Notations and Conventions

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Equality

$$
\begin{aligned}
x = y &\quad \text{(exactly equal)} \\
x \approx y &\quad \text{(approximately equal)} \\
x \sim y &\quad \text{(equal apart from a dimensionless constant)} \\
x \propto y &\quad \text{(equal apart from a constant)}
\end{aligned}
$$

Inverse temperature $\beta \equiv 1/k_{\mathrm{B}}T$

In most cases, the inverse temperature is included in the definition of the Hamiltonian $\mathcal{H}$.

Field variables

A function of field variables, such as the Ising model Hamiltonian that depends on Ising spins, e.g., $S_1, S_2, \cdots$, may be expressed as

$$\begin{aligned} &\mathcal{H}(S_1, S_2, \cdots, S_N) \\ &\quad = \mathcal{H}(\{S_i | i \in \Omega\}) \quad (\Omega = \{1, 2, \cdots, N\} \\ &\quad = \mathcal{H}(\{S_i\}_{i\in\Omega}) \end{aligned}$$

When the definition of the space Ω is clear from the context, or when it does not have to be specified, we may drop it and use the simpler symbols such as

$$\mathcal{H}(\{S_i\}), \quad \mathcal{H}(\mathbf{S}), \quad \mathcal{H}(S), \quad \cdots$$

Tr (trace) and $\int$ (integral) for functional integrals

For functional integrals with respect to the field variables, we often use the both symbols for the same meaning, i.e.,

$$\mathop{\mathrm{Tr}}_{\phi} f[\phi(\mathbf{x})] \equiv \int D\phi(\mathbf{x})\, f[\phi(\mathbf{x})]$$

Fourier transformation and Greens' functions

$$a = (\text{lattice constant}), \quad L = (\text{system size}), \quad N \equiv \frac{L^d}{a^d} = (\#\text{ of sites})$$

$$\tilde{\phi}_{\mathbf{k}} = \int_0^L d^d\mathbf{r}\, e^{-i\mathbf{kr}}\phi_{\mathbf{r}} = a^d \sum_{\mathbf{r}} e^{-i\mathbf{kr}}\phi_{\mathbf{r}}$$

$$\phi_{\mathbf{r}} = \int_{-\pi/a}^{\pi/a} \frac{d^d\mathbf{k}}{(2\pi)^d}\, e^{i\mathbf{kr}}\tilde{\phi}_{\mathbf{k}} = L^{-d} \sum_{\mathbf{k}} e^{i\mathbf{kr}}\tilde{\phi}_{\mathbf{k}}$$

The tilde ˜ is often dropped when there is no fear of confusion.

$$G(\mathbf{r}', \mathbf{r}) \equiv \langle \phi_{\mathbf{r}'}\phi_{\mathbf{r}} \rangle, \quad G_{\mathbf{k}',\mathbf{k}} \equiv L^{-d}\langle \phi_{\mathbf{k}'}\phi_{\mathbf{k}} \rangle$$

For translationally and rotationally symmetric case,

$$G(\mathbf{r}', \mathbf{r}) = G(|\mathbf{r}' - \mathbf{r}|), \quad G_{\mathbf{k}',\mathbf{k}} = \delta_{\mathbf{k}'+\mathbf{k},\mathbf{0}} G_{|\mathbf{k}|}, \quad G_{|\mathbf{k}|} \equiv L^{-d}\langle |\phi_{\mathbf{k}}|^2 \rangle$$

1

$\acute{X}$(acute) and X'(prime)

We use both for the same meaning, because the position of the mark for the prime sometimes interferes with other superscripts and look messy.

“Rank”

The word “rank” can mean two things: the number if indices of a tensor and the number of linearly independent column/row vectors of a matrix. To avoid confusion, we use the word only for the latter. For the number of indices of a tensor, we use “degree”. So, a third degree tensor is a tensor with three indices and a rank-n matrix is a matrix with n independent column/row vectors.

Normal order product

We use the symbol $[\![\cdots]\!]$ for the normal-order product. In text books, colons $(: \cdots :)$ are more often used. (There is no reason. Just a matter of taste.)

Lecture 1: Introduction

Phase transitions, critical phenomena and universality

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To begin with

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

[1-1] Various Phenomena described by Ising model

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

Ferromagnets

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

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

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

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

represents the ferromagnet at least qualitatively.

Real gases

Real gas is described by Schrödinger equation,

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

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

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

Lenard-Jone gas

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

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

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

Lattice gas model

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

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

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

Universality

- The phase diagram one obtains from the LJ model agrees with the phase diagram determined by real experiments. The agreement can be made even quantitatively accurate for noble gases by choosing right values for ϵ and σ.
- This observation shows that the microscopic mechanism and the macroscopic properties are related to each other **only through a few parameters**. We may call this the **universality of statistical mechanical phenomena**.
- Moreover, when we focus on the critical phenomena, one can infer even the **exact** values of real systems from a very simplified model. For example, the value of the critical index β is estimated for the lattice-gas model to be $\beta \approx 0.3272$, and the experimental result can be fit well by assuming this estimate.
- This observation is an example of the **universality of critical phenomena**.

[1-2] Percolation

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

Forest fire and percolation

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

Generating function of the bond percolation (1)

- Let us consider the average cluster size defined by

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

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

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

$$\overline{Q}_c \equiv \sum_c Q_c / \sum_c 1. \tag{8}$$

- The angular bracket denotes the statistical average,

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

where the summation runs over all possible connection graphs.

Generating function of the bond percolation (2)

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

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

where $|G|$ is the number of the connections in G, $N_{\rm B}$ is the total number of the nearest neighbor pairs of sites, and $v \equiv p/(1-p)$.

- To obtain compact expression of the average cluster size,

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

Generating function of the bond percolation (3)

- The generating function of bond-percolation

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

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

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

Relation among percolation, Ising and Potts models

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

Potts model

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

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

where

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

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

Fortuin-Kasteleyn formula (1)

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

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

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

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

where

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

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

Fortuin-Kasteleyn formula (2)

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

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

- By using a simplifying notation

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

we obtain

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

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

Fortuin-Kasteleyn formula (3)

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

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

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

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

Fortuin-Kasteleyn formula (4)

- When $H = 0$,

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

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

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

[1-3] Summary

- Many cooperative macroscopic phenomena do have good explanation without referring to details of the microscopic mechanisms.
- The essential macroscopic properties can be understood by models in terms of intermediate-scale degrees of freedom.
- Often the same model can describe the essence of multiple phenomena with completely different microscopic origins.
- These observations may be phrased as the *universality of statistical mechanical phenomena*.
- In particular, the universality holds exactly in the critical phenomena. (*universality of critical phenomena*)

Homework

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

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

where

$$M \equiv \sum_i S_i \tag{25}$$

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

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

Lecture 2: Meanfield approximation, variational principle and Landau expansion

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[2-1] Mean-field approximation

In this lecture we will see:

- Molecular-field theory does not gives us the free energy.
- Gibbs-Bogoliubov-Feynman inequality give us a very systematic and frexible framework for constructiong the mean-field-type approximations.

Molecular field theory revisited

- In the molecular-field theory, the effect of **environment** is replaced by an additional term, in the case of Ising ferromagnet, we focus on a single spin, say S_0, and replace the Hamiltonian as

$$\mathcal{H} = -J \sum_{ij} S_i S_j - H \sum_i S_i \ \rightarrow \ \mathcal{H}_{\mathbf{MF}} = -H_{\mathrm{MF}} S_0 - H S_0$$

- It is also argued that the right choice of the effective field is

$$H_{\mathrm{MF}} = J \sum_j \langle S_j \rangle$$

- The uniformity condition $m = \langle S_i \rangle$ (independent of i) yields,

$$m = \tanh(\beta(H + zJm)) \quad (z = (\text{number of nearest-neighbors}))$$

Why should we complain?

- In principle, we have multiple solutions of the self-consistent equation.
- The molecular-field theory does not tell us which solution we should choose.
- If the theory allowed us to compute the free energy for each solution, we would be able to tell which one to take.

Gibbs-Bogoliubov-Feynman (GBF) inequality

Theorem 1 (GBF inequality)

For two Hamiltonians $\mathcal{H}(S)$ and $\mathcal{H}_0(S)$ defined on the same space $S \in \Omega$,

$$F_{\mathrm{v}} \equiv F_0 + \langle \mathcal{H} - \mathcal{H}_0 \rangle_0 \geq F, \tag{1}$$

where F and F_0 are the free-energies of $\mathcal{H}$ and $\mathcal{H}_0$ respectively and $\langle \cdots \rangle_0$ is the thermal average with respect to $\mathcal{H}_0$.

Variational calculation

When $\mathcal{H}(S)$ is the Hamiltonian of the system that we want to study but is not solvable, by taking $\mathcal{H}_0(\mathbf{\Lambda}, S)$ for $\mathcal{H}_0$ in (1) that also depends on a list of parameters $\mathbf{\Lambda}$ and is solvable for any $\mathbf{\Lambda}$, $F_v(\mathbf{\Lambda})$ gives us the upper bound of the correct free energy. (And it is computable!)

GBF inequality from information-scientific view-point

Theorem 2 (Relation to Kullback-Leibler divergence)

The "error" in the variational free-energy is proportional to the Kullback-Leibler divergence of the thermodynamic distribution of $\mathcal{H}_0$ relative to that of $\mathcal{H}$.

More precisely,

$$F_{\rm v} - F = k_{\rm B} T \ I_{\rm KL}[\rho_0|\rho] \tag{2}$$

where

$$\rho_0 \equiv e^{-\beta\mathcal{H}_0}/Z_0, \quad \text{and} \quad \rho \equiv e^{-\beta\mathcal{H}}/Z \tag{3}$$

and

$$I_{\rm KL}[P|Q] \equiv \sum_S P(S) \log \frac{P(S)}{Q(S)} \tag{4}$$

(Z and Z_0 are partition functions of $\mathcal{H}$ and $\mathcal{H}_0$ respectively.)

Proof of Theorem 2

$$I_{\mathrm{KL}}\left[Z_0^{-1}e^{-\beta\mathcal{H}_0}\middle|Z^{-1}e^{-\beta\mathcal{H}}\right]$$

$$= \sum_S \left(\frac{e^{-\beta\mathcal{H}_0(S)}}{Z_0} \log\left(\frac{e^{-\beta\mathcal{H}_0(S)}}{Z_0}\right) - \frac{e^{-\beta\mathcal{H}_0(S)}}{Z_0} \log\left(\frac{e^{-\beta\mathcal{H}(S)}}{Z}\right)\right)$$

$$= -\log Z_0 + \langle -\beta\mathcal{H}_0\rangle_0 + \log Z - \langle -\beta\mathcal{H}\rangle_0$$

$$= \beta F_0 - \beta\langle\mathcal{H}_0\rangle_0 - \beta F + \beta\langle\mathcal{H}\rangle_0$$

$$= \beta(F_{\mathrm{v}} - F)$$

Kullback-Leibler information measure is positive

$$
\begin{aligned}
I_{\mathrm{KL}}[P|Q] \\
&= \sum_S P(S) \log \frac{P(S)}{Q(S)} = -\sum_S P(S) \log \frac{Q(S)}{P(S)} \\
&\geq -\sum_S P(S) \left(\frac{Q(S)}{P(S)} - 1 \right) \quad \text{(because } \log(x) \leq x - 1) \\
&= \sum_S (Q(S) - P(S)) = 1 - 1 = 0
\end{aligned}
$$

Remark

This inequality together with Theorem 2 proves Theorem 1.

Quantum extention

- Though the theorems have been proved for classical systems, the corresponding quantum version of them can be also proved.
- For the extension, the KL divergence must be generaized to

$$I_{\mathrm{KL}}[P|Q] \equiv \mathrm{Tr}\left(P(\log P - \log Q)\right) \quad (5)$$

  where P and Q are now density operators satisfying $\mathrm{Tr}\left(P\right) = \mathrm{Tr}\left(Q\right) = 1$.
- Only non-trivial part in the proof of the quantum extension is the positivity of the KL information. The rest is straight-forward simply by replacing $\sum_S$ by Tr.

Proof of quantum extention (1)

Theorem 3 (Positivity of quantum KL divergence)

For any density operators P and Q,

$$I_{\mathrm{KL}}[P|Q] \equiv \mathrm{Tr}\left(P \log P - P \log Q\right) \geq 0 \tag{6}$$

Proof:

- Let us take the basis set in which P is diagonal, i.e., $P_{ij} = p_i \delta_{ij}$.
- For some unitary operator U, $Q_{ij} = u_{ik} q_k u^*_{jk}$
- With this u_{ij},

$$I_{KL}[P|Q] = \sum_i \left\{ p_i \log p_i - p_i \sum_j a_{ij} \log q_j \right\} \quad (a_{ij} \equiv |u_{ij}|^2)$$

Proof of quantum extention (2)

- Now, notice that $a_{ij} \geq 0, \quad \sum_i a_{ij} = \sum_j a_{ij} = 1.$
- Let us define $p'_{ij} = p_i a_{ij}, \quad q'_{ij} = q_j a_{ij}.$
- Then, these can be regarded as the classical distribution function in the squared Hilbert space $H \times H \equiv \{ (ij) \,|\, i,j \in H\}$:

$$p'_{ij} \geq 0,\ q'_{ij} \geq 0,\ \sum_{ij} p'_{ij} = \sum_{ij} q'_{ij} = 1$$

- Now, we can see

$$\sum_{ij} p'_{ij} \log p'_{ij} = \sum_i p_i \log p_i + \sum_{ij} p_i a_{ij} \log a_{ij}$$
$$\sum_{ij} p'_{ij} \log q'_{ij} = \sum_{ij} p_i a_{ij} \log q_j + \sum_{ij} p_i a_{ij} \log a_{ij},$$

- Thus we have obtained $I_{KL}[P|Q] = \sum_{ij} p'_{ij} \log(p'_{ij}/q'_{ij}) \geq 0$ (because the RHS is the classical KL information). (QED)

Variational approximation to the Ising model (1)

- For the target Hamiltonian $\mathcal{H} \equiv -J\sum_{ij} S_i S_j - H\sum_i S_i$, let us take the "trial" Hamiltonian $\mathcal{H}_0 \equiv -\Lambda \sum_i S_i$. where Λ is a variational parameter.
- Then, our variational free energy is

$$
\begin{aligned}
F_{\mathrm{v}} &= F_0 + \langle \mathcal{H} - \mathcal{H}_0 \rangle_0 \\
&= \langle \mathcal{H} \rangle_0 - S_0 T
\end{aligned}
$$

where $S_0 \equiv T^{-1}(\langle \mathcal{H}_0 \rangle_0 - F_0)$ is the entropy of the $\mathcal{H}_0$ system

- By introducing $m \equiv \langle S_i \rangle_0 = \tanh \beta\Lambda$,

$$
\langle \mathcal{H}_0 \rangle_0 = -\frac{z}{2} NJm^2 - HNm \qquad S_0 = N\sigma(m) \tag{7}
$$

$$
\sigma(m) \equiv -k_{\mathrm{B}} \left(\frac{1+m}{2} \log \frac{1+m}{2} + \frac{1-m}{2} \log \frac{1-m}{2} \right) \tag{8}
$$

Variational approximation to the Ising model (2)

Variational free-energy density

$$f_{\rm v} \equiv \frac{F_{\rm v}}{N} = -\frac{zJm^2}{2} - Hm - T\sigma(m)$$

- The GBF inequality tells us that we should minimize $f_{\rm v}$ with respect to λ. Since $f_{\rm v}$ depends on λ only through m, the stational condition $\partial f_{\rm v}/\partial\lambda = 0$ leads to $\partial f_{\rm v}/\partial m = 0$.
- From this, we obtain the same as the molecular-field approx.:

$$\frac{\partial f_{\rm v}}{\partial m} = 0 \quad \Rightarrow \quad m = \tanh \beta H_{\rm MF} \quad (H_{\rm MF} \equiv zJm + H). \tag{9}$$

Mean-field free energy — Landau expansion

- We have also obtained the explicit expression for the free energy.
- Since its behavior near $m \approx 0$ is most important for the critical phenomena, let us expand f_{v} with respect to m.

$$f_{\mathrm{v}} = -\frac{zJ}{2}m^2 - Hm - k_{\mathrm{B}}T\left(\log 2 - \frac{m^2}{2} - \frac{m^4}{12}\right) \tag{10}$$

- From the condition (coefficient of m^2) $= 0$, we obtain $k_{\mathrm{B}}T_c = zJ$.
- Near $T \approx T_c$, we can get the Landau expansion:

$$f_{\mathrm{v}} \approx f_{\mathrm{v}}^0 + tm^2 + um^4 - Hm \tag{11}$$

where $f_v^0 \equiv -zJ\log 2,\ t \equiv (k_{\mathrm{B}}T - zJ)/2$ and $u \equiv zJ/12$

[2-2] Summary of Lecture 2

- Molecular-field theory does not give us the free energy.
- Gibbs-Bogoliubov-Feynman inequality give us a very systematic and frexible framework for constructiong the mean-field-type approximations that also provides the free energy.
- Landau expansion is useful in having a clear view of the phase transitions.

