can be found in (1.1.1), we follow the following steps:

[1] Generate random configurations of spins, initiate variables

[2] Importance Sampling to choose efficient configurations.

We select $P=e^{-\beta E(s)}$ as the probability distribution. (see Sec.1.2)

[3] Generate a Markov chain to sample all these configurations stochastically.

We define a "random walker" to sweep the space of configurations {s} rather than choose them independently. The random walker is achieved in Sec.2.

[4] Data storage

In order to store the transition probability p defined in Sec.2, we make a look-up table to

store 2⁵ values for every site. Because in 2D Ising model, we have 4 nearest neighbours around a site and each site can have two possible values. Adding the site itself we have

2⁵ possible values.

[5] Perform a sufficient number of iterations for thermalization.

[6] Carry out measurements and store the associated numbers.

[7] Compute total averages and statistical errors.

The program is put in the appendix, and you can also refer it to reference 2. Some result of the program is seen in the figure below



Fig 3.1

Reference

1.Ma, W.K. "Computational Physics" (Science Press) (2005)

2.Dagotto E., et al. Nanoscale phase separation and colossal magnetoresistance (physics of manganites) (Springer, 2002)(463s)

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Appendix: MC Code for the Ising Model

The following Fortran90 code performs a single walker Monte Carlo for the 2D Ising model. The code employs the Fortran90 random number generator, but we strongly suggest to use a more efficient one

program ising use tables implicit none integer :: i, j, ix, iy, n ! auxiliary variables integer :: niter, nterm ! Constants for the run real(kind(0.d0)) :: ran ! Random number real(kind(0.d0)) :: beta ! 1/T real(kind(0.d0)) :: ener, e0, e2, se ! Average of energy real(kind(0.d0)) :: magnet, m0, m2, sm ! Average of magnetization write(*,*)'Linear size of the lattice (ns):' read(*,*) ns write(*,*)'Number of thermalization steps (nwarmup):'

read(*,*) nterm write(*,*)'Number of measurements (niter):' read(*,*) niter write(*,*)'Temperature (T):' read(*,*) xt $x_j = 1.d0$ 1_ ! Tables for neighbors !-1 1 ! | ! 2 - (x,y) - 0 ! 3 1 1 ! Coordinates of neighbors in any direction n are given by ! (nnx(x,n),nny(y,n)) n=0,...,3!do ix=0.ns-1 nnx(ix,0)=ix+1nnx(ix,1)=ixnnx(ix,2)=ix-1 nnx(ix,3)=ix enddo do iy=0,ns-1 nny(iy,0)=iy nny(iy,1)=iy+1nny(iy,2)=iy nny(iy,3)=iy-1 enddo ! Periodic boundary conditions nnx(ns-1,0) = 0nnx(0,2) = ns-1nny(ns-1,1) = 0nny(0,3) = ns-1!--! Build transition probabilities and local energies !beta = 1.d0/xtdo i=-1,1,2 ! Spin in the site can have value -1 or 1 do n=-4,4 ! Sum of the spins in neighboring sites -4,...,0,...,4 site_e(i,n)=-xj*dble(i*n) $w(i,n) = exp(-beta^*xj^*2^{*i^*n})$ enddo enddo !___ ! Random starting configuration do ix=0,ns-1 do iy=0,ns-1 si(ix,iy)=1we recommend using a more efficient random number generator (see Knuth) call random_number(ran)

```
print *,'--- MEASUREMENT ----'
e0 = 0.d0
e2 = 0.d0
m_{0=0.d0}
m_{2=0.d0}
do i=1,niter
do n=1.5 !decorrelation steps, arbitrarily set to 5
call metropolis()
enddo
call metropolis()
! Calculate observables and add to averages
ener = 0.d0
magnet = 0.d0
do ix=0,ns-1
do iy=0,ns-1
n = 0
do j=0,3 !Sum of 4 first neighbor spins of site (ix,iy)
n = n + si(nnx(ix,j), nny(iy,j))
enddo
ener=ener+site_e(si(ix,iy),n)
magnet = magnet + si(ix, iy)
enddo
enddo
ener=ener/2.d0 !Tables count spins twice
e0=e0+ener
e2=e2+ener*ener
m0=m0+abs(magnet)
m2=m2+magnet*magnet
enddo
! Averages and statistical errors
e0=e0/dble(niter)
e2=e2/dble(niter)
se=sqrt((e2-e0*e0)/dble(niter))
m0=m0/dble(niter)
m2=m2/dble(niter)
sm=sqrt((m2-m0*m0)/dble(niter))
! Output
print *,xt,'ENER=',e0,' Err=',se
print *,xt,'M=',m0,' Err=',sm
open(20,file='evst.dat',status='unknown',position='append')
write(20,*) xt,e0,se
close(20)
open(20,file='mvst.dat',status='unknown',position='append')
write(20,*) xt,m0,sm
close(20)
end
!-
subroutine metropolis()
use tables
implicit none
integer :: i, i0, ix, iy, n
real(kind(0.d0)) :: ran
do ix=0.ns-1
```

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1. What's the relation between observables and correlation function?