Homework

- Veryfy (7) and (8).
- At the point where we have arrived at (9), m is just a variational parameter and its physical meaning is not yet clear. Give the reason why we can interprete it as the magnetization.
- Following the example of the Ising model in the lecture, obtain the Landau expansion of the 3-state Potts model by taking the trial Hamiltonian

$$\mathcal{H}_0 \equiv -\Lambda \sum_i \delta_{S_i,1}. \tag{12}$$

  This time, the order parameter should be $m \equiv \langle \delta_{S_i,1} \rangle - 1/3$. What is the essential difference from the Ising case?
- Submit your report on one of these problems at the beginning of the next lecture.

Lecture 3: ϕ^4 theory and Ornstein-Zernike form

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To begin with ...

- The mean-field theory discussed in the previous section does not tell us about the spatial correlation.
- In this lecture, starting from the Ising model, we derive ϕ^4 model, which, we expect, the same long-range behavior as the Ising model.
- We then apply the GBF variational approximation to the ϕ^4 Hamiltonian, to obtain the mean-field expression for the two-point correlation function. (Ornstein-Zernike form)

[3-1] ϕ^4 field theory

- We first see a very "hand-waving" derivation of ϕ^4 field theory starting from the Ising model and using the coarse-graining.
- We next see an alternative derivation which looks less hand-waving, based on the Hubbard-Stratonovich transformation.
- Since the ϕ^4 theory is obtained by the coarse-graining of the Ising model, they are supposed to share the same long-range behavior, while they may differ quantitatively for short-range physics.
- In particuar, we expect, ϕ^4 model belongs to the same universality class as the Ising model, as has been verified by a number of arguments and numerical calculations.

A hand-waving derivation by coarse-graining (1)

- Let us consider the Ising model on d-dimensional hyper-cubic lattice. (Hereafter, we use symbols like $\mathbf{r}$ and $\mathbf{R}$ to spacify lattice points in stead of i and j.)
- Divide the whole lattice into cells of size ab, where a is the lattice constant, and denote the one located at $\mathbf{R}$ as $\Omega_{ab}(\mathbf{R})$. $(b \gg 1)$
- Consider the cell average of spins

$$\phi_{\mathbf{R}} = \left(\frac{1}{b}\right)^d \sum_{\mathbf{r}\in\Omega_{ab}(\mathbf{R})} S_{\mathbf{r}} \tag{1}$$

- Consider the coarse-grained Hamiltonian $\tilde{\mathcal{H}}$ defined as

$$e^{-\tilde{\mathcal{H}}(\phi)} \equiv \sum_{\mathbf{S}} \Delta(\mathbf{S}|\phi) e^{-\mathcal{H}(\mathbf{S})}$$

where $\phi \equiv \{\phi_{\mathbf{R}}\}$, $\mathbf{S} \equiv \{S_{\mathbf{r}}\}$, and $\Delta(\mathbf{S}|\phi)\,(=0,1)$ takes 1 if and only if the condition (1) is satisfied for all cells.

A hand-waving derivation by coarse-graining (2)

- Let us guess, by intuition, what $\tilde{\mathcal{H}}$ should be like.
- There must be two parts: a single-cell part reflecting the physics inside each cell and a multiple-cell part for interactions.
- For one-cell part, the entropic effect gives rise to ϕ^2 and ϕ^4 terms (as in means-field approx.) whereas the interaction will produce $-\phi^2$.
- For multiple-cell part, the interaction among cells is represented by terms that depend on the gradient, $\nabla_{\mathbf{R}}\phi$. The mirror-image symmetry allows only even order terms. So, we expect $|\nabla\phi|^2$ in the lowest order.
- Putting these together and including the Zeeman term, we obtain

$$\tilde{H}(\phi) \equiv a^d \sum_{\mathbf{R}} \left(\rho|\nabla\phi|^2 + t\phi^2 + u\phi^4 - h\phi\right) \tag{2}$$

$$= \int_a^L d^d\mathbf{R} \left(\rho|\nabla\phi|^2 + t\phi^2 + u\phi^4 - h\phi\right) \tag{3}$$

(ρ, u are positive constants. t can be either positive or negative, depending on the temperature.)

Derivation by the Hubbard-Stratonovich transformation

$$Z_{\rm Ising} = \sum_S e^{K\sum_{(\mathbf{r},\mathbf{r}')} S_\mathbf{r} S_{\mathbf{r}'}} = \sum_S e^{\frac{K}{2}\mathbf{S}^\mathsf{T} C \mathbf{S} - \frac{cKN}{2}} \quad \left(C_{\mathbf{r},\mathbf{r}'} = \begin{cases} c & (|\mathbf{r}-\mathbf{r}'|=0) \\ 1 & (|\mathbf{r}-\mathbf{r}'|=a) \\ 0 & (\text{otherwise}) \end{cases} \right)$$

$$\stackrel{*}{=} \sum_S \int D\phi\, e^{-\frac{1}{2K}\phi^\mathsf{T} C^{-1}\phi + \phi\mathbf{S}} \quad \text{(HS transformation)}$$

$$= \int D\phi\, e^{-\frac{1}{2K}\phi^\mathsf{T} C^{-1}\phi} \prod_\mathbf{r} (2\cosh\phi_\mathbf{r})$$

$$\stackrel{*}{\approx} \int D\phi\, e^{-K^{-1}\sum_\mathbf{r}(\alpha\phi_\mathbf{r}^2 + \beta(\nabla\phi_\mathbf{r})^2)} e^{-\sum_\mathbf{r}(-\frac{1}{2}(\phi_\mathbf{r})^2 + \frac{1}{12}(\phi_\mathbf{r})^4)}$$

$$= \int D\phi\, e^{-\tilde{\mathcal{H}}(\phi)} = Z_{\phi^4}$$

$$\tilde{\mathcal{H}}(\phi) = \sum_\mathbf{r} \left(\frac{\beta}{K}|\nabla\phi_\mathbf{r}|^2 + \left(\frac{\alpha}{K} - \frac{1}{2}\right)|\phi_\mathbf{r}|^2 + \frac{1}{12}|\phi_\mathbf{r}|^4 \right)$$

Supplement: Hubbard-Stratonovich transformation (1)

For an arbitrary positive definite symmetric matrix A and a vector $\mathbf{B}$, we can show the following,

$$
\begin{aligned}
&\int D\phi\, e^{-\frac{1}{2}\sum_{\mathbf{r},\mathbf{r}'} A_{\mathbf{r},\mathbf{r}'}\phi_{\mathbf{r}}\phi_{\mathbf{r}'}+\sum_{\mathbf{r}} B_{\mathbf{r}}\phi_{\mathbf{r}}} \\
&\qquad = \int D\phi\, e^{-\frac{1}{2}\phi^{\mathsf{T}}A\phi+\mathbf{B}^{\mathsf{T}}\phi} \\
&\qquad = \int D\boldsymbol{\xi}|A|^{-1/2}e^{-\frac{1}{2}\boldsymbol{\xi}^{\mathsf{T}}\boldsymbol{\xi}+\boldsymbol{\eta}^{\mathsf{T}}\boldsymbol{\xi}} \quad (\boldsymbol{\xi}\equiv A^{1/2}\phi,\ \boldsymbol{\eta}\equiv A^{-1/2}\mathbf{B}) \\
&\qquad = \int D\boldsymbol{\xi}|A|^{-1/2}e^{-\frac{1}{2}(\boldsymbol{\xi}-\boldsymbol{\eta})^2+\frac{1}{2}(\boldsymbol{\eta})^2} \\
&\qquad = (2\pi)^{\frac{N}{2}}|A|^{-1/2}e^{\frac{1}{2}(\boldsymbol{\eta})^2} = (2\pi)^{\frac{N}{2}}|A|^{-1/2}e^{\frac{1}{2}\mathbf{B}^{\mathsf{T}}A^{-1}\mathbf{B}}
\end{aligned}
$$

By taking KC for A^{-1} and $\mathbf{S}$ for $\mathbf{B}$,

$$
e^{\frac{K}{2}\mathbf{S}^{\mathsf{T}}C\mathbf{S}} \sim \int D\phi\, e^{-\frac{1}{2K}\phi^{\mathsf{T}}C^{-1}\phi+\phi^{\mathsf{T}}\mathbf{S}}
$$

Supplement: Hubbard-Stratonovich transformation (2)

The matrix C is defined as $C \equiv cI + \Delta$ where Δ is the connection matrix

$$\Delta_{\mathbf{r},\mathbf{r}'} \equiv \begin{cases} 1 & (|\mathbf{r} - \mathbf{r}'| = a) \\ 0 & (\text{Otherwise}) \end{cases}$$

We need its inverse, which we can compute as

$$\begin{aligned} C^{-1} &= \frac{1}{c}\left(I + \frac{1}{c}\Delta\right)^{-1} \\ &= \frac{1}{c}\left(I - \frac{1}{c}\Delta + \frac{1}{c^2}\Delta^2 + \cdots\right) \end{aligned}$$

This decays exponentially as a function of distance; truncation would not change things qualitatively, leading to what have been used in the main text

$$C^{-1} \approx \frac{1}{c}I - \frac{1}{c^2}\Delta \quad \left(\phi^{\mathsf{T}} C^{-1}\phi \approx \sum_{\mathbf{r}}\left(\frac{1}{c}(\phi_{\mathbf{r}})^2 + \frac{1}{2c^2}(\nabla\phi)^2\right)\right)$$

The meaning of ϕ in the HS derivation

For an arbitrary vector $\boldsymbol{\xi}$, we have

$$\begin{aligned}
\langle \boldsymbol{\xi}^{\mathsf{T}} \mathbf{S} \rangle_{\text{Ising}} &= Z_0^{-1} \frac{\partial}{\partial h} \sum_{\mathbf{S}} e^{\mathbf{S}^{\mathsf{T}} K \mathbf{S} + h \boldsymbol{\xi}^{\mathsf{T}} \mathbf{S}} \\
&= Z_0^{-1} \frac{\partial}{\partial h} \int D\phi \sum_{\mathbf{S}} e^{-\frac{1}{2}\phi^{\mathsf{T}} K^{-1} \phi + \phi^{\mathsf{T}} \mathbf{S} + h \boldsymbol{\xi}^{\mathsf{T}} \mathbf{S}} \quad \text{(HS transformation)} \\
&= Z_0^{-1} \frac{\partial}{\partial h} \int D\phi' \sum_{\mathbf{S}} e^{-\frac{1}{2}(\phi' - h\boldsymbol{\xi})^{\mathsf{T}} K^{-1} (\phi' - h\boldsymbol{\xi}) + \phi'^{\mathsf{T}} \mathbf{S}} \quad (\phi' \equiv \phi + h\boldsymbol{\xi}) \\
&= Z_0^{-1} \frac{\partial}{\partial h} \int D\phi' \sum_{\mathbf{S}} e^{-\frac{1}{2}\phi'^{\mathsf{T}} K^{-1} \phi' + h \boldsymbol{\xi}^{\mathsf{T}} K^{-1} \phi' + \phi'^{\mathsf{T}} \mathbf{S}} \quad \text{(Expand in } h\text{)} \\
&= Z_0^{-1} \int D\phi \, e^{-\tilde{\mathcal{H}}_{\phi^4}(\phi)} \, \boldsymbol{\xi}^{\mathsf{T}} K^{-1} \phi = \langle \boldsymbol{\xi}^{\mathsf{T}} K^{-1} \phi \rangle_{\phi^4} \quad \text{(Remove } ' \text{)}
\end{aligned}$$

This means $\quad \phi_r \leftrightarrow \sum_{r'} K_{r,r'} S_r. \quad$ (A local sum of spins)

[3-2] Variational approximation to ϕ^4 model

- Similar to the Ising model, generally it is impossible to obtain the exact solution of ϕ^4 model by analytical means. So, we need some approximation. The simplest one is the mean-field type approximation as always.

- We will first move to the momentum space.

- Then, we will apply the GBF variational principle by taking the Gaussian theory as the trial Hamiltonian.

- As a result, we will obtain the mean-field evaluation of the spatial correlation function, which is called Ornstein-Zernike form.

Switching to the momentum space

Starting from (4), $\mathcal{H} = a^d \sum_{\mathbf{r}} \left(\rho |\nabla \phi_{\mathbf{r}}|^2 + t\phi_{\mathbf{r}}^2 + u\phi_{\mathbf{r}}^4 - h\phi_{\mathbf{r}} \right),$

by Fourier transformation $\phi_{\mathbf{r}} = L^{-d} \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}} \tilde{\phi}_{\mathbf{k}}$, we obtain

$$\begin{aligned} \mathcal{H} &= \frac{1}{L^d} \sum_{\mathbf{k}} (\rho k^2 + t) |\tilde{\phi}_{\mathbf{k}}|^2 \\ &+ \frac{u}{L^{3d}} \sum_{\mathbf{k}_1 \cdots \mathbf{k}_4} \delta_{\sum_{\mu=1}^4 \mathbf{k}_\mu, \mathbf{0}} \tilde{\phi}_{\mathbf{k}_1} \tilde{\phi}_{\mathbf{k}_2} \tilde{\phi}_{\mathbf{k}_3} \tilde{\phi}_{\mathbf{k}_4} - h\tilde{\phi}_{\mathbf{0}}. \end{aligned} \tag{4}$$

Switching to continuous wave numbers,

$$\begin{aligned} \mathcal{H} &= \int \frac{d^d\mathbf{k}}{(2\pi)^d} (\rho k^2 + t) \tilde{\phi}_{\mathbf{k}}^* \tilde{\phi}_{\mathbf{k}} \\ &+ u \int \frac{d^d\mathbf{k}_1 \cdots d^d\mathbf{k}_4}{(2\pi)^{4d}} \delta \left(\sum_{\mu} \mathbf{k}_\mu \right) \tilde{\phi}_{\mathbf{k}_1} \cdots \tilde{\phi}_{\mathbf{k}_4} - h\tilde{\phi}_{\mathbf{0}} \end{aligned} \tag{5}$$

Supplement: Convention (Fourier transformation)

In this lecture, we use the following conventions:

$$a = (\text{lattice constant}), \quad L = (\text{system size}), \quad N \equiv \frac{L^d}{a^d} = (\#\text{ of sites})$$

$$\tilde{\phi}_{\mathbf{k}} = \int_0^L d^d\mathbf{r}\, e^{-i\mathbf{k}\mathbf{r}} \phi_{\mathbf{r}} = a^d \sum_{\mathbf{r}} e^{-i\mathbf{k}\mathbf{r}} \phi_{\mathbf{r}}$$

$$\phi_{\mathbf{r}} = \int_{-\pi/a}^{\pi/a} \frac{d^d\mathbf{k}}{(2\pi)^d} e^{i\mathbf{k}\mathbf{r}} \tilde{\phi}_{\mathbf{k}} = L^{-d} \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}} \tilde{\phi}_{\mathbf{k}}$$

The tilde ˜ is often dropped when there is no fear of confusion.

$$G(\mathbf{r}', \mathbf{r}) \equiv \langle \phi_{\mathbf{r}'} \phi_{\mathbf{r}} \rangle, \quad G_{\mathbf{k}',\mathbf{k}} \equiv L^{-d} \langle \phi_{\mathbf{k}'} \phi_{\mathbf{k}} \rangle$$

For translationally and rotationally symmetric case,

$$G(\mathbf{r}', \mathbf{r}) = G(|\mathbf{r}' - \mathbf{r}|), \quad G_{\mathbf{k}',\mathbf{k}} = \delta_{\mathbf{k}'+\mathbf{k},\mathbf{0}} G_{|\mathbf{k}|}, \quad G_{|\mathbf{k}|} \equiv L^{-d} \langle |\phi_{\mathbf{k}}|^2 \rangle$$

GBF variational approximation (1)

Let us consider a trial Hamiltonian with variational parameter $\epsilon_{\mathbf{k}}$,

$$\mathcal{H}_0 \equiv \frac{1}{L^d} \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} |\phi_{\mathbf{k}}|^2 \tag{6}$$

$$Z_0 = \int D\phi\, e^{-\frac{1}{L^d} \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} |\phi_{\mathbf{k}}|^2} = \prod_{\mathbf{k}} \zeta_{\mathbf{k}}$$

$$\langle |\phi_{\mathbf{k}}|^2 \rangle_0 = \frac{L^d}{2\epsilon_{\mathbf{k}}}, \quad \zeta_{\mathbf{k}} \equiv \left(\frac{\pi L^d}{\epsilon_{\mathbf{k}}} \right)^{1/2}$$

$$E_0 = \frac{1}{L^d} \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \langle |\phi_{\mathbf{k}}|^2 \rangle_0 = \sum_{\mathbf{k}} \frac{\epsilon_{\mathbf{k}}}{L^d} \frac{L^d}{2\epsilon_{\mathbf{k}}} = \sum_{\mathbf{k}} \frac{1}{2} \quad \text{(Equipartition)}$$

$$-TS_0 = F_0 - E_0 = -\sum_{\mathbf{k}} \frac{1}{2} \log \frac{\pi L^d}{\epsilon_{\mathbf{k}}} = \frac{1}{2} \sum_{\mathbf{k}} \log \epsilon_{\mathbf{k}}$$

(Additive constants have been omitted.)

GBF variational approximation (2)

$$\langle \mathcal{H} \rangle_0 = \frac{1}{L^d} \sum_{\mathbf{k}} (\rho k^2 + t) \langle |\phi_{\mathbf{k}}|^2 \rangle_0 + \frac{u}{L^{3d}} \sum_{\mathbf{k}_1 \cdots \mathbf{k}_4} \delta_{\sum \mathbf{k}, \mathbf{0}} \langle \phi_{\mathbf{k}_1} \phi_{\mathbf{k}_2} \phi_{\mathbf{k}_3} \phi_{\mathbf{k}_4} \rangle_0$$

$$= \frac{1}{L^d} \sum_{\mathbf{k}} (\rho k^2 + t) \langle |\phi_{\mathbf{k}}|^2 \rangle_0 + \frac{3u}{L^{3d}} \sum_{\mathbf{k}, \mathbf{k}'} \langle |\phi_{\mathbf{k}}|^2 \rangle_0 \langle |\phi_{\mathbf{k}'}|^2 \rangle_0 \quad \text{(Wick)}$$

In terms of $G_{\mathbf{k}} \equiv L^{-d} \langle |\phi_{\mathbf{k}}|^2 \rangle_0 = (2\epsilon_{\mathbf{k}})^{-1}$, we obtain

$$F_{\mathrm{v}} = \langle \mathcal{H} \rangle_0 - TS_0 = \sum_{\mathbf{k}} (\rho k^2 + t) G_{\mathbf{k}} + \frac{3u}{L^d} \left(\sum_{\mathbf{k}} G_{\mathbf{k}} \right)^2 + \frac{1}{2} \sum_{\mathbf{k}} \log \epsilon_{\mathbf{k}}$$

Thus we have, $f_{\mathrm{v}} = B + 3uA^2 + \frac{1}{2L^d} \sum_{\mathbf{k}} \log \epsilon_{\mathbf{k}},$ (7)

where $A \equiv \frac{1}{L^d} \sum_{\mathbf{k}} G_{\mathbf{k}}$, and $B \equiv \frac{1}{L^d} \sum_{\mathbf{k}} (\rho k^2 + t) G_{\mathbf{k}}$.

Stationary condition

$$0 = \frac{\partial F_v}{\partial \epsilon_{\mathbf{k}}} = \left(\rho k^2 + t + \sigma\right) \frac{\partial G_{\mathbf{k}}}{\partial \epsilon_{\mathbf{k}}} + \frac{1}{2\epsilon_{\mathbf{k}}}$$

$$\left(\sigma \equiv 6uA = \frac{6u}{L^d} \sum_{\mathbf{k}} G_{\mathbf{k}}\right)$$

$\cdots$ Spatial fluctuation shifts the transition point.

$$= \left(\rho k^2 + t + \sigma\right) \left(-\frac{1}{2\epsilon_{\mathbf{k}}^2}\right) + \frac{1}{2\epsilon_{\mathbf{k}}}$$

$$\Rightarrow \quad \epsilon_{\mathbf{k}} = \rho k^2 + t + \sigma = \rho(k^2 + \kappa^2) \quad \left(\kappa \equiv \sqrt{\frac{t + \sigma}{\rho}}\right)$$

Ornstein-Zernike form

$$G_k \propto \frac{1}{k^2 + \kappa^2}, \quad \kappa \propto \sqrt{T - T_c}$$

Supplement: Wick's theorem

Theorem 1 (Wick)

When the distribution function is gaussian, any multi-point correlator factorizes in pairs.

Example 2 (4-point correlator)

Ex: When the Hamiltonian is $\mathcal{H} = \frac{1}{2}\phi^{\mathsf{T}} A \phi$ with A being a positive definit matrix,

$$\begin{aligned}\langle \phi_1\phi_2\phi_3\phi_4 \rangle &= \langle \phi_1\phi_2 \rangle \langle \phi_3\phi_4 \rangle + \langle \phi_1\phi_3 \rangle \langle \phi_2\phi_4 \rangle + \langle \phi_1\phi_4 \rangle \langle \phi_2\phi_3 \rangle \\ &= \Gamma_{12}\Gamma_{34} + \Gamma_{13}\Gamma_{24} + \Gamma_{14}\Gamma_{23}\end{aligned}$$

where $\Gamma \equiv A^{-1}$ and $\langle \cdots \rangle \equiv \dfrac{\int D\phi \, e^{-\mathcal{H}(\phi)} \ldots}{\int D\phi \, e^{-\mathcal{H}(\phi)}}$

Supplement: Proof of Wick's theorem

If we define $\Xi \equiv \int D\phi\, e^{-\frac{1}{2}\phi^{\mathsf{T}}A\phi+\boldsymbol{\xi}^{\mathsf{T}}\phi}$, the correlation function can be expressed as its derivatives,

$$\left\langle \phi_{k_1}\phi_{k_2}\cdots\phi_{k_{2p}} \right\rangle = \Xi^{-1} \left(\frac{\partial}{\partial \xi_{k_1}} \cdots \frac{\partial}{\partial \xi_{k_{2p}}} \Xi \right)\Bigg|_{\boldsymbol{\xi}\to\mathbf{0}} .$$

Now notice that $\Xi \propto e^{\frac{1}{2}\boldsymbol{\xi}^{\mathsf{T}}\Gamma\boldsymbol{\xi}}$, which can be expanded as

$$\Xi = 1 + \sum_{ij} \frac{\Gamma_{ij}}{2}\xi_i\xi_j + \frac{1}{2}\sum_{ij}\sum_{kl}\frac{\Gamma_{ij}}{2}\frac{\Gamma_{kl}}{2}\xi_i\xi_j\xi_k\xi_l + \cdots$$

Therefore, the $2p$-body correlation becomes

$$\frac{1}{p!}\sum_{i_1j_1}\sum_{i_2j_2}\cdots\sum_{i_pj_p}\frac{\Gamma_{i_1j_1}}{2}\frac{\Gamma_{i_2j_2}}{2}\cdots\frac{\Gamma_{i_pj_p}}{2}\delta_{\{k_1,k_2,\cdots,k_{2p}\},\{i_1,j_1,i_2,j_2,\cdots,i_p,j_p\}}$$

$$= \sum \Gamma_{i_1j_1}\Gamma_{i_2j_2}\ldots\Gamma_{i_pj_p} \quad \text{(Summation over all pairings of } \{k_1,\cdots,k_{2p}\}\text{)}$$

Real-space correlation function

$$G_{\mathbf{k}} = L^{-d}\langle|\phi_{\mathbf{k}}|^2\rangle = \frac{1}{2\epsilon_{\mathbf{k}}} = \frac{1}{2(\rho k^2 + t + \sigma)}$$

$$G(\mathbf{r}' - \mathbf{r}) \equiv \langle\phi_{\mathbf{r}'}\phi_{\mathbf{r}}\rangle = L^{-2d}\sum_{\mathbf{k},\mathbf{k}'} e^{i\mathbf{k}'\mathbf{r}'}e^{i\mathbf{k}\mathbf{r}}\langle\phi_{\mathbf{k}'}\phi_{\mathbf{k}}\rangle$$

$$= L^{-2d}\sum_{\mathbf{k},\mathbf{k}'} e^{i\mathbf{k}'\mathbf{r}'}e^{i\mathbf{k}\mathbf{r}}\delta_{\mathbf{k}'+\mathbf{k},\mathbf{0}}G_{\mathbf{k}} = L^{-2d}\sum_{\mathbf{k}} e^{-i\mathbf{k}(\mathbf{r}'-\mathbf{r})}\frac{L^d}{2\epsilon_{\mathbf{k}}}$$

$$G(\mathbf{r}) = \int \frac{d^d\mathbf{k}}{(2\pi)^d}\frac{e^{i\mathbf{k}\mathbf{r}}}{2\epsilon_{\mathbf{k}}} = \frac{1}{2}\int \frac{d^d\mathbf{k}}{(2\pi)^d}\frac{e^{i\mathbf{k}\mathbf{r}}}{\rho k^2 + t + \sigma}$$

$$\overset{*}{\sim} \begin{cases} \frac{1}{\rho}\frac{\kappa^{d-2}}{(\kappa r)^{\frac{d-1}{2}}}e^{-\kappa r} \quad \left(\kappa r \gg 1,\ \kappa \equiv \sqrt{\frac{t+\sigma}{\rho}}\right) & (T > T_c) \\ \frac{1}{\rho}\frac{1}{r^{d-2}} & (T = T_c) \end{cases}$$

($* \cdots$ see supplement)

Mean-field values of ν and η

$$G(r) \sim \begin{cases} \frac{1}{\rho} \frac{\kappa^{d-2}}{(\kappa r)^{\frac{d-1}{2}}} e^{-\kappa r} \quad \left(\kappa r \gg 1,\ \kappa \equiv \sqrt{\frac{t+\sigma}{\rho}}\right) & (T > T_c) \\ \frac{1}{\rho} \frac{1}{r^{d-2}} & (T = T_c) \end{cases}$$

Mean-field value of ν

$$\text{For } T > T_c, \quad G(r) \propto \frac{1}{r^{\frac{d-1}{2}}} e^{-r/\xi}, \quad \xi \propto \frac{1}{|T - T_c|^{\nu}}, \quad \nu_{\mathrm{MF}} = \frac{1}{2}$$

Mean-field value of η

$$\text{At } T = T_c, \quad G(r) \propto \frac{1}{r^{d-2+\eta}}, \quad \eta_{\mathrm{MF}} = 0$$

Supplement: Evaluation of the asymptotic form ($T > T_c$)

$$\int d\mathbf{k}\,\frac{e^{i\mathbf{kr}}}{k^2+\kappa^2} = \int d\mathbf{k}\,e^{i\mathbf{kr}}\int_0^\infty dt e^{-t(k+\kappa^2)}$$

$$= \int_0^\infty dt\,e^{-t\kappa^2}\int d\mathbf{k} e^{-tk^2+i\mathbf{rk}}$$

$$= \int_0^\infty dt\,e^{-t\kappa^2}\int d\mathbf{k} e^{-t(\mathbf{k}-\frac{i}{2t}\mathbf{r})^2-\frac{\mathbf{r}^2}{4t}} = \int_0^\infty dt\,\left(\frac{\pi}{t}\right)^{\frac{d}{2}} e^{-\kappa^2 t-\frac{r^2}{4t}}$$

(Here we define u so that $t \equiv \frac{r}{2\kappa}u$ and $\kappa^2 t + \frac{r^2}{4t} = \frac{\kappa r}{2}(u+u^{-1})$.)

$$= \int_0^\infty du\,\left(\frac{\pi}{u}\right)^{\frac{d}{2}}\left(\frac{2\kappa}{r}\right)^{\frac{d}{2}-1} e^{-\frac{\kappa r}{2}(u+u^{-1})}$$

(For $\kappa r \gg 1$, we use $u+u^{-1} \approx 2+\epsilon^2$ where $\epsilon \equiv u-1$.)

$$\approx \pi^{\frac{d}{2}}\left(\frac{2\kappa}{r}\right)^{\frac{d}{2}-1} e^{-\kappa r}\left(\frac{2\pi}{\kappa r}\right)^{\frac{1}{2}} \qquad \sim \frac{\kappa^{d-2}}{(\kappa r)^{\frac{d-1}{2}}}e^{-\kappa r}$$

Supplement: Evaluation of the asymptotic form ($T = T_c$)

As before, we have

$$\int d\mathbf{k}\, \frac{e^{i\mathbf{kr}}}{k^2+\kappa^2} = \int_0^\infty dt\, \left(\frac{\pi}{t}\right)^{\frac{d}{2}} e^{-\kappa^2 t - \frac{r^2}{4t}}$$

Here, by setting $\kappa = 0$ ($T = T_c$),

$$= \int_0^\infty dt\, \left(\frac{\pi}{t}\right)^{\frac{d}{2}} e^{-\frac{r^2}{4t}}$$

(By defining $\eta \equiv \frac{r^2}{4t}$)

$$= \left(\frac{r^2}{4}\right)^{1-\frac{d}{2}} \pi^{\frac{d}{2}} \Gamma\left(\frac{d}{2}-1\right) \sim \frac{1}{r^{d-2}}$$

Gaussian MF approximation below T_c (1)

- To deal with the spontaneous magnetization below T_c, we must introduce a symmetry-breaking field η as a new variational parameter,

$$\mathcal{H}_0 = L^{-d} \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} |\phi_{\mathbf{k}}|^2 - \eta \phi_{\mathbf{k}=\mathbf{0}}$$

- It is, then, a little tedious but not hard to see that (7) is replaced by

$$f_{\rm v} \stackrel{*}{=} B + tm^2 + u(3A^2 + 6Am^2 + m^4) + \frac{1}{2L^d} \sum_{\mathbf{k}} \log \epsilon_{\mathbf{k}}, \qquad (8)$$

where $m \equiv \langle \phi_{\mathbf{r}} \rangle_0$ and, as before,

$$A \equiv \frac{1}{L^d} \sum_{\mathbf{k}} \frac{1}{2\epsilon_{\mathbf{k}}}, \quad B \equiv \frac{1}{L^d} \sum_{\mathbf{k}} \frac{\rho \mathbf{k}^2 + t}{2\epsilon_{\mathbf{k}}}$$

Gaussian MF approximation below T_c (2)

- From $\partial f_{\mathrm{v}}/\partial m = 0$, we obtain

$$
\begin{aligned}
& t + 6uA + 2um^2 = 0 \\
\text{or} \quad & m^2 = -\frac{t+\sigma}{2u} \quad (\sigma \equiv 6uA)
\end{aligned}
\tag{9}
$$

- From $\partial f_{\mathrm{v}}/\partial \epsilon_{\mathbf{k}} = 0$ ($\mathbf{k} \neq \mathbf{0}$), we obtain

$$\epsilon_{\mathbf{k}} = \rho k^2 + t + 6u(A + m^2).$$

Using (9), $\epsilon_{\mathbf{k}} = \rho k^2 - 2(t+\sigma) = \rho(k^2 + \acute{\kappa}^2) \quad \left(\acute{\kappa}^2 \equiv \frac{2(t+\sigma)}{\rho}\right)$

- Thus, we have obtained the Ornstein-Zernike type Green's function

$$G_k = \frac{1}{2\epsilon_{\mathbf{k}}} = \frac{1}{2(k^2 + \acute{\kappa}^2)} \quad (T < T_c)$$

The correlation length is $1/\sqrt{2}$ times smaller than the high-T side.

Supplement: Wick's theorem with symmetry-breaking field

For deriving (8), since the external field distorts the Gaussian distribution, which is the precondition to the Wick's theorem, we must apply the theorem to the fluctuation $\delta\phi_{\mathbf{r}} \equiv \phi_{\mathbf{r}} - \langle \phi_{\mathbf{r}} \rangle_0$, not ϕ itself. In the momentum space, by defining $\delta\phi_{\mathbf{k}} \equiv \phi_{\mathbf{k}} - \bar{\phi}_{\mathbf{0}}\delta_{\mathbf{k}}$ ($\delta_{\mathbf{k}} \equiv \delta_{\mathbf{k},\mathbf{0}}$, $\bar{\phi}_{\mathbf{0}} = L^d m$),

$$
\begin{aligned}
&\langle \phi_{\mathbf{k}_1}\phi_{\mathbf{k}_2}\phi_{\mathbf{k}_3}\phi_{\mathbf{k}_4} \rangle_0 \\
&\quad = \langle (\bar{\phi}_0\delta_{\mathbf{k}_1} + \delta\phi_{\mathbf{k}_1})(\bar{\phi}_0\delta_{\mathbf{k}_2} + \delta\phi_{\mathbf{k}_2})(\bar{\phi}_0\delta_{\mathbf{k}_3} + \delta\phi_{\mathbf{k}_3})(\bar{\phi}_0\delta_{\mathbf{k}_4} + \delta\phi_{\mathbf{k}_4}) \rangle_0 \\
&\quad = \bar{\phi}_0^4 \delta_{\mathbf{k}_1}\delta_{\mathbf{k}_2}\delta_{\mathbf{k}_3}\delta_{\mathbf{k}_4} + \bar{\phi}_0^2 \left(\delta_{\mathbf{k}_1}\delta_{\mathbf{k}_2} \langle \delta\phi_{\mathbf{k}_3}\delta\phi_{\mathbf{k}_4} \rangle_0 + 5 \text{ similar terms} \right) \\
&\quad + \left(\langle \phi_{\mathbf{k}_1}\phi_{\mathbf{k}_2} \rangle_0 \langle \phi_{\mathbf{k}_3}\phi_{\mathbf{k}_4} \rangle_0 + 2 \text{ similar terms} \right)
\end{aligned}
$$

Therefore, we obtain

$$
\begin{aligned}
&\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} \delta_{\sum \mathbf{k}} \langle \phi_{\mathbf{k}_1}\phi_{\mathbf{k}_2}\phi_{\mathbf{k}_3}\phi_{\mathbf{k}_4} \rangle_0 \\
&\quad = \bar{\phi}_0^4 + 6\bar{\phi}_0^2 \sum_{\mathbf{k}_1} \langle \delta\phi_{\mathbf{k}_1}\delta\phi_{-\mathbf{k}_1} \rangle_0 + 3 \sum_{\mathbf{k}_1,\mathbf{k}_3} \langle \phi_{\mathbf{k}_1}\phi_{-\mathbf{k}_1} \rangle_0 \langle \phi_{\mathbf{k}_3}\phi_{-\mathbf{k}_3} \rangle_0
\end{aligned}
$$

Exercise

- Consider an Ising model with only 4 spins.

$$\mathcal{H} = -K(S_1S_2 + S_3S_4) - K'(S_1S_3 + S_2S_4 + S_1S_4 + S_2S_3)$$

By coarse-graining

$$\phi_1 \equiv \frac{1}{2}(S_1 + S_2) \text{ and } \phi_2 \equiv \frac{1}{2}(S_3 + S_4),$$

obtain the **exact** effective Hamiltonian in terms of ϕ_1 and ϕ_2, and verify the existence of terms proportional to ϕ^2, ϕ^4 and $|\nabla\phi|^2 (= (\phi_1 - \phi_2)^2)$, respectively. (If necessary, solve numerically by setting some numerical values of your choice to K and K'.)