Ans:

Take a magnetism system as an example,

 $G = \langle m_i m_j \rangle - \langle m_i \rangle \cdot \langle m_j \rangle$ As to Ising mode, we have $G = \langle m_i m_j \rangle$

$$\langle m_i m_j \rangle = \frac{\beta^{-2}}{Z} \frac{\partial}{\partial B} \frac{\partial}{\partial B} Z$$

And $\langle m_j \rangle = -\frac{\partial}{\partial B} F, F = -KTInZ,$

Therefore,

$$\chi = \frac{\partial}{\partial h}m = -\frac{\partial}{\partial h}\frac{\partial}{\partial h}F = \beta^{-2}\frac{\partial}{\partial h}\frac{\partial}{\partial h}F = kT\left(\frac{1}{Z}\frac{\partial}{\partial h}\frac{\partial}{\partial h}Z - \frac{1}{Z}\left(\frac{\partial}{\partial h}Z\right)\cdot\frac{1}{Z}\frac{\partial}{\partial h}Z\right) = \frac{1}{kT}\left(\langle m_{i}m_{j}\rangle - \langle m_{i}\rangle\cdot\langle m_{j}\rangle\right) = \frac{1}{kT}G$$

Therefore, G=kTχ

2. How MFT, especially Brag-William Model, draw solution of critical exponent? (Group 3)

Ans:

[1] β

We need to solve a transcendental equation when trying to obtain L(definition see below)

Especially when there is no outfield, we have

$$L := \tanh\left(\frac{T_c}{T} \cdot L\right), L \text{ satisfies } \frac{1}{2}(L+1) = \frac{N_+}{N}, \text{ where } N_+ \text{ is the total number of spin}$$
$$-up \text{ particles}$$
$$\xrightarrow{\text{evaluate at point}}$$

tanh(0.75 *L*)

evaluate at point





[2]α

Partition Function has the following expression:

 $\frac{lnZ}{N} = \beta \left(\frac{1}{2} \gamma L^2 + WL\right) - \frac{1+L}{2} \ln \frac{1+L}{2} - \frac{(1-L)}{2} \ln \left(\frac{1-L}{2}\right),$ where γ is the coordination number, W is magnetism energy and J is the energy of spin interaction.

$$T > T_{c}, L = 0; T < T_{c}, L = L_{0}$$

$$U = -\frac{\partial}{\partial \beta} \ln Z = \begin{cases} 0 & T > T_{c} \\ -\frac{1}{2} N \gamma J L_{0}^{2} & T < T_{c} \end{cases}$$

$$C = \frac{d}{dT} U = \begin{cases} 0 & T > T_C \\ -\frac{1}{2} N \gamma d \frac{d}{dT} L_0^2 & T < T_C \end{cases}$$

Therefore, heat capacity experience mutation at T_c [3] γ

When there exists outfiled, the transcendental equation is L=tanh $\left(\frac{T_c}{T}L + \frac{B}{k_B T}\right)$ $T > T_c, B \to 0$, we have $I \ll 1$ (the trend can also draw from fig 1),

thus we can replace tank with x, so
$$L = \frac{B}{k_B(T - T_c)}$$

 $M = N\mu L \approx \frac{N\mu B}{k_B(T - T_c)}$, therefore $\chi = \left(\frac{\partial M}{\partial B}\right)_T = \frac{N}{k_B(T - T_c)} \sim (T - T_c)^{-1}$
Therefore $\gamma = -1$
[4] δ

$$T = T_{C,} we have L = \tanh\left(\frac{B}{k_{B}T} + L\right) \sim B + L - \frac{1}{3}(B + L)^{3} \Rightarrow B \sim L^{3} \Rightarrow M \sim L \sim B^{\frac{1}{3}}$$

Therefore, $\delta = \frac{1}{3}$

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Advanced Statistic Physics Homework 1 By Maple 13

1.Derive the correlation function of Ising model with variable r or N.