Lecture 4: Introduction to Renormalization Group

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To begin with ...

- There are cases where we can rely on the mean-field theory even for the critical behavior. (Ginzburg criterion)
- In one dimension, we may be able to carry out coarse-graining and obtain correct critical behavior. However, in higher dimensions, similar approaches would not yield computationally tractable solutions.
- Real-space renormalization group transformation can be approximately carried out (Migdal-Kadanoff RG) and produces a non-trivial (non-MF) evaluates of critical exponents. However, they do not generally agree with the correct values, nor they provide a way to systematically improve the approximation.

[4-1] When can MF be valid? — Ginzburg criterion

- First, we will elucidate the meaning of the asymptotic validity and draw a general criterion.
- Then, we will check whether the mean-field theory satisfies the criterion in a self-consistent way.
- We will find that it is indeed self-consistent in some cases, but not in general. (Ginzburg criterion)

Asymptotic validity of MF approximation

- Consider a system just below the critical temperature, where there is a finite but small spontaneous magnetization.
- The mean-field (MF) description should be valid when the relative fluctuation is negligible, i.e., $\delta\phi_{\mathbf{r}} \ll \langle \phi_{\mathbf{r}} \rangle$
- Typically, this condition is **not** satisfied at the scale of lattice constant, e.g., for the Ising model, $\langle \phi_{\mathbf{r}} \rangle \approx 0$ and $\delta\phi_{\mathbf{r}} = \sqrt{\langle \delta\phi_{\mathbf{r}}^2 \rangle} \approx 1$.
- However, the MF description can still be qualitatively correct at larger length-scales relevant to the critical behavior, i.e., ξ.
- So, we consider the local average of ϕ, i.e., $\bar{\phi}_{\mathbf{R}} \equiv \frac{1}{b^d} \sum_{\mathbf{r} \in \Omega_b(\mathbf{R})} \phi_{\mathbf{r}}$
- The condition for asymptotic validity of MF is $\delta\bar{\phi}_{\mathbf{R}} \ll \langle \bar{\phi}_{\mathbf{R}} \rangle$ for some $b \sim \xi$.

Self-consistency of mean-field approximation (1)

- For $\langle\bar{\phi}\rangle$, below T_c, we have $\langle\bar{\phi}\rangle^2_{\rm MF} \sim m^2 \sim \dfrac{|\Delta t|}{u} \sim \dfrac{\rho}{u\xi^2}$
- For the amplitude of the fluctuation, we have

$$\langle(\delta\bar{\phi})^2\rangle_{\rm MF} = \left(\frac{a}{b}\right)^{2d} \sum_{\mathbf{r},\mathbf{r}'\in\Omega_b(\mathbf{R})} \langle\delta\phi_{\mathbf{r}'}\delta\phi_{\mathbf{r}}\rangle \overset{*}{\sim} \frac{\xi^2}{\rho b^d} \quad (* \text{ see supplement})$$

- Thus, the validity condition becomes $\dfrac{\rho}{u\xi^2} \gg \dfrac{1}{\rho\xi^{d-2}} \left(\xi^{d-4} \gg \dfrac{u}{\rho^2}\right)$
- For $d > 4$, the condition is asymptotically satisfied as one approaches the critical point, whereas it is not for $d < 4$.

Ginzburg criterion (Upper critical dimension)

The MF approximation to ϕ^4 model cannot be correct asymptotically below 4 dimensions while it can be correct above 4.

Supplement: MF estimate of fluctuation (1)

In Lecture 3, we saw

$$\langle \delta\phi_{\mathbf{r}'}\delta\phi_{\mathbf{r}} \rangle \sim \frac{1}{\rho}\frac{\kappa'^{d-2}}{(\kappa' r)^{\frac{d-1}{2}}} e^{-\kappa'|\mathbf{r}'-\mathbf{r}|} \qquad (\kappa' \approx \sqrt{-\Delta t})$$

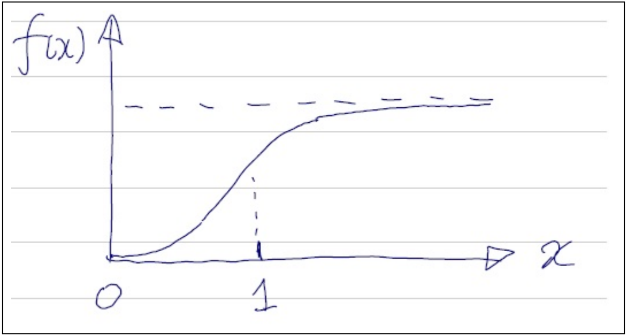
from which we obtain

$$\langle (\delta\bar{\phi})^2 \rangle = \left(\frac{a}{b}\right)^{2d} \sum_{\mathbf{r},\mathbf{r}'\in\Omega_b(\mathbf{R})} \langle \delta\phi_{\mathbf{r}'}\delta\phi_{\mathbf{r}} \rangle \sim \left(\frac{a}{b}\right)^{d} \sum_{\Delta\mathbf{r}} \frac{\rho^{-1}\kappa'^{d-2}}{(\kappa'|\Delta\mathbf{r}|)^{\frac{d-1}{2}}} e^{-\kappa'|\Delta\mathbf{r}|}$$

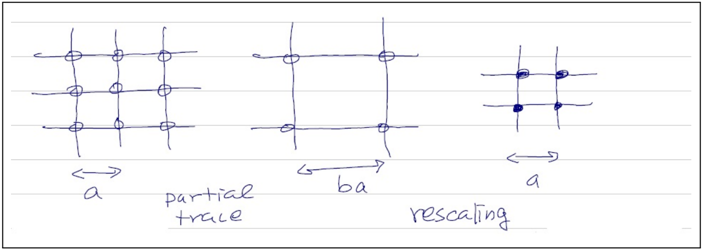
$$\sim \frac{1}{b^d}\int_0^b dr\, r^{d-1}\frac{\rho^{-1}\kappa'^{d-2}}{(\kappa' r)^{\frac{d-1}{2}}} e^{-\kappa' r} \sim \frac{1}{b^d}\frac{1}{\rho\kappa'^2}\int_0^{\kappa' b} dx\, x^{\frac{d-1}{2}} e^{-x}$$

$$\sim \frac{f(\kappa' b)}{\rho\kappa'^2 b^d} \quad \left(f(x) \sim \begin{cases} x^{\frac{d+1}{2}} & (x \ll 1) \\ f_\infty \text{ (a dimension-less constant)} & (x \gg 1) \end{cases} \right)$$

Supplement: MF estimate of fluctuation (2)



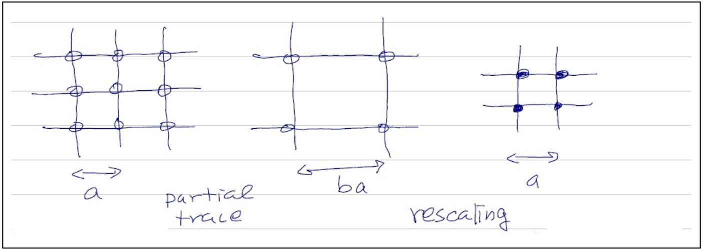
[4-2] General renormalization group (RG) transformation



- In the derivation of the Ginzburg criterion, we introduced the coarse-graining transformation as a Gedankenexperiment.
- The RG transformation consists of two steps: (i) coarse-graining and (ii) rescaling. Schematically,

$$\mathcal{H}_a(S\,|\,\mathbf{K},L) \xrightarrow{\text{(i)}} \mathcal{H}_{ab}(\tilde{S}\,|\tilde{\mathbf{K}},L) \xrightarrow{\text{(ii)}} \mathcal{H}_a(\acute{S}\,|\acute{\mathbf{K}},b^{-1}L)$$

[4-2] General Renormalization Group Transformation



- In the coarse-graining step, we define coarse-grained field and carry out the configuration-space summation of the partition function, with the constraint imposed by the coarse-grained fields.
- In the rescaling step, we redefine the length-scale and the field variables by multiplying them with scaling factors so that the effective Hamiltonian may be the same form as the original one.

Coarse-graining

In the coarse-graining step of the RG procedure, we first define "coarse-grained field", $\tilde{S}_{\mathbf{R}}$, which is defined in terms of $S_{\mathbf{r}}$ in the neighborhood of $\mathbf{R}$, i.e., $\tilde{S}_{\mathbf{R}} = \Sigma(\{S_{\mathbf{r}}\}_{\mathbf{r}\in\Omega_b(\mathbf{R})})$, with some function $\Sigma(\cdots)$. More formally,

$$e^{-\mathcal{H}_a(S|\mathbf{K},L)} \to e^{-\mathcal{H}_{ab}(\tilde{S}|\tilde{\mathbf{K}},L)} \equiv \sum_S \Delta(\tilde{S}\,|\Sigma(S))e^{-\mathcal{H}_a(S|\mathbf{K},L)},$$

where $\mathbf{K}$ is a set of parameters such as $\mathbf{K} \equiv (\beta, H)$.

Example 1 (Ising chain with $b = 3$)

$$\Sigma(S_1, S_2, S_3) = S_2 \quad \text{(Simple decimation)}$$
$$\Sigma(S_1, S_2, S_3) = (S_1 + S_2 + S_3)/3 \quad \text{(Local Average)}$$
$$\Sigma(S_1, S_2, S_3) = \mathrm{sign}(S_1 + S_2 + S_3) \quad \text{(Majority rule)}$$

Example: Coarse-graining of Ising chain ($b = 2$)

- Consider the Ising model of size $L \equiv 2^g$ in one dimension.

$$\mathcal{H}_a(S|\mathbf{K}, L) = -K \sum_{i=0}^{L-1} S_i S_{i+1} - h \sum_{i=0}^{L-1} S_i \qquad (\mathbf{K} \equiv (K, h))$$

- For even L, let us adopt the decimation for the coarse-graining:

$$\tilde{S}_i = S_i \quad (\text{for } i = 0, 2, 4, \cdots, L-2)$$

- Then, $e^{-\mathcal{H}_{2a}(\tilde{S}|\tilde{K},L)} = \sum_{S_1, S_3, \cdots, S_{L-1}} e^{-\mathcal{H}_a(S|K,L)}$. For $h = 0$ we have

$$e^{-\mathcal{H}_{2a}(\tilde{S}|\tilde{K},L)} = \sum_{S_1} e^{K(S_0+S_2)S_1} \sum_{S_3} e^{K(S_2+S_4)S_3} \cdots \sum_{S_{L-1}} e^{K(S_{L-2}+S_0)S_{L-1}}$$

$$\sim e^{\tilde{K} S_0 S_2} e^{\tilde{K} S_2 S_4} \cdots e^{\tilde{K} S_{L-2} S_0} \sim e^{-\mathcal{H}_{2a}(\tilde{S}|\tilde{K},L)} \quad (\tilde{K} \equiv \mathrm{ath}(\mathrm{th}^2 K))$$

Example: Rescaling of Ising chain ($b = 2$)

- Let us use $t \equiv e^{-2K}$ in stead of K for the parameter. Then, the effect of the coarse-graining on t is

$$\tilde{t} = \frac{2t}{1+t^2}.$$

- The rescaling in the present case is simply

$$\acute{\mathbf{r}} \equiv \mathbf{r}/2, \quad \acute{S}_{\acute{\mathbf{r}}} \equiv \tilde{S}_{\mathbf{r}}, \quad \text{and} \quad \acute{t} \equiv \tilde{t}.$$

- Together with the coarse-graining, we obtain the whole RG transformation,

$$\mathcal{H}_a(S|t,L) \xrightarrow[b=2]{RG} \mathcal{H}_a(\acute{S}|\acute{t},L/2), \quad \text{with} \quad \acute{t} = \frac{2t}{1+t^2}.$$

Example: Critical exponent ν

- From the whole RG procedure, we can deduce

$$e^{-r/\xi(t)} \sim \langle S_{\mathbf{r}} S_{\mathbf{0}} \rangle_t = \langle S_{\acute{\mathbf{r}}} S_0 \rangle_{\acute{t}} \sim e^{-\acute{r}/\xi(\acute{t})}$$

- Because $\acute{r} = r/2$,

$$\xi(t) = 2\xi(\acute{t}) \quad \left(\acute{t} = \frac{2t}{1+t^2} \right).$$

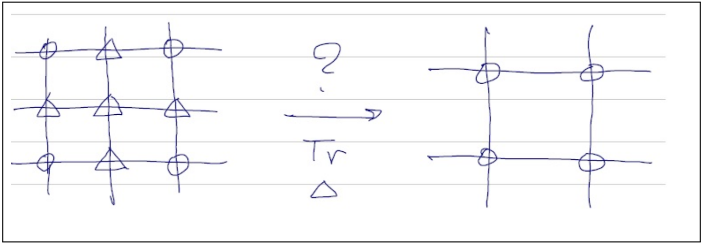
- Since $\acute{t} \approx 2t$ near the fixed-point $t = 0$,

$$\xi(t) \approx 2\xi(2t).$$

- Therefore, for $t \approx 0$,

$$\xi(t) \sim \frac{1}{t} \qquad \Rightarrow \nu = 1 \quad \text{(Exact!)}$$

Can we do the same in 2D case? (1)



Can we do the same in 2D case? (2)

- Coarse-graining by decimation.

$$\tilde{S}_{\mathbf{r}} \equiv S_{\mathbf{r}} \quad \text{for } \mathbf{r} \in \Omega' \equiv \{(2ma, 2na) | m, n = 0, 1, 2, \cdots, L/2\}$$

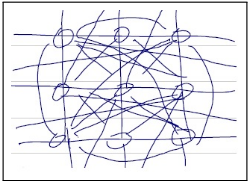
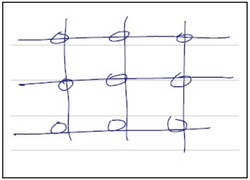
- The partial trace can be taken (at least formally)

$$e^{-\tilde{\mathcal{H}}_{2a}(\tilde{\mathbf{S}}, \tilde{K})} \equiv \operatorname*{Tr}_{\{S_{\mathbf{r}}\}_{\mathbf{r} \in \Omega \setminus \Omega'}} e^{-\mathcal{H}_a(\mathbf{S}, K)}$$

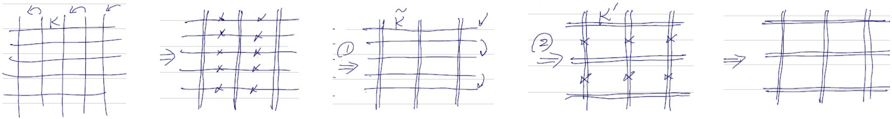
- In general, unlike the 1D case, $\tilde{H}_{2a}$ contains terms other than the two-body nearest-neighbor interactions. For example, it contains the long-range interaction $-K_{\mathbf{r}\mathbf{r}'} S_{\mathbf{r}'} S_{\mathbf{r}}$ where $|\mathbf{r} - \mathbf{r}'| > a$, as well as many-body interactions such as $-K_{\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3\mathbf{r}_4} S_{\mathbf{r}_1} S_{\mathbf{r}_2} S_{\mathbf{r}_3} S_{\mathbf{r}_4}$.
- Therefore, it is not feasible to study such a model (unless we use machines).

Can we do the same in 2D case? (3)

The renormalized Hamiltonian

is more like  than  .

[4-3] Migdal-Kadanoff approximation for 2D Ising model



- Bunch up two vertical lines.
- Take the partial trace of intermediate spins ($\times$). (Step ①)

$$\mathrm{th}\,\tilde{K} = \mathrm{th}^2\,K$$

- Bunch up two horizontal lines. (Step ②)

$$\acute{K} = 2\tilde{K}$$

- Take the partial trace of intermediate spins ($\times$).

simple Migdal-Kadanoff

$$\acute{t} = \frac{2t^2}{1+t^4} \quad (t \equiv \mathrm{th}\,K,\ \acute{t} \equiv \mathrm{th}\,\acute{K})$$

RG fixed point and $1/\nu$ (general argument)

- Suppose some RG transformation (RGT) yields

$$\acute{t} = R_b(t) \quad (b\text{: the rescaling factor, e.g., } R_2(t) = \tfrac{2t^2}{1+t^4})$$

- We define the RG fixed-point t_c by $t_c = R_b(t_c)$.
- Then, the 'deviation' from the fixed-point changes by RGT as

$$\delta t \to \delta\acute{t} = \acute{t} - t_c = R_b(t) - R_b(t_c) \approx \lambda \delta t \quad (\lambda \equiv R_b'(t_c))$$

- The correlation length after RGT must be smaller than the original by factor b. So, we obtain $\xi(\lambda\delta t) \approx b^{-1}\xi(\delta t)$, which leads to

$$\xi(\delta t) \propto (\delta t)^{-\nu} \text{ where } \lambda^{-\nu} = b^{-1} \quad \text{or} \quad \nu \equiv \frac{\log b}{\log \lambda}\,. \tag{1}$$

RG fixed point and $1/\nu$ (numerical estimates)

- For the Migdal-Kadanoff RGT for 2D Ising model, we have

$$R_2(t_c) = \frac{2t_c^2}{1+t_c^4} = t_c \rightarrow \ t_c = 0.54368\cdots$$

$$(\text{cf: } \ t_c^{\mathrm{exact}} = \sqrt{2} - 1 = 0.4142\cdots)$$

- With some arithmatics, we can get

$$R_2'(t_c) = \frac{2(1-t_c)}{t_c} \approx 1.676$$

$$\rightarrow y_t \equiv 1/\nu \approx \log 1.676 / \log 2 \approx 0.747$$

$$(\text{cf: } \ y_t^{\mathrm{exact}} = 1, \ y_t^{\mathrm{mean\ field}} = 2)$$

Not bad, but ad-hoc (not obvious how to improve).