Ans:

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

$$Z = e^{\beta J\sum_{i=1}^{N} s_{i}s_{i}}$$
[1]Taking free border condition, define $\eta_{i} = s_{i}s_{i}$ then $\eta_{i} = \begin{cases} -1 & S_{i} = -S_{i+1} \\ 1 & S_{i} = S_{i+1} \end{cases}$
So, $Z = \sum_{\{\eta_{i}\}} e^{\beta J\sum_{i=1}^{N} \eta_{i}} = 2[2\cosh(\kappa)]^{N-1}$, $\kappa = \beta J$
Correlation Function:G[N]=<
$$S_{i}S_{j} > = \frac{1}{Z}\sum_{i=1}^{N} \eta_{i}e^{\kappa\sum_{i=1}^{N} \eta_{i}} = \frac{\partial^{N}}{\partial \kappa^{N}} Z = (\tanh(\kappa))^{N} = e^{-Nin(\coth(\kappa))} = e^{-N\xi}$$
 $\xi = \frac{1}{\ln(\coth(\kappa))}$ is correlation length,
Thus, we can plot the relation of correlation function and r or N
 $G := \exp(-N)$, $define \xi = 1$

$$\sum_{i=1}^{N} plot(\exp(-N), N = 0..10)$$



2. Taking period border condition, when the number of spots is 10, what is Z?

Ans:

$$S_{1} = S_{N+1'} so Z = \sum_{\substack{\{s \\ i\}}} e^{K \sum_{\substack{s \ i \ i \ +1}} + s \sum_{\substack{s \ i \ i \ +1}} e^{K \left(\eta_{1} + \eta_{2} + \dots + \eta_{10}\right) + K \eta_{1} \eta_{2} \dots \eta_{10}} = 2$$
$$\sum_{a=0}^{\infty} \frac{K^{a}}{a!} \left(\sum_{\eta} e^{K \eta} \eta_{a}\right)^{10} = (2 \cosh K)^{11} + (2 \sinh K)^{11}$$

3.How do Energy, heat capacity, magnetization intensity, magnetic susceptibility, correlation function and partition function change with K? Draw its picture, and can you conclude that 1D Ising model has no phase change?

Ans:

[1] Taking no regard of outfield

1. Energy

$$Z := \beta \rightarrow 2 \left(2 \cosh(\beta \cdot J) \right)^{N-1}$$

$$Z := \beta \rightarrow 2 \left(2 \cosh(\beta J) \right)^{N-1}$$

$$F := \beta \rightarrow -\frac{\partial}{\partial \beta} \ln(Z(\beta))$$

$$(1)$$

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Class Homework

(5)

$$-\frac{9\sinh\left(\frac{1}{KT}\right)}{\cosh\left(\frac{1}{KT}\right)}$$

$$\int diff((5), T)$$

$$\frac{9}{\kappa T^2} - \frac{9\sinh\left(\frac{1}{\kappa T}\right)^2}{\cosh\left(\frac{1}{\kappa T}\right)^2 \kappa T^2}$$
(6)

>
$$eval\left((6), \left[T = \frac{1}{\kappa \cdot \beta} \right] \right)$$

9 $\kappa \beta^{2} - \frac{9 \sinh(\beta)^{2} \kappa \beta^{2}}{\cosh(\beta)^{2}}$ (7)

> eval((7), [K=1])

$$9\beta^{2} - \frac{9\sinh(\beta)^{2}\beta^{2}}{\cosh(\beta)^{2}}$$
(8)

> smartplot((8))







So, 1 D Ising has no phase change at none-zero temperature, or 1 D Ising model has no phase change;

Fig 5 x:T, y: ξ

0.07

0.08

0.10

0.09

4. Partition Function

 $3. \times 10^{13}$

 $2. \times 10^{13}$

 $1. \times 10^{13}$

0-

0.05

Т

 $Z = 2 \left(2 \cosh(K) \right)^{N-1} \xrightarrow{\text{evaluate at point}} Z = 1024 \cosh(K)^9 \rightarrow$