An improvement of MKRG

- Consider the MKRG step in which b lines, instead of 2, are bunched up at a time. The resulting RG transformation will be

$$\tilde{K} = bK \text{ and } \operatorname{th} \acute{K} = \operatorname{th}^b \tilde{K}, \quad \text{or}$$
$$\operatorname{th} \acute{K} = \operatorname{th}^b(bK)$$

(The order of bunching and tracing was changed.)

- "bunching-up" two lines to one might be too crude. It may become less harmful if we bunch-up as small number of lines as possible.
- For $b = 1 + \lambda$ ($\lambda \ll 1$), defining $t \equiv \operatorname{th} K$, we obtain

$$\acute{t} = R_b(t) = t + \lambda(1 - t^2) \operatorname{ath} t + \lambda t \log t, \quad \text{or}$$
$$\frac{dR_b}{d \log t} = (1 - t^2) \operatorname{ath} t + t \log t \equiv f(t)$$

Infinitesimal RG (general argument)

- In general, suppose some RG transformation with continuous scaling factor $b = e^{\lambda}$ yields

$$\lim_{\lambda \to 0} \frac{dR(t)}{d\lambda} = f(t).$$

- Obviously, the fixed-point is determined by $t_c = f(t_c)$.
- Starting from the previously obtained expression for $1/\nu$, we get

$$y_t = \frac{1}{\nu} = \frac{\log \left(\frac{dR_b}{dt} \right)_{t_c}}{\log b} = \frac{1}{\lambda} \left(\frac{dR_{1+\lambda}}{dt} - 1 \right)$$
$$= \frac{d}{dt} \left(\frac{R_{1+\lambda} - t}{\lambda} \right) = \frac{d}{dt} \left(\frac{R_{1+\lambda} - R_1}{\lambda} \right) = \left(\frac{d}{dt} f(t) \right)_{t_c}$$

Infinitesimal MKRG (numerical estimates)

- From $t_c = f(t_c) = (1 - t_c^2)\,\mathrm{ath}\, t_c + t_c \log t_c,$, we obtain

$$t_c = \sqrt{2} - 1 = t_c^{\mathrm{exact}} \quad !$$

- As for y_t, we have

$$y_t = f'(t_c) = 0.7535 \cdots ,$$

slightly closer to $y_t^{\mathrm{exact}} = 1$ than the simple MKRG with $b = 2$.

Better, but still ad-hoc (not obvious how to further improve).

Exercise

- By solving the 1D Ising model, compute the correlation function $G(r) \equiv \langle S_r S_0 \rangle$ and the correlation length ξ. Verify $\xi \propto t^{-1}$.

hint:

$$\langle S_r S_0 \rangle = \mathrm{Tr}\left(T^{L-r} \sigma T^r \sigma \right) \Big/ \mathrm{Tr}\left(T^L \right)$$

where

$$T_{S'S} \equiv e^{KS'S} \quad (2 \times 2 \text{ matrix})$$

$$\sigma = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Lecture 5: Tensor-Network Renormalization Group (TNRG)

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May 13, 2019

In this lecture, we see ...

- The MKRG was manageable, but is rather crude an approximation. Even worse, we do not know when we can expect this approximation to be good or how we can improve systematically.

- Real-space renormalization group method based on tensor-network representation (TNRG) provides us with a method for computing the partition function. While TNRG is also an approximation, it comes with a method for systematic improvements, and may produce the exact critical exponents in the limit.

[5-1] Tensor-network renormalization group (TNRG)

- Most of statistical-mechanical models on lattices are tensor networks.
- Quantum many-body states on lattices are also described by tensor networks.
- As we have seen, after renormalization transformation, we need infinitely many parameters to describe the resulting system.
- By working with the TN representation, and introducing "data compression" at all length scales, we can overcome both the faults in the real-space RG.

What is a tensor network?

- When an object is expressed as the result of (full or partial) contraction of tensor-product of multiple tensors, we call such an expression a "tensor-network". An expression such as

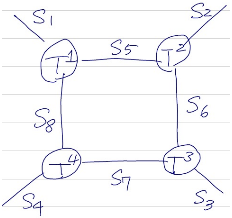
$$\mathrm{Cont}\left(\prod_k T^k\right) \equiv \sum_{(S_i)_{i\in\Omega}} \prod_k T^k_{S_{i_1^k}, S_{i_2^k}, \cdots, S_{i_{n_k}^k}} \quad (1)$$

  is a tensor-network, where Ω is a subset of all indices, $\{i_\alpha^k\}$, appearing multiple times (typically twice) in the summand.

- Example:

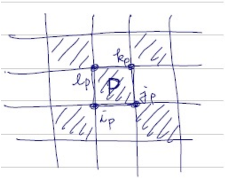
$$T_{S_1,S_2,S_3,S_4} =$$

$$\sum_{S_6,S_7,S_8,S_9} T^1_{S_1,S_8,S_5} T^2_{S_2,S_5,S_6} T^3_{S_3,S_6,S_7} T^4_{S_4,S_7,S_8}$$



Statistical-mechanical models are tensor networks

The partition function of the Ising model on the square lattice can be expressed as

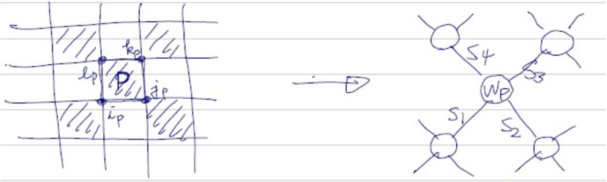


$$Z = \sum_{S} \prod_{p:\text{shaded square}} W(S_{i_p}, S_{j_p}, S_{k_p}, S_{l_p})$$

$$W(S_1, S_2, S_3, S_4) \equiv e^{K(S_1 S_2 + S_2 S_3 + S_3 S_4 + S_4 S_1)}$$

- We can regard $W(S_1, S_2, S_3, S_4)$ as a degree-4 tensor.
- Then, the above equation is a tensor network representation of the partition function.

Graphical notation

- In TN-related discussions, we use more diagrams than equations because it is often much easier to grasp the idea.
- 

- For tensors, we often use bulkier symbols than just dots such as circles, triangles, squares, etc, while we use simple lines for indices. (This is more natural from the information-scientific point of view because tensors are the carriers of most of the information.)

Wave function can be represented as TN (1)

- Consider a quantum many-body system defined on a lattice.
- A local quantum degree of freedom, say S_i, is defined on each site.
- Accordingly, we have a local Hilbert space $H_i \equiv \{|S_i\rangle_i\}$ associated with each site, e.g., H_i is 2-dimensional for $S = 1/2$ spin models.
- The whole Hilbert space is the product of them $H \equiv \bigotimes_i H_i$.
- Any global wave function $|\Psi\rangle$ can be expanded as

$$|\Psi\rangle \equiv \sum_{\{S_i\}} C_{S_1,S_2,\cdots,S_N}|S_1, S_2, \cdots, S_N\rangle \equiv \sum_{\mathbf{S}} C_{\mathbf{S}}|\mathbf{S}\rangle$$

where $|S_1, S_2, \cdots, S_N\rangle \equiv |S_1\rangle_1 \otimes |S_2\rangle_2 \otimes \cdots \otimes |S_N\rangle_N$.

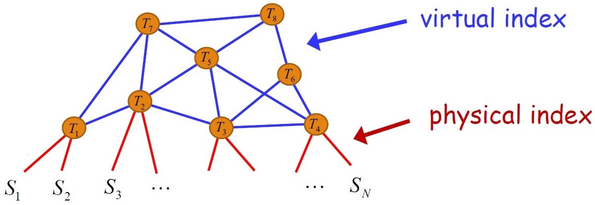
- Now, $C_{S_1,S_2,\cdots,S_N}$ can be viewed as a degree-N tensor. It may be approximated by some tensor network, i.e,

$$C_{\mathbf{S}} \approx \mathrm{Cont}\left(\prod_k T^k\right)$$

Wave function can be represented as TN (2)

$$C_{\mathbf{S}} \approx \mathrm{Cont}\left(\prod_k T^k\right)$$

$$=$$



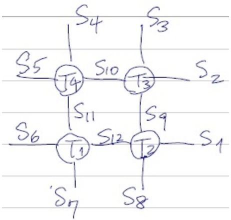
Note that $C_{\mathbf{S}}$ has d^N parameters ($d = 2$ for $S = 1/2$ spin systems), whereas the tensor network can be specified by only $O(N)$ number of parameters. By the tensor network representation, we may be able to reduce the computation for large N down to a manageable level.

Trivial Tensor-network RG

- Let us condider classical systems, and ask how we can use the tensor network for RG.
- How can we replace the original tensor lattice into something similar but with the unit cell bigger than the original?
- Let us solve this problem starting from the trivial TNRG:

$$\acute{T}_{\acute{S}_1,\acute{S}_2,\acute{S}_3,\acute{S}_4} \equiv \sum_{S_9,S_{10},S_{11},S_{12}} T^1_{S_1,S_9,S_{12},S_8} \times T^2_{S_2,S_3,S_{10},S_9} T^3_{S_{10},S_4,S_5,S_{11}} T^4_{S_{12},S_{11},S_6,S_7}$$

where $\acute{S}_1 \equiv (S_1, S_2)$, $\acute{S}_2 \equiv (S_3, S_4), \cdots$



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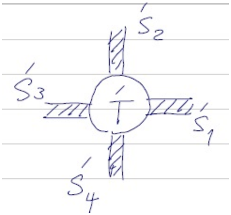
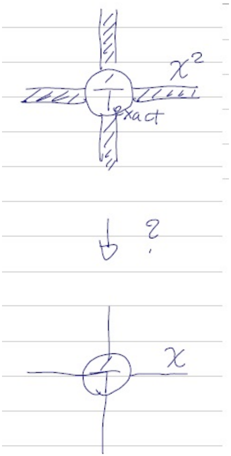


What's wrong with trivial TNRG?

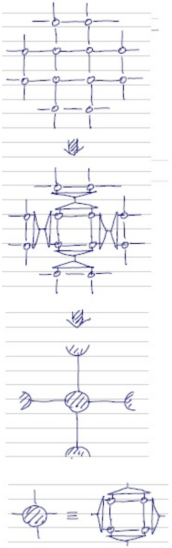
- Using $\acute{T}$, we can exactly express the original partition function with lattice constant twice larger than the original, which is good.
- However, the dimension of each index of the new tensor is χ^2 where χ is the index dimension of the original tensor.
- To be more specific, to handle an $L \times L$ system we end up with a big tensor with χ^L-dimensional indices. (We cannot go to so large L.)
- To make the whole procedure practically useful for larger systems, we need to make the index dimension back to χ in each iteration.



Data compression is necessary!

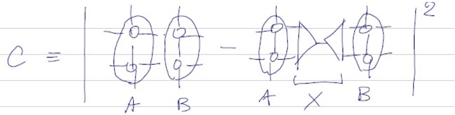
Rank-reducer

- What we need is a 'rank-reducer'.
- A rank-reducer is a tensor whose rank (when viwed as a matrix) is χ in stead of χ^2, and whose insertion keep things unchanged.
- If such a thing exists, we can define triangle operators as illustrated in the figure by SVD.
- Then, by cutting the network at the reduced indices, we can define the renormalized tensor with index dimension χ, as we disired.
- Now, we must ask whether such a magical rank-reducer exists or not, and if it does, how we can compute it.



Low-rank approximation (LRA)

- How can we optimize the rank-reducer X for the given rank χ?
- For the cost function, we take the amplitude of the local disturbance caused by the insertion of X, i.e.,



- Let us regard A and B as $\chi^4 \times \chi^2$ matrices and the rank-reducer X as a $\chi^2 \times \chi^2$ matrix whose rank is χ (or less).

Low-rank approximation problem

Suppose 3 integers, l, m, n, that satisfy $l < m < n$. For two given $n \times m$ matrices A and B, find a rank-l, $m \times m$ matrix X that minimizes

$$C(X) \equiv |AB^{\mathrm{T}} - AXB^{\mathrm{T}}|^2. \quad (2)$$

Solution to LRA problem (1)

- We want the rank-l matrix X that minimizes

$$C \equiv |AB^{\mathrm{T}} - AXB^{\mathrm{T}}|^2.$$

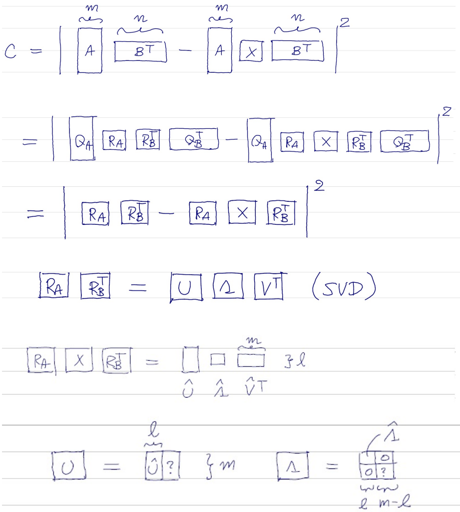
- Consider the QR-decomposition,

$$A = Q_A R_A, \quad B = Q_B R_B.$$

- Then, $C \equiv |R_A R_B^{\mathrm{T}} - R_A X R_B^{\mathrm{T}}|^2$
- Consider SVD: $R_A R_B^{\mathrm{T}} = U \Lambda V^{\mathrm{T}}$.
- If X satisfies

$$R_A X R_B^{\mathrm{T}} = \hat{U} \hat{\Lambda} \hat{V}^{\mathrm{T}}, \qquad (3)$$

it is optimal. $(*)$ (Here, $\hat{U}$, $\hat{\Lambda}$, and $\hat{V}$ are truncated matrices at the l-th row and/or column.)



Solution to LRA problem (2)

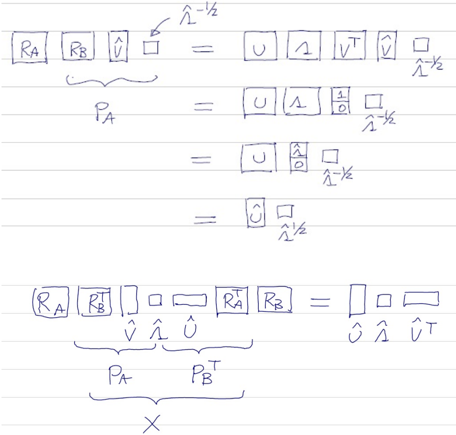
- Now, let us define "triangule operators," P_A and P_B, by

$$P_A \equiv R_B^{\mathrm{T}} \hat{V} \hat{\Lambda}^{-\frac{1}{2}},$$
$$P_B \equiv R_A^{\mathrm{T}} \hat{U} \hat{\Lambda}^{-\frac{1}{2}}$$

- Then, because $R_A R_B^{\mathrm{T}} = U \Lambda V^{\mathrm{T}}$,

$$R_A P_A = \hat{U} \hat{\Lambda}^{\frac{1}{2}},$$
$$R_B P_B = \hat{V} \hat{\Lambda}^{\frac{1}{2}}.$$

- Therefore, $X \equiv P_A P_B^{\mathrm{T}}$, satisfies Eq.(3), $R_A X R_B^{\mathrm{T}} = \hat{U} \hat{\Lambda} \hat{V}^{\mathrm{T}}$, and therefore is the optimal rank-reducer.



Supplement: Theorem for Low-Rank Approximation (LRA)

Theorem 1 (Eckhart-Young-Mirsky)

For a given $n \times m$ matrix A, consider its approimation by a rank-l ($l \leq m \leq n$) matrix X and its error $E^2 = |A - X|^2$ where $|A|^2 \equiv \mathrm{Tr}\, A^{\mathsf{T}} A$. Let $A = U \Lambda V^{\mathsf{T}}$ be the singular value decomposition (SVD) of A with an $n \times m$ diagonal matrix Λ and n and m dimensional unitaries, U and V, respectively. Then,

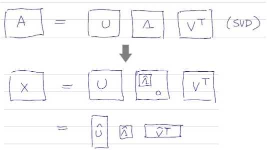
$$E^2 \geq \lambda_{l+1}^2 + \lambda_{l+2}^2 + \cdots + \lambda_m^2$$

where λ_i is the i-th largest singular value. The lower bound is attained by $X \equiv \hat{U} \hat{\Lambda} \hat{V}^{\mathsf{T}}$ where '^' represents truncation at the l-th row/column.