0.06



5. Magnetism Intensity =0

6. Magnetism susceptibility =0

[2]Considering Outfield

First we should derive the partition function by using the matrix method - Taking the periodic border condition,

$$E = -J \sum_{i=1}^{N} s_{i} s_{i+1} - W \sum_{i=1}^{N} s_{i}$$
$$Z = \sum_{s} \sum_{1}^{N} \sum_{2}^{N} \dots \sum_{N} e^{-\beta \left(-J \sum_{i=1}^{N} s_{i+1} - W \sum_{i=1}^{N} s_{i} \right)} = \sum_{s} \sum_{1}^{N} \sum_{2}^{N} \dots \sum_{N} \Pi e^{\beta J s_{i+1} + \frac{\beta W}{2} \left(s_{i} + s_{i+1} \right)}$$

Define matrix

$$\begin{cases} \beta^{JS}s_{i+1} + \frac{\beta W}{2} \left(s_{i} + s_{i+1}\right) \\ \left(s_{i} | P | s_{i+1}\right) = e^{\beta^{J}s_{i+1} + \frac{\beta W}{2} \left(s_{i} + s_{i+1}\right)} \end{cases}$$
Then Z=tr(P^{N}), $W = \mu B$
and $P = \begin{bmatrix} e^{\beta \cdot J + \beta \cdot \mu \cdot B} & e^{-\beta \cdot J} \\ e^{-\beta \cdot J} & e^{\beta \cdot J - \beta \cdot \mu \cdot B} \end{bmatrix} \xrightarrow{\text{eigenvalues}} \begin{bmatrix} \left(\frac{1}{2} e^{\beta J - \beta \mu B} + \frac{1}{2} e^{\beta J + \beta \mu B} + \frac{1}{2} e^{\beta J - \beta \mu B} + \frac{1}{2} e^{\beta J - \beta \mu B} e^{\beta J + \beta \mu B} + \left(e^{\beta J + \beta \mu B}\right)^{2} + 4 \left(e^{-\beta J}\right)^{2} \end{bmatrix}, \begin{bmatrix} \left(\frac{1}{2} e^{\beta J - \beta \mu B} + \frac{1}{2} e^{\beta J - \beta \mu B} e^{\beta J - \beta \mu B} + \left(e^{\beta J - \beta \mu B}\right)^{2} + 4 \left(e^{-\beta J}\right)^{2} \end{bmatrix}$

$$\begin{split} \lambda_{1} &\coloneqq \frac{1}{2} e^{\beta J - \beta \mu B} + \frac{1}{2} e^{\beta J + \beta \mu B} \\ &\quad + \frac{1}{2} \sqrt{\left(e^{\beta J - \beta \mu B}\right)^{2} - 2 e^{\beta J - \beta \mu B} e^{\beta J + \beta \mu B} + \left(e^{\beta J + \beta \mu B}\right)^{2} + 4 \left(e^{-\beta J}\right)^{2}} \\ \frac{1}{2} e^{\beta J - \beta \mu B} + \frac{1}{2} e^{\beta J + \beta \mu B} \\ &\quad + \frac{1}{2} \sqrt{\left(e^{\beta J - \beta \mu B}\right)^{2} - 2 e^{\beta J - \beta \mu B} e^{\beta J + \beta \mu B} + \left(e^{\beta J + \beta \mu B}\right)^{2} + 4 \left(e^{-\beta J}\right)^{2}} \\ \lambda_{2} &\coloneqq \frac{1}{2} e^{\beta J - \beta \mu B} + \frac{1}{2} e^{\beta J + \beta \mu B} \\ &\quad - \frac{1}{2} \sqrt{\left(e^{\beta J - \beta \mu B}\right)^{2} - 2 e^{\beta J - \beta \mu B} e^{\beta J + \beta \mu B} + \left(e^{\beta J + \beta \mu B}\right)^{2} + 4 \left(e^{-\beta J}\right)^{2}} \\ \frac{1}{2} e^{\beta J - \beta \mu B} + \frac{1}{2} e^{\beta J + \beta \mu B} \\ &\quad - \frac{1}{2} \sqrt{\left(e^{\beta J - \beta \mu B}\right)^{2} - 2 e^{\beta J - \beta \mu B} e^{\beta J + \beta \mu B} + \left(e^{\beta J + \beta \mu B}\right)^{2} + 4 \left(e^{-\beta J}\right)^{2}} \\ F = -KT ln \left(\lambda_{1}^{N} + \lambda_{2}^{N}\right) \end{split}$$
(14)

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$$M = -\frac{\partial}{\partial B}F = \frac{NKT \left(\lambda_{1}^{N-1} \frac{\partial}{\partial B}\lambda_{1} + \lambda_{2}^{N-1} \frac{\partial}{\partial B}\lambda_{2}\right)}{\lambda_{1}^{N} + \lambda_{2}^{N}}$$

$$= \frac{\partial}{\partial B}\lambda_{1,2} = \beta\mu \left(e^{\beta J}\sinh(\beta\mu B) \pm \frac{e^{2\beta J}\sinh(\beta\mu B)\cosh(\beta\mu B)}{\left(e^{-2\beta J} + e^{2\beta J}\sinh^{2}(\beta J)\right)^{\frac{1}{2}}}\right) =$$

$$\pm \frac{\beta\mu e^{\beta J}\sinh(\beta\mu B)\lambda_{1,2}}{\left(e^{-2\beta J} + e^{2\beta J}\sinh^{2}(\beta\mu B)\right)^{\frac{1}{2}}}$$

$$M := \frac{N\cdot\mu\cdot\sinh(\beta\cdot\mu\cdot B)\left(\lambda_{1}^{N} - \lambda_{2}^{N}\right)}{\left(e^{4\beta\cdot J} + (\sinh(\beta\cdot\mu\cdot B))^{2}\right)^{\frac{1}{2}}\left(\lambda_{1}^{N} + \lambda_{2}^{N}\right)} \xrightarrow{evaluate at point B = 2, \mu = 1, I = 2, J = 0, N = 100}$$

$$M := \frac{N\cdot\mu\cdot\sinh(\beta\cdot\mu\cdot B)\left(\sum_{1}^{2}\left(\lambda_{1}^{N} + \lambda_{2}^{N}\right)\right)^{\frac{1}{2}}\left(\lambda_{1}^{N} + \lambda_{2}^{N}\right)}{\left(100\sinh(\beta B)\left(\left(\frac{1}{2}e^{-\beta B} + \frac{1}{2}e^{\beta B} + \frac{1}{2}\sqrt{\left(e^{-\beta B}\right)^{2} - 2e^{-\beta B}e^{\beta B} + \left(e^{\beta B}\right)^{2} + 4}\right)^{100}\right)\right)\right)^{100}$$

$$\left(1$$

$$+\sinh(\beta B)\left(\left(\frac{1}{2}e^{-\beta B} + \frac{1}{2}e^{\beta B} + \frac{1}{2}\sqrt{\left(e^{-\beta B}\right)^{2} - 2e^{-\beta B}e^{\beta B} + \left(e^{\beta B}\right)^{2} + 4}\right)^{100}\right)\right)^{1/2}$$


$$\left(e^{4\beta} \left(\left(\frac{1}{2} + \frac{1}{2} e^{2\beta} + \frac{1}{2} \sqrt{1 - 2 e^{2\beta} + (e^{2\beta})^2 + 4 (e^{-\beta})^2} \right)^{100} + \left(\frac{1}{2} + \frac{1}{2} e^{2\beta} - \frac{1}{2} \sqrt{1 - 2 e^{2\beta} + (e^{2\beta})^2 + 4 (e^{-\beta})^2} \right)^{100} \right) + \sinh(\beta) \left(\left(\frac{1}{2} + \frac{1}{2} e^{2\beta} + \frac{1}{2} \sqrt{1 - 2 e^{2\beta} + (e^{2\beta})^2 + 4 (e^{-\beta})^2} \right)^{100} + \left(\frac{1}{2} + \frac{1}{2} e^{2\beta} - \frac{1}{2} \sqrt{1 - 2 e^{2\beta} + (e^{2\beta})^2 + 4 (e^{-\beta})^2} \right)^{100} \right)^{2} \right)^{1/2}$$