$\Lambda \equiv$

$$\begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \lambda_m \\ 0 & \cdots & \cdots & 0 \\ \vdots & & & \vdots \\ 0 & \cdots & \cdots & 0 \end{pmatrix}.$$

$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_m \geq 0$



Supplement: LRA used in the derivation

Theorem 2 (LRA)

Consider an $m \times m$ matrix Y expressed as $Y = R_A R_B^T$ with R_A and R_B, and consider its SVD, $Y = U\Lambda V^{\mathrm{T}}$. Then, Y's optimal LRA of the form $R_A X R_B^{\mathrm{T}}$ with rank l ($l < m$) matrix X is obtained when $R_A X R_B^{\mathrm{T}} = \hat{U}\hat{\Lambda}\hat{V}^{\mathrm{T}}$.

Proof: When the condition of the theorem is satisfied,

$$|Y - R_A X R_B^{\mathrm{T}}|^2 = |U\Lambda V^{\mathrm{T}} - \hat{U}\hat{\Lambda}\hat{V}^{\mathrm{T}}|^2$$
$$= |U\Lambda V^{\mathrm{T}} - U\tilde{\Lambda}V^{\mathrm{T}}|^2 = |\Lambda - \tilde{\Lambda}|^2 = \sum_{k=l+1}^{m} \lambda_k^2,$$

where $\tilde{\Lambda}$ is Λ with singular values λ_k ($k > l$) replaced by 0. Therefore, $R_A X R_B^{\mathrm{T}}$ saturates the inequality of the EYM theorem.

Summary of the TNRG procedure

1. QR-decomposition of A and B matrices.

   $$A = Q_A R_A, \ \ B = Q_B R_B$$

2. SVD. $\quad R_A R_B^{\mathrm{T}} = U \Lambda V^{\mathrm{T}}$

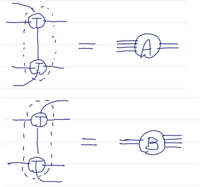
3. Compute the "triangle operators".

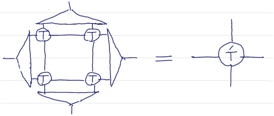
   $$P_A \equiv R_B^{\mathrm{T}} \hat{V} \hat{\Lambda}^{-\frac{1}{2}},$$
   $$P_B \equiv R_A^{\mathrm{T}} \hat{U} \hat{\Lambda}^{-\frac{1}{2}}$$

4. Do the same for other directions.

5. Using the triangular operators, contract four original tensors to obtain the new element tensor $\acute{T}$.

6. Repeat these till the desired system size has been reached.



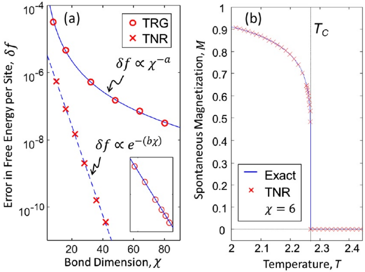


TNRG provides accurate estimates

- The free energy can be obtained to the accuracy of nearly 8 digits. ("TRG" in the figure.)

  ("TRG" is essentially the same, but technically different way of realizing TNRG from the one discussed in this lecture. See Levin and Nave, Phys. Rev. Lett. 99, 120601 (2007) for details.)

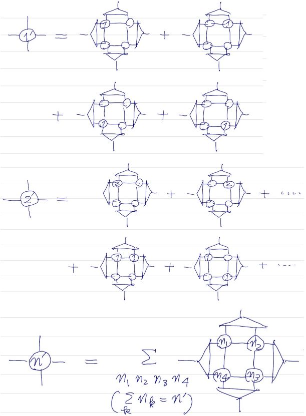
- An improvement ("TNR") pushes it even up to 10 digits.



[Evenbly and Vidal, Physical Review Letters 115, 180405 (2015)]

How we can compute other quantities

From the method described so far, we can obtain F, E, S and C. What about the magnetization, M, χ, and the Binder ratio?



- Define "impurity tensors",

$$T^{(0)} \equiv T, \quad T^{(n)} \equiv 0 \ (n > 1)$$
$$T^{(1)}_{S_1 S_2 S_3 S_4} \equiv T_{S_1 S_2 S_3 S_4} \times m(S_1, S_2, S_3, S_4)$$

where $m = (S_1 + S_2 + S_3 + S_4)/2$.

- Define "renormalized impurity tensors":

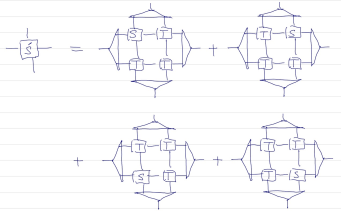
$$\acute{T}^{(n)} \equiv \sum_{\substack{n_1 n_2 n_3 n_4 \\ (\sum_k n_k = n)}} \mathrm{Cont}(T^{(n_1)} T^{(n_2)} T^{(n_3)} \times T^{(n_4)} \times \text{(triangle tensors)})$$

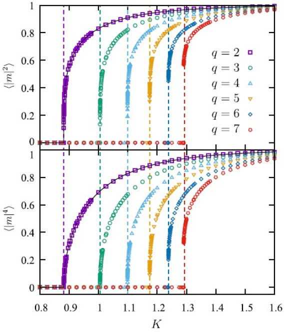
- At the end of all iterations,

$$\langle M^n \rangle = \sum_{S_1 S_2} T^{(n)}_{S_1 S_2 S_1 S_2} / \sum_{S_1 S_2} T^{(0)}_{S_1 S_2 S_1 S_2}$$

Application of TNRG to q-state Potts model (1)

- q-state Potts model in 2D. [S. Morita and N.K., Computational Physics Communications, 236 65-71 (2019).]
- n-th moments of magnetization are computed (e.g., magnetization ($n = 1$), susceptibility ($n = 2$), Binder ratio ($n = 4$), etc)
- The result of 20 RG iterations (i.e., $L = 2^{20} \approx 10^6$) was obtaind for $q = 2, 3, \cdots, 7$ for the truncation dimension ('bond-dimension') $\chi = 48$.



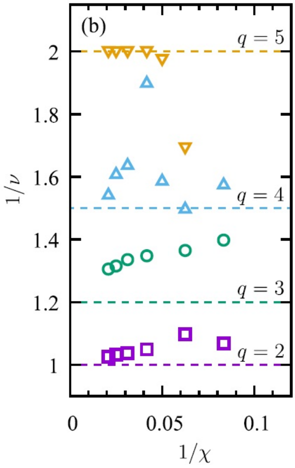


Application of TNRG to q-state Potts model (2)

- According to the finite-size scaling (FSS), which we will discuss later, the Binder ratio is defined as $U_4 \equiv \langle M^4 \rangle / \langle M^2 \rangle^2$ depends on T and L as

$$\left(\frac{dU_4}{dT} \right)_{T=T_c} = \frac{1}{\nu} \log L + a + bL^{-\omega} + \cdots$$

- For first-order transitions, $1/\nu = d$ is expected.
- The 1st order nature of the transition of 5-state Potts model has been confirmed. (CF: $\xi \approx 2500$ at T_c).



[S. Morita and N.K., Comp. Phys. Comm. 236, 65-71 (2019).]

Summary

- Tensor-network RG (TNRG) is a scheme that realizes **“data compression”** at every length scale.
- With TNRG, we can systematically improve the real-space RG by adjusting the compression level, i.e., by increasing the cut-off dimension χ (often called “bond-dimension”).
- TNRG provides us with rather accurate estimates of various quantities and critical indices.
- While we have seen just one way of implementing the idea, there are many proposals for realizing TNRG. (MERA, TRG, TNR, loop-TNR, etc)

Lecture 6: General Framework of Renormalization Group — Fixed Points and Scaling Operators

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May 27, 2019

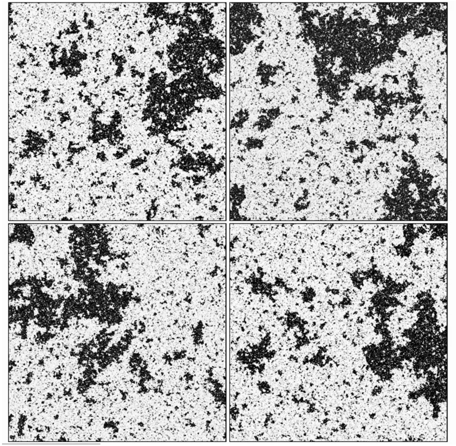
In this lecture, we see ...

- Having seen a few examples of the real-space RG transformations, we formulate it as a general framework for discussing the phase diagram and the critical phenomena.
- As an exactly-treatable example of the RG framework, we consider the Gaussian model, which is easy to solve and provides us the starting point for perturbative renormalization group.

[6-1] Fixed-point and scaling operators

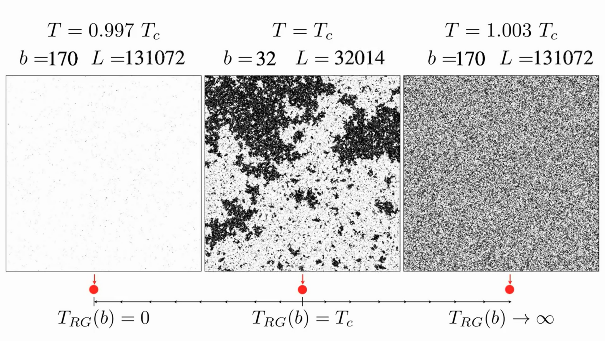
- As a Gedunkenexperiment, we consider a generic Hamiltonian, and its exact renormalization group transformation. (As long as it exists, it doesn't matter whether or not we can actually compute such things.)
- We'll see that the RGT defines a "RG-flow" in the parameter space, which provides us with a framework of understanding the phase diagram.

Critical point is scale-invariant



“https://youtu.be/fi-g2ET97W8” by Douglas Ashton

RG flow



“https://youtu.be/MxRddFrEnPc” by Douglas Ashton

Generic Hamiltonian

- Any Hamiltonian is expressed as an expansion w.r.t. local operators.

$$\mathcal{H}_a(S|\mathbf{K}, L) = -\sum_{\mathbf{x}} \sum_{\alpha} K_\alpha S_\alpha(\mathbf{x}) \qquad (1)$$

where $\{S_\alpha\}$ spans the space of all local operators, i.e.,

$$\forall Q(\mathbf{x})\ \exists q_\alpha\ \left(Q(\mathbf{x}) = \sum_\alpha q_\alpha S_\alpha(\mathbf{x}) \right) \qquad (2)$$

- Example: A generic model defined with Ising spins.

$$\begin{array}{ll}
K_1 = H & S_1(\mathbf{x}) = S_\mathbf{x} \\
K_2 = J_x & S_2(\mathbf{x}) = S_\mathbf{x}\, S_{\mathbf{x}+\mathbf{a}_x} \\
K_3 = J_y & S_3(\mathbf{x}) = S_\mathbf{x}\, S_{\mathbf{x}+\mathbf{a}_y} \\
K_4 = Q & S_4(\mathbf{x}) = S_\mathbf{x}\, S_{\mathbf{x}+\mathbf{a}_x}\, S_{\mathbf{x}+2\mathbf{a}_x} \\
K_5 = Q & S_5(\mathbf{x}) = S_\mathbf{x}\, S_{\mathbf{x}+\mathbf{a}_x}\, S_{\mathbf{x}+\mathbf{a}_y} \\
\vdots & \vdots
\end{array}$$

($\mathbf{a}_x, \mathbf{a}_y, \cdots$: lattice unit vectors)

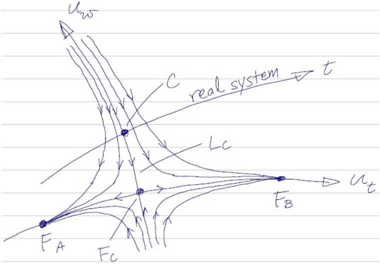
RG flow diagram

- The RGT

$$\mathcal{H}_a(\phi, \mathbf{K}) \to \mathcal{H}_a(\acute{\phi}, \acute{\mathbf{K}})$$

can be regarded as a map from the parameter space onto itself

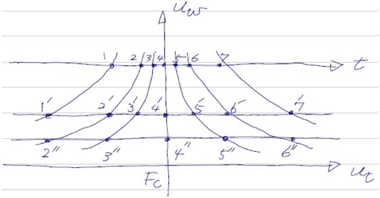
$$\mathbf{K} \to \acute{\mathbf{K}} \equiv \mathcal{R}_b \mathbf{K}$$



- An RG trajectory is a RGT-invariant curve.
- We assume that the trajectory is continuous. (In other words, the RGT is defined for continuous b, such that $\mathcal{R}_{b_1}\mathcal{R}_{b_2} = \mathcal{R}_{b_1 b_2}$.)
- A trajectry converging to the unstable fixed point $(\mathrm{F_C})$ is called a critical line $(\mathrm{L_C})$. The parameter along it is called irrelevant (u_w).
- The parameter along a trajectry emanating from the unstable fixed point is called relevant. (u_t).

Critical properties are controled by unstable fixed-point

- RGT with b maps the points $1, 2, \cdots, 7$ to $1', 2', \cdots, 7'$.
- RGT with $b' > b$ maps the narrower region including only $2, 3, 4, 5, 6,$ to $2'', 3'', \cdots, 6''$, distributed in the same range of u_t, but closer to the $u_w = 0$ line.



- In this way, a narrower region is mapped closer to the $u_w = 0$ line. So, the critical properties on the t-axis, is identical to the property around the unstable fixed point ("$\mathrm{F_C}$") on the $u_w = 0$ line.
- The irrelevant fields of our system determine how far we must approach to the critical point to observe the correct critical behavior.
- Applying a small irrelevant field does not qualitatively change the nature of the critical point, while a relevant field does.

Expansion around unstable fixed point

- Consider the local Hamiltonian $\mathcal{H}_a(\mathbf{S}(\mathbf{x}), \mathbf{x})$ and its fixed point form:

$$\mathcal{H}_a^*(\mathbf{S}(\mathbf{x}), \mathbf{x}) \equiv \mathcal{H}_a(\mathbf{S}(\mathbf{x}), \mathbf{x}|\mathbf{K}^*). \tag{3}$$

(In what follows, we drop some or all of the parameters, a, $\mathbf{x}$ and $\mathbf{S}(\mathbf{x})$, and use the abbreviation like $\mathcal{H}^*$ for $\mathcal{H}_a^*(\mathbf{S}(\mathbf{x}), \mathbf{x})$.)

- Let us denote the RGT by $\mathcal{R}_b$ where b is the renormalization factor. Then, $\mathcal{R}_b(\mathcal{H}^*) = \mathcal{H}^*$.
- Let us expand the Hamiltonian around this fixed point.

$$\mathcal{H} = \mathcal{H}^* - \sum_\alpha h_\alpha S_\alpha(\mathbf{x}) = \mathcal{H}^* - \mathbf{h} \cdot \mathbf{S} \tag{4}$$

where h_α is the deviation of the parameter K_α from its fixed-point value, i.e., $h_\alpha \equiv K_\alpha - K_\alpha^*$

Linearization of RGT

- Now consider the transformation applied to the local Hamiltonian near the fixed point:

$$\mathcal{R}_b(\mathcal{H}^* - \mathbf{h}\cdot\mathbf{S}(\mathbf{x})) = \mathcal{H}^* - \acute{\mathbf{h}}\cdot\mathbf{S}(\mathbf{x})$$

- To the lowest order, $\acute{\mathbf{h}}$ depends linearly on $\mathbf{h}$ in the lowest order, i.e., a linear operator T_b exists such that

$$\acute{\mathbf{h}} \approx T_b\mathbf{h}.$$

- We assume that T_b is diagonalizable with real eigenvalues.

$$P^{-1}T_bP = \begin{pmatrix} \lambda_1 & & \\ & \lambda_2 & \\ & & \ddots \end{pmatrix} \equiv \Lambda_b$$

Scaling fields and scaling operators

- By defining

$$\mathbf{u} \equiv P^{-1}\mathbf{h}, \text{ and } \phi \equiv P^{\mathsf{T}}\mathbf{S}$$

we obtain

$$\mathbf{u}\cdot\phi = (P^{-1}\mathbf{h})^{\mathsf{T}}(P^{\mathsf{T}}\mathbf{S}) = \mathbf{h}^{\mathsf{T}}(P^{-1})^{\mathsf{T}}P^{\mathsf{T}}\mathbf{S} = \mathbf{h}\cdot\mathbf{S}.$$

In addition, $\mathbf{u}$ transforms as

$$\acute{\mathbf{u}} \equiv \mathcal{R}_b\mathbf{u} = P^{-1}\acute{\mathbf{h}} = P^{-1}T_b\mathbf{h} = P^{-1}T_bP\mathbf{u} = \Lambda_b\mathbf{u},$$

namely, $\acute{u}_\mu = b^{y_\mu}u_\mu$ with $y_\mu \equiv \log_b \lambda_\mu$.