2. Magnetism susceptibility

$$\begin{split} M &:= \frac{N \cdot \mu \cdot \sinh(\beta \cdot \mu \cdot \beta) \left(\lambda_{1}^{N} - \lambda_{2}^{N}\right)}{\left(e^{4\beta \cdot j} + (\sinh(\beta \cdot \mu \cdot \beta))^{2}\right)^{\frac{1}{2}} \left(\lambda_{1}^{N} + \lambda_{2}^{N}\right)} \\ 3.5.nergy \\ Z &:= \lambda_{1}^{N} + \lambda_{2}^{N} \\ \left(\frac{1}{2} e^{\beta \cdot - \beta \mu \beta} + \frac{1}{2} e^{\beta \cdot + \beta \mu \beta} \right)^{2} - 2 e^{\beta \cdot - \beta \mu \beta} e^{\beta \cdot + \beta \mu \beta} + \left(e^{\beta \cdot + \beta \mu \beta}\right)^{2} + 4 \left(e^{-\beta \cdot i}\right)^{2}\right)^{N} \\ &+ \left(\frac{1}{2} e^{\beta \cdot - \beta \mu \beta} + \frac{1}{2} e^{\beta \cdot + \beta \mu \beta} - \frac{1}{2} \sqrt{\left(e^{\beta \cdot - \beta \mu \beta} + \frac{1}{2} e^{\beta \cdot - \beta \mu \beta} e^{\beta \cdot + \beta \mu \beta} + \left(e^{\beta \cdot + \beta \mu \beta}\right)^{2} + 4 \left(e^{-\beta \cdot i}\right)^{2}\right)^{N}} \\ &+ \left(\frac{1}{2} e^{\beta \cdot - \beta \mu \beta} + \frac{1}{2} e^{\beta \cdot - \beta \mu \beta} e^{\beta \cdot + \beta \mu \beta} + \left(e^{\beta \cdot + \beta \mu \beta}\right)^{2} + 4 \left(e^{-\beta \cdot i}\right)^{2}\right)^{N} \\ &= -\frac{1}{2} \sqrt{\left(e^{\beta \cdot - \beta \mu \beta}\right)^{2} - 2 e^{\beta \cdot - \beta \mu \beta} e^{\beta \cdot + \beta \mu \beta} + \left(e^{\beta \cdot + \beta \mu \beta}\right)^{2} + 4 \left(e^{-\beta \cdot i}\right)^{2}} \right)^{N} \\ \hline E &:= -\frac{\partial}{\partial \beta} \ln(Z) \\ \xrightarrow{evaluate at point B = 1, \mu = 1, i = 1, N = 100} \\ &- \left(100 \left(\frac{1}{2} + \frac{1}{2} e^{2\beta} + \frac{1}{2} \sqrt{1 - 2 e^{2\beta} + \left(e^{-\beta}\right)^{2}} + 100 \left(\frac{1}{2} + \frac{1}{2} e^{2\beta}\right)^{2} + 4 \left(e^{-\beta}\right)^{2}\right) + 100 \left(\frac{1}{2} + \frac{1}{2} e^{2\beta} - \frac{1}{2} \sqrt{1 - 2 e^{2\beta} + \left(e^{2\beta}\right)^{2} - 8 \left(e^{-\beta}\right)^{2}} \right) \right) / \left(\left(\frac{1}{2} + \frac{1}{2} e^{2\beta} - \frac{1}{4} \frac{-4 e^{2\beta} + 4 \left(e^{2\beta}\right)^{2} - 8 \left(e^{-\beta}\right)^{2}}{\sqrt{1 - 2 e^{2\beta} + \left(e^{2\beta}\right)^{2} + 4 \left(e^{-\beta}\right)^{2}}} \right) \right) / \left(\left(\frac{1}{2} + \frac{1}{2} e^{2\beta} + \frac{1}{2} \sqrt{1 - 2 e^{2\beta} + \left(e^{2\beta}\right)^{2} + 4 \left(e^{-\beta}\right)^{2}} \right) \right) \\ \end{pmatrix}$$





5.Correlation function G

 $G = \langle s_{i} \rangle = \frac{\left(k \cdot T\right)^{2}}{Z} \frac{\partial}{\partial B} \frac{\partial}{\partial B} Z \xrightarrow{evaluate at point B = 1, \mu = 1, l = 1, J = 1, N = 100}$



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$$\left(\frac{\frac{1}{2} + \frac{1}{2} e^{2\beta} + \frac{1}{2} \sqrt{1 - 2 e^{2\beta} + (e^{2\beta})^2 + 4 (e^{-\beta})^2}}\right)^{10} + \left(\frac{1}{2} + \frac{1}{2} e^{2\beta}\right)^{10}$$

$$-\frac{1}{2} \sqrt{1 - 2 e^{2\beta} + (e^{2\beta})^2 + 4 (e^{-\beta})^2}^{10}$$

$$\rightarrow$$

$$7. \times 10^{86}$$

$$6. \times 10^{86}$$

$$4. \times 10^{86}$$

$$3. \times 10^{86}$$

$$2. \times 10^{86}$$

$$1. \times 10^{86}$$

$$\frac{1}{2} + \frac{1}{2} e^{2\beta} + \frac{1}{2} e^{2\beta} = \frac{1}{2} e^{2\beta}$$

$$\frac{1}{2} + \frac{1}{2} e^{2\beta} + \frac{1}{2} e^{2\beta} = \frac{1}{2} e^{2\beta}$$