$u_\mu =$ "scaling field", $\phi_\mu =$ "scaling operator",

$y_\mu =$ "scaling eigenvalue" $\left(\begin{array}{ll} y_\mu > 0 & \rightarrow u_\mu \text{ is relevant} \\ y_\mu < 0 & \rightarrow u_\mu \text{ is irrelevant} \end{array}\right)$

Scaling dimensions

- We have seen that we can formulate the RGT for a general Hamiltonian expanded around a fixed point

$$\mathcal{H}(\phi) = \mathcal{H}^*(\phi) - \mathbf{u} \cdot \phi,$$

as

$$\acute{\mathcal{H}}(\acute{\phi}) \equiv \mathcal{R}_b \mathcal{H}(\phi) = \mathcal{H}^*(\acute{\phi}) - \sum_{\mu} b^{y_\mu} u_\mu \acute{\phi}_\mu.$$

- The scaling property of ϕ_μ is determined by y_μ through the condition

$$\int d\mathbf{x} u_\mu(\mathbf{x}) \phi_\mu(\mathbf{x}) = \int d\acute{\mathbf{x}} \acute{u}_\mu(\acute{\mathbf{x}}) \acute{\phi}_\mu(\acute{\mathbf{x}}) + (\text{short length-scale term})$$

with $\acute{\mathbf{x}} = b^{-1}\mathbf{x}$ and $\acute{u}_\mu = b^{y_\mu} u_\mu$. Namely,

$$\acute{\phi}_\mu(\acute{\mathbf{x}}) \approx b^{x_\mu} \phi_\mu(\mathbf{x}) \quad \text{with} \quad x_\mu = d - y_\mu$$

which is called "scaling dimension" of the scaling operator ϕ_μ.

Scaling form of correlation functions

- For correlation function in the long-length scale, we have

$$G_\mu(|\acute{\mathbf{x}} - \acute{\mathbf{y}}|, \acute{\mathbf{K}}) = \langle \acute{\phi}_\mu(\acute{\mathbf{x}}) \acute{\phi}_\mu(\acute{\mathbf{y}}) \rangle_{\mathcal{H}(\acute{\phi}, \acute{\mathbf{K}})}$$
$$\approx b^{2x_\mu} \langle \phi_\mu(\mathbf{x}) \phi_\mu(\mathbf{y}) \rangle_{\mathcal{H}(\phi, \mathbf{K})} = b^{2x_\mu} G_\mu(|\mathbf{x} - \mathbf{y}|, \mathbf{K}),$$

or $$G_\mu(r, \mathbf{K}) \approx \frac{1}{b^{2x_\mu}} G_\mu\left(\frac{r}{b}, \acute{\mathbf{K}}\right)$$

- Let us consider the case where b is large enough that all irrelevant field in $\acute{\mathbf{K}}$ are regarded as zero.
- When we have only one non-zero relevant field, say t,

$$G_\mu(r, t) \approx \frac{1}{b^{2x_\mu}} G_\mu\left(\frac{r}{b}, b^{y_t} t\right).$$

By choosing $b = r$, we obtain

$$G_\mu(r, t) \approx \frac{1}{r^{2x_\mu}} g_\mu\left(\frac{r}{t^{-1/y_t}}\right) \quad (g_\mu(x) \equiv G_\mu(1, x^{y_t}))$$

Critical exponents ν and η

- Let us consider what we can deduce from the scaling form

$$G_\mu(r,t) \approx \frac{1}{r^{2x_\mu}} g_\mu \left(\frac{r}{t^{-1/y_t}} \right).$$

- First, by comparing it with the defining equation of the correlation length, $G_\mu(r,t) \propto r^{-\omega} e^{-r/\xi(t)}$ we can derive

$$\xi(t) \propto t^{-\frac{1}{y_t}} \quad \Rightarrow \quad \nu = \frac{1}{y_t}.$$

- Second, by taking the limit $t \to 0$,

$$G_\mu(r, t=0) \approx \frac{1}{r^{2x_\mu}} g_\mu(0) \tag{5}$$

which means

$$d - 2 + \eta_\mu = 2x_\mu$$

Order parameters and critical exponent β

- Consider the expectation value of a scaling field ϕ_μ

$$m_\mu(\mathbf{u}) \equiv \langle \phi_\mu(\mathbf{x}) \rangle_{\mathbf{u}} \approx \langle b^{-x_\mu} \acute{\phi}_\mu(\acute{\mathbf{x}}) \rangle_{\mathbf{u}} = b^{-x_\mu} m_\mu(\acute{\mathbf{u}}).$$

It follows that $m_\mu(\mathbf{0}) = 0$ if $x_\mu \neq 0$, which we assume below.

- Suppose that spontaneous "magnetization" exists (i.e., $\langle \phi_\mu \rangle > 0$) slightly away from the critical point. When we have only one non-zero relevant field $t \equiv u_\nu$,

$$m_\mu(t) \approx b^{-x_\mu} m_\mu(b^{y_t} t).$$

- By choosing $b = (t/t_0)^{-1/y_t}$, with t_0 being any constant, we obtain

$$m_\mu(t) \propto t^{\frac{x_\mu}{y_t}},$$

Thus, the critical exponent β is related to the scaling dimensions, i.e.,

$$\beta = \frac{x_\mu}{y_t}.$$

[6-2] Gaussian model and Gaussian fixed point

- Consider the Gaussian model:

$$\mathcal{H}_a(\phi|\rho,t) \equiv \int_a^L d^d\mathbf{x}\left(\rho(\nabla\phi_{\mathbf{x}})^2 + t\phi_{\mathbf{x}}^2 - h\phi_{\mathbf{x}}\right)$$
$$= \int_{\pi/L}^{\pi/a} \frac{d^d\mathbf{k}}{(2\pi)^d}(\rho k^2 + t)\phi_{\mathbf{k}}^2 - h\phi_{\mathbf{0}}.$$

(∗ The lower-bound of the integrals symbolically specifies the short-range cutoff.)

- We will apply the RG transformation:

Partial Trace: $\mathcal{H}_a(\phi|\rho,t,h) \to \mathcal{H}_{ba}(\tilde{\phi}|\tilde{\rho},\tilde{t},\tilde{h})$

Rescaling: $\mathcal{H}_{ba}(\tilde{\phi}|\tilde{\rho},\tilde{t},\tilde{h}) \to \mathcal{H}_a(\acute{\phi}|\acute{\rho},\acute{t},\acute{h})$

$$\left(\phi'_{\mathbf{k}'} = b^{-y}\tilde{\phi}_{\mathbf{k}} \quad (\mathbf{k}' \equiv b\mathbf{k})\right)$$

Partial trace of short-range fluctuation

- (Partial trace) $\mathcal{H}_a(\phi|\rho, t, h) \to \mathcal{H}_{ab}(\tilde{\phi}|\tilde{\rho}, \tilde{t}, \tilde{h})$

  Since each wave-number component is independent from the others, the summation over $\phi_{\mathbf{k}}$ for $|\mathbf{k}| > \pi/2a$ results simply in a multiplicative constant:

$$e^{-\mathcal{H}_{ba}(\tilde{\phi}|\tilde{\rho},\tilde{t},\tilde{h})} \equiv \int d\{\phi_{\mathbf{k}}\}_{|\mathbf{k}|>\frac{\pi}{ba}} e^{-\int_{\pi/L}^{\pi/a} \frac{d^d\mathbf{k}}{(2\pi)^d} \left(\rho k^2 + t\right)\phi_{\mathbf{k}}^2 + h\phi_{\mathbf{0}}}$$

$$\sim e^{-\int_{\pi/L}^{\pi/ba} \frac{d^d\mathbf{k}}{(2\pi)^d} \left(\rho k^2 + t\right)\phi_{\mathbf{k}}^2 + h\phi_{\mathbf{0}}},$$

or $$\mathcal{H}_{ba}(\tilde{\phi}|\tilde{\rho}, \tilde{t}) = \int_{\pi/L}^{\pi/ba} \frac{d^d\mathbf{k}}{(2\pi)^d} \left(\rho k^2 + t\right) \phi_{\mathbf{k}}^2 - h\phi_{\mathbf{0}}.$$

  In short, the partial trace amounts to

$$\tilde{\phi}_{\mathbf{k}} = \phi_{\mathbf{k}} \quad \left(\text{for } |\mathbf{k}| < \frac{\pi}{ba}\right), \quad (\tilde{\rho}, \tilde{t}, \tilde{h}) = (\rho, t, h).$$

Rescaling

- (Rescaling) $\mathcal{H}_{ba}(\tilde{\phi}|\tilde{\rho},\tilde{t}) \to \mathcal{H}_a(\acute{\phi}|\acute{\rho},\acute{t})$ $\left(\acute{\phi}_{\acute{\mathbf{k}}} = b^{-y_h}\tilde{\phi}_{\mathbf{k}}\ (\acute{\mathbf{k}} \equiv b\mathbf{k})\right)$

$$\mathcal{H}_a(\acute{\phi}|\acute{\rho},\acute{t},\acute{h}) = \int_{b\pi/L}^{\pi/a} \frac{d^d\acute{\mathbf{k}}}{(2\pi)^d} b^{-d}\left(\rho b^{-2}k'^2 + t\right) b^{2y_h}\acute{\phi}^2_{\acute{\mathbf{k}}} - h\phi_{\mathbf{0}}$$
$$= \int_{b\pi/L}^{\pi/a} \frac{d^d\acute{\mathbf{k}}}{(2\pi)^d} b^{-(d+2)+2y_h}\left(\rho\acute{\mathbf{k}}^2 + b^2 t\right)\acute{\phi}^2_{\acute{\mathbf{k}}} - b^{y_h}h\acute{\phi}_{\mathbf{0}}$$

The exponent y_h should be chosen so that ρ is unchanged by the RG transformation. Namely, $y_h = (d+2)/2$.
Then,

$$\mathcal{H}_a(\acute{\phi}|\acute{\rho},\acute{t},\acute{h}) = \int_{b\pi/L}^{\pi/a} \frac{d^d\acute{\mathbf{k}}}{(2\pi)^d}\left(\rho\acute{k}^2 + \acute{t}\right)\acute{\phi}^2_{\acute{\mathbf{k}}} - \acute{h}\acute{\phi}_{\mathbf{0}}$$

with $\acute{t} \equiv b^2 t$, and $\acute{h} \equiv b^{y_h}h$.

RG transformation of the Gaussian model

To summarize,

- By RG transformation,

$$\mathcal{H}_a(\phi|\rho, t, h) = \int_{b\pi/L}^{\pi/a} \frac{d^d\mathbf{k}}{(2\pi)^d} \left(\rho k^2 + t\right) \phi_{\acute{\mathbf{k}}}^2 - h\phi_{\mathbf{0}}$$

is transformed into

$$\mathcal{H}_a(\acute{\phi}|\acute{\rho}, \acute{t}, \acute{h}) = \int_{b\pi/L}^{\pi/a} \frac{d^d\acute{\mathbf{k}}}{(2\pi)^d} \left(\rho \acute{k}^2 + \acute{t}\right) \acute{\phi}_{\acute{\mathbf{k}}}^2 - \acute{h}\acute{\phi}_{\mathbf{0}}$$

with

$$\acute{\mathbf{k}} = b\mathbf{k}, \quad \acute{\phi}_{\acute{\mathbf{k}}} = b^{-y_h}\tilde{\phi}_{\mathbf{k}}, \quad \acute{t} = b^{y_t}\tilde{t}, \quad \acute{h} = b^{y_h}h \tag{6}$$

with

$$y_t \equiv 2 \quad \text{and} \quad y_h \equiv \frac{d+2}{2}. \tag{7}$$

RGT on $\phi_{\mathbf{x}}$

- While in [6-1] we saw $x_\mu = d - y_\mu$ in general, its direct derivation in the case of Gaussian model clarifies the meaning of RGT.
- Considering the Fourier components of $\acute{\phi}_{\acute{\mathbf{x}}}$,

$$\acute{\phi}_{\acute{\mathbf{x}}} = \acute{L}^{-d} \sum_{\acute{k}}^{\pi/a} e^{i\acute{\mathbf{k}}\acute{\mathbf{x}}} \acute{\phi}_{\acute{\mathbf{k}}} = b^d L^{-d} \sum_{\mathbf{k}}^{\pi/ab} e^{i\mathbf{k}\mathbf{x}} b^{-y} \phi_{\mathbf{k}}$$

$$= b^{d-y} L^{-d} \sum_{\mathbf{k}}^{\pi/ab} e^{i\mathbf{k}\mathbf{x}} \phi_{\mathbf{k}} = b^x [\phi_{\mathbf{x}}]_{k<\frac{\pi}{ab}}$$

- Here, $[\phi_{\mathbf{x}}]_{k<k^*} \equiv L^{-d} \sum_{\mathbf{k}}^{k^*} e^{i\mathbf{k}\mathbf{x}} \phi_{\mathbf{k}}$ is something one obtains after filtering out the short wave-length part $(k > k^*)$ from $\phi_{\mathbf{x}}$. Therefore, $\phi_{\mathbf{x}}$ and $[\phi_{\mathbf{x}}]_{k<k^*}$ are identical in the renormalized description.

Implication of RGT

- In [6-1], we saw, in general,

$$\nu = \frac{1}{y_t}$$

$$d - 2 + \eta_\mu = 2x_\mu$$

- For the Gaussian model, we have derived

$$y_t = 2 \quad \text{and} \quad y_h = \frac{d+2}{2}$$

- Therefore, for the gaussian model

$$\nu = \frac{1}{2} \quad \text{and} \quad \eta = 0.$$

Homework (Submit your report on one of the following)

- By an argument similar to the one resulting in $\beta_\mu = x_\mu / y_t$, show that the critical exponent γ_μ that describes the temperature-dependence of the susceptibility, $\chi_\mu \equiv \partial \langle \phi_\mu(\mathbf{x}) \rangle / \partial u_\mu \propto t^{-\gamma_\mu}$, is related to the scaling dimensions/eigenvalues as $\gamma_\mu = \dfrac{y_\mu - x_\mu}{y_t} = \dfrac{2y_\mu - d}{y_t}$.
- Consider a system for which the susceptibility χ_μ diverges as one approaches the critical point keeping the condition $u_\mu = 0$. Does application of infinitesimal field u_μ qualitatively change the critical properties? Can we say the opposite, i.e., that the field does not essentially change the nature of the transition whenever $\chi_\mu < \infty$?
- In the rescaling of the Gaussian model, we fixed y_h so that the ρ would not change. In principle, we should be able to obtain some RGT by fixing other parameters in stead of ρ. What would we have obtained, for example, if we had fixed t rather than ρ?

Lecture 7: Consequences of Renormalization Group

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June 3, 2019

In this lecture, we see ...

- The free energy (and therefore all the quantities derived from it) can be expressed as the sum of a singular part and a regular part.
- The critical phenomena can be systematically derived from the singular part of the free energy.
- By RG flow diagram, we can understand cross-over phenomena, which is the scale-dependent critical phenomena.
- From RG, we can derive "finite-size scaling (FSS)," which is useful in estimating scaling dimensions through numerical simulation of finite systems.

[7-1] Singular part of free energy

- The free energy of a finite system can be split into two non-singular parts: the first part is purely extensive, whereas the second is RGT invariant and becomes singular in the thermodynamic limit. The latter is called the singular part of the free energy (though it is non-singular for finite systems).

Singular part of free energy

- As we see later, the RGT invariant function produces a singularity that explains critical behaviors.
- However, the free energy itself cannot be RGT invariant at the critical point due to cotribution from short-range fluctuations.
- These observations motivate the following form for the free energy:

$$F(\mathbf{K}, L) = F_{\mathrm{s}}(\mathbf{K}, L) + L^d \gamma(\mathbf{K}) \tag{1}$$

where F_{s} is RGT-invariant

$$F_{\mathrm{s}}(\acute{\mathbf{K}}, \acute{L}) = F_{\mathrm{s}}(\mathbf{K}, L) \tag{2}$$

and $\gamma(\mathbf{K})$ is a non-singular function of $\mathbf{K}$

Example: 1D Ising model (1)

- The partition function can be expressed with the transfer matrix as

$$Z = \mathrm{Tr}\; T^L \quad \left(T_{S_1,S_2} \equiv e^{KS_1S_2 + h(S_1+S_2)/2} = \begin{pmatrix} e^{K+h} & e^{-K} \\ e^{-K} & e^{K-h} \end{pmatrix} \right)$$

- The eigenvalues of T are

$$\lambda_\pm \equiv e^K \left(\cosh h \pm \sqrt{\sinh^2 h + e^{-4K}} \right) \tag{3}$$

- The correlation length is then

$$\xi^{-1} = -\log \frac{\lambda_-}{\lambda_+} \approx 2\sqrt{h^2 + t^2} \qquad \left(t \equiv e^{-2K} \right). \tag{4}$$

- $Z = \mathrm{Tr}\; T^L = \lambda_+^L + \lambda_-^L = \lambda_+^L \left(1 + \left(\frac{\lambda_-}{\lambda_+} \right)^L \right)$

Example: 1D Ising model (2)

- $F = Lf + \Delta F \quad \left(f \equiv -\log \lambda_+,\ \Delta F \equiv -\log \left(1 + e^{-L/\xi} \right) \right)$
- Notice that ΔF is obviously RGT-invariant. However, we cannot take f and ΔF as γ and $F_{\rm s}$, respectively, because f is singular.
- Notice also that, for $\xi \gg L$, we have $\Delta F \approx -\log 2 + \dfrac{L}{2\xi}$.
- Therefore, by subtracting $L/2\xi$ from ΔF and add it to Lf, we can make both terms non-singular*, while keeping ΔF RGT-invariant:

$$F = F_{\rm s} + L\gamma \qquad (5)$$

with $F_{\rm s} \equiv \Delta F - \dfrac{L}{2\xi} \quad \left(f_{\rm s} \equiv \lim_{L\to\infty} \dfrac{F_{\rm s}}{L^d} = -\dfrac{L}{2\xi} \right)$, and $\gamma \equiv f + \dfrac{1}{2\xi}$

(*) Since F is the free energy of a finite system, it must be regular. Therefore, regularity of γ automatically means regularity of $F_{\rm s}$ even if it produces a singularity in the $L \to \infty$ limit. In addition, strictly speaking, γ is singular, but this singularity is physically uninportant, because it can be removed by adding a constant to the Hamiltonian.

[7-2] Scaling form

- It is convenient to introduce the scaling form of the singular part of the free energy.
- From it, we can systematically derive various scaling relations.

Finite system

- The RGT invariance, $F_{\mathrm{s}}(\mathbf{K}, L) = F_{\mathrm{s}}(\acute{\mathbf{K}}, \acute{L})$, can be rewritten in terms of scaling field, u_μ,

$$F_{\mathrm{s}}(u_1, u_2, \cdots, L) = F_{\mathrm{s}}(u_1 b^{y_1}, u_2 b^{y_2}, \cdots, L/b). \tag{6}$$

- By setting $b = L/L_0$ where L_0 is some constant length scale, and dropping the L_0 dependence of the function, we may write

$$F_{\mathrm{s}}(u_1, u_2, \cdots, L) = \tilde{F}_{\mathrm{s}}(u_1 L^{y_1}, u_2 L^{y_2}, \cdots), \tag{7}$$

which is called the "scaling form" of F_{s}.

Infinite system

- Another way of rewriting F_{s} is

$$F_{\mathrm{s}}(u_1, u_2, \cdots, L) = L^d f_{\mathrm{s}}(u_1, u_2, \cdots, L)$$
$$= (L/b)^d f_{\mathrm{s}}(u_1 b^{y_1}, u_2 b^{y_2}, \cdots, L/b).$$

- Let us assign a special role to the first scaling field, u_1, which we assume to be relevant, and denote it as t ($t \equiv u_1$).
- By taking b so that $tb^{y_t} = t_0$ is a constant,

$$f_{\mathrm{s}}(u_1, u_2, \cdots, L) = t^{\frac{d}{y_t}} f_{\mathrm{s}}(t_0, u_2 t^{-y_2/y_1}, \cdots, L t^{1/y_t})$$

- In the thermodynamic limit, the L dependence on the both side should vanish. Then, by also droping the t_0 dependence,

$$f_{\mathrm{s}}(u_1, u_2, u_3, \cdots) = t^{\frac{d}{y_t}} \tilde{f}_{\mathrm{s}} \left(u_2 t^{-\frac{y_2}{y_1}}, u_3 t^{-\frac{y_3}{y_1}}, \cdots \right) \quad (8)$$

which is called the scaling form of the free energy density.

Singularity of various quantities (1)

- We can derive various scaling properties from (7) (or (8)).
- Below, we consider only the vicinity of the critical point which allows us to set all irrelevant fields zero.
- As an example, we consider the case where we have only two relevant fields, $t \equiv u_1$ and $h \equiv u_2$ (like $t \propto T - T_c$ and $h \propto H$ in the Ising model). So, our singular part of the free energy becomes

$$F_{\rm s}(t, h, L) = \tilde{F}_{\rm s}(tL^{y_t}, hL^{y_h}) \tag{9}$$

Singularity of various quantities (2)

$$F_{\mathrm{s}}(t,h,L) = \tilde{F}_{\mathrm{s}}(tL^{y_t}, hL^{y_h})$$

- For the "specific heat", we have

$$c(t,L) \propto -\frac{1}{L^d}\left(\frac{\partial^2 F_{\mathrm{s}}}{\partial t^2}\right)_{h\to 0} \sim -L^{-d+2y_t}\tilde{F}_{\mathrm{s}}^{(2,0)}(tL^{y_t},0)$$

$$\left(\tilde{F}_{\mathrm{s}}^{(m,n)} \equiv \frac{\partial^m}{\partial t^m}\frac{\partial^n}{\partial h^n}\tilde{F}_{\mathrm{s}}\right)$$

$$\sim L^{2y_t-d}\left(tL^{y_t}\right)^{-\frac{2y_t-d}{y_t}} \times \left(-\left(tL^{y_t}\right)^{\frac{2y_t-d}{y_t}}\tilde{F}_{\mathrm{s}}^{(2,0)}(tL^{y_t},0)\right)$$

$$= t^{-\frac{2y_t-d}{y_t}}\tilde{c}(tL^{y_t}) \qquad \left(\tilde{c}(x) \equiv -x^{\frac{2y_t-d}{y_t}}\tilde{F}_{\mathrm{s}}^{(2,0)}(x,0)\right)$$

- Since $\lim_{L\to\infty} c(t,L)$ is independent of L, $c(t,\infty) \propto t^{-\alpha}$ where

$$\alpha = \frac{2y_t - d}{y_t} = 2 - d\nu \quad \left(\nu \equiv \frac{1}{y_t}\right) \tag{10}$$

Singularity of various quantities (3)

- For "magnetization", we have

$$m \propto -\frac{1}{L^d}\left(\frac{\partial F_{\rm s}}{\partial h}\right)_{h\to 0} = -L^{-d+y_h} F_{\rm s}^{(0,1)}(tL^{y_t},0)$$
$$= t^{\frac{d-y_h}{y_t}} \tilde{m}(tL^{y_t}) \propto t^{\beta}$$
$$\text{with} \quad \beta \equiv \frac{d-y_h}{y_t} \tag{11}$$

- For "magnetic susceptibility", we have

$$\chi \propto -\frac{1}{L^d}\left(\frac{\partial^2 F_{\rm s}}{\partial h^2}\right)_{h\to 0} = -L^{-d+2y_h} F_{\rm s}^{(0,2)}(tL^{y_t},0)$$
$$= t^{-\frac{2y_h-d}{y_t}} \tilde{\chi}(tL^{y_t}) \propto t^{-\gamma}$$
$$\text{with} \quad \gamma \equiv \frac{2y_h-d}{y_t} \tag{12}$$

Scaling relations

- From (10), (11) and (12),

$$\alpha + 2\beta + \gamma = 2. \qquad \text{(Rushbrooke)} \tag{13}$$

- Similarly, we can also derive that

$$\gamma = \beta(\delta - 1) \qquad \text{(Griffiths)} \tag{14}$$

where δ is the exponent that characterize the magnetic-field dependence of the magnetization at the critical temperature,

$$m(t = 0, h) \propto h^{1/\delta}$$

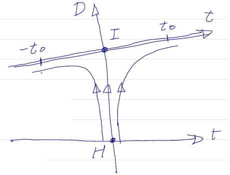
[7-3] Cross-over phenomena

- A cross-over phenomenon is the behavior of the system in which a weak but relevant scaling field manifests itself.
- We can understand it from the scaling form.
- We can also derive the form of the phase boundary near the critical point.

Example: Heisenberg model with anisotropy (1)

- 3D classical Heisenberg model

$$\mathcal{H} = -J \sum_{(ij)} \mathbf{S}_i \cdot \mathbf{S}_j - D \sum_{(ij)} S_i^z S_j^z$$



where $\mathbf{S} \equiv (S_i^x, S_i^y, S_i^z)^{\mathrm{T}}$ ($|\mathbf{S}| = 1$).

- If $D = 0$, the system has a critical point, corresponding to the fixed point "H".
- The anisotropic operator is relevant at H.
- If the anisotoropy is strong enough, we can regard the system as an Ising model, whose critical point is represented by "I".
- Accordingly, there is a RG trajectory (critical line) starting from H and ending at I.

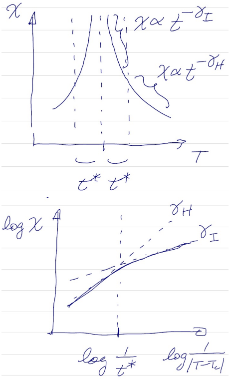
Example: Heisenberg model with anisotropy (2)

- By (8), the free energy around "H" is

$$f_s(t, D) = t^{\frac{d}{y_t}} \tilde{f}_s\left(Dt^{-\phi}\right) \quad (15)$$

where ϕ is cross-over exponent $\phi \equiv \frac{y_D}{y_t}$.

- Eq.(15) can be re-written as $f_s = t^{\frac{d}{y_t}} \tilde{f}_s(t/t^*(D))$ with a "cross-over temperature" $t^*(D) \propto D^{1/\phi}$. Then, f_s behaves like an isotropic Heisenberg model ($D = 0$) when $t \gg t^*$, whereas it qualitatively deviates from the Heisenberg-like behavior when $t \ll t^*$.

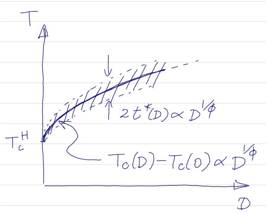


$$\gamma_{3DI} = 1.237075(10)$$
$$\gamma_{3DH} \approx 1.35(*)$$
$$\gamma_{3DXY} = 1.3177(5)$$

(*) Kaupuzs, cond-mat/0101156

Example: Heisenberg model with anisotropy (3)

- Now, we consider the shape of the phase boundary in the $D - T$ phase diagram.
- We again use $f_{\mathrm{s}}(t, D) = t^{d/y_t^H} \tilde{f}_{\mathrm{s}}(Dt^{-\phi})$, where $\phi \equiv y_D^H / y_t^H$. where we put superscript "H" to make it clear that y_t^H is the value at H.
- Wnen $D > 0$, the system should show the Ising-like critical behavior. Then, we obtain
$$f_{\mathrm{s}}(t, D) \sim (t - t_c(D))^{d/y_t^I}.$$



$\phi \approx 1.2$ for 3D Heisenberg model.

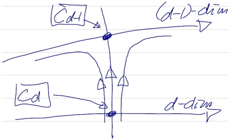
- Now, to satisfy both of these forms at the same time, f_{s} must have the following form near the criticality.

$$f_{\mathrm{s}} \propto t^{\frac{d}{y_t^H}} \left(tD^{-\frac{1}{\phi}} - x_0 \right)^{\frac{d}{y_t^I}} \propto D^{\frac{d}{\phi}\left(\frac{1}{y_t^H} - \frac{1}{y_t^I}\right)} \left(t - x_0 D^{\frac{1}{\phi}} \right)^{\frac{d}{y_t^I}}$$

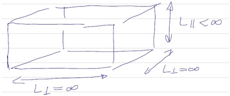
Therefore, $t_c(D) \propto D^{1/\phi} = D^{y_t^H / y_t^I}$

Dimensional crossover

- Some systems have phase transitions even when the size is finite in one direction. However, the critical properties are different from the case where the system is infinite in all directions.



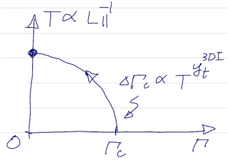
- Though the system size is not a "field" in the conventional terminology, we can treat $(\text{size})^{-1}$ as if it were a relevant field.



- In doing so, the scaling eigenvalue of $D \equiv L_{\parallel}^{-1}$, where $L_{\parallel}$ is the size that is finite, is obviously 1.

- Therefore, we have $\phi = 1/y_t$ for the crossover exponent, which leads to $t^* \propto L_{\parallel}^{-y_t}$ for the crossover temperature, and $t_c(L_{\parallel}) \propto L_{\parallel}^{-y_t}$ for the transition temperature near the $L_{\parallel} = \infty$ critical point.

Quantum critical point



- By Feynman's path integral formulation, d-dimensional quantum system can be represented as $(d+1)$-dimensional classical system with size $1/T$ in the new direction.
- In some special cases, the extra dimension, called the "imaginary time", is essentially equivalent to one of the spatial directions.
- For example, the 2-dimensional transverse field Ising model $\mathcal{H} = -J \sum_{(ij)} S_i^z S_i^z - \Gamma \sum_i S_i^x$ has a quantum phase transition at $T = 0$ and $\Gamma = \Gamma_c$, and it can be mapped to 3-dimensional classical Ising model with the size $1/T$ in the 3rd dimension.
- Then, we can apply the dimensional cross-over to this system:

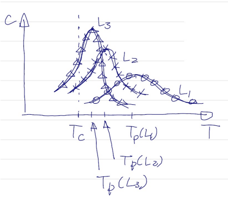
$$t^*(T) \propto t_c(T) \propto L_{\parallel}^{-y_t^{3DI}} \propto T^{y_t} \qquad (16)$$

where $t \equiv \Gamma - \Gamma_c$ and y_t is for the 3D Ising model.

[7-4] Finite-size scaling

- As we have seen, the RGT-invariant quantity can be used to characterize a critical phenomena.
- We'll see a practical way for obtaining the critical indices (scaling dimensions).
- We can define such a computable RGT-invariant quantity as a difference in the free energy of two system-sizes.

Specific heat (1)



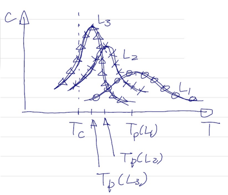
- Suppose we have obtained $F_{\rm s}(\mathbf{K}, L)$ as a function of $\mathbf{K}$ and L, and it has the form $F_{\rm s}(\mathbf{K}, L) = \tilde{F}_{\rm s}(tL^{y_t}, hL^{y_h}, \cdots)$.
- From $\tilde{F}_{\rm s}$, the scaling form of the specific heat is

$$c \approx \frac{-T}{L^d}\frac{\partial^2 F_{\rm s}}{\partial T^2} \sim L^{2y_t - d}\tilde{c}(tL^{y_t}). \tag{17}$$

- If $c(T, L)$ diverges at the critical point for $L \to \infty$, we expect that c has a peak around $T \approx T_{\rm c}$ even if L is finite.
- This is compatible with (17) only if $\tilde{c}$ has a peak itself.

Specific heat (2)

$$c(T, L) \sim L^{2y_t - d} \tilde{c}(tL^{y_t}).$$



- Suppose $\tilde{c}(x)$ has a peak at $x = x_p$. It means that $c(T, L)$ has a peak when $tL^{y_t} = x_p$.
- Let $T_{\rm c}(L)$ be the temperature at which $c(T, L)$ has the peak. Then,

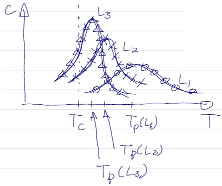
$$T_{\rm c}(L) - T_{\rm c} \propto t_{\rm c}(L) \propto L^{-y_t}. \qquad (18)$$

- The height of the peak also carries some information on the critical behavior, i.e., it is proportional to

$$c(T_{\rm c}(L), L) \propto L^{2y_t - d} \qquad (19)$$

Specific heat (3)

- More directly, by plotting c/L^{2y_t-d} against $(T - T_{\rm c})L^{y_t}$, we expect that curves corresponding to varying system sizes fall on top of each other.
- Of course, to do this, we need to choose the right values for $T_{\rm c}$ and y_t, which we do not know initially.
- We can fix these values by some trials-and-errors, like using an analog camera and adjusting the focus.



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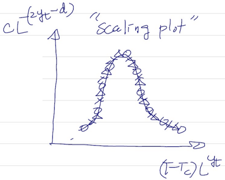

Remark: Practical substitute of $F_{\rm s}$

- So far, we have been implicitly assuming that we can compute $F_{\rm s}$.
- But it is not usually true even for finite systems. That's why people often simply use F itself in the place of $F_{\rm s}$ in numerical calculation. (This is equivalent to using the specific heat itself instead of its singular part.)
- This "approximation" is bad when the divergence is "weak."
- We had better use the following quantity, not F, in the place of $F_{\rm s}$:

$$\begin{aligned}\Delta_b F(\mathbf{K}, L) &\equiv (b^d F(\mathbf{K}, L/b) - F(\mathbf{K}, L))/(b^d - 1) \\ &= (b^d F_{\rm s}(\mathbf{K}, L/b) - F_{\rm s}(\mathbf{K}, L))/(b^d - 1).\end{aligned}$$

The last expression tells us that $\Delta_b F$ is RGT-invariant, i.e., free from the regular part, while the second expression is computable.

Exercise

- Consider the 1-dimensional q-state Potts model. Following the similar argument as in the lecture, obtain the singular part of the free energy.
- Consider $S = 1$ Ising model which is described by the same form of the Hamiltonian as the conventional Ising model, whereas each spin variable takes one of three values, $-1, 0, 1$ instead of two. Confirm that $\xi f_s = -1/2$ for this model, the same as the $S = 1/2$ Ising model.
- Derive Griffiths' scaling relation (14).

Lecture 8: Operator Product Expansion

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In this lecture, we see ...

- Product of two scaling operators can be expanded in terms of scaling operators. (OPE)
- Such an expansion determines the RG-flow structure around the fixed point (will be discussed in the next lecture).
- For the Gaussian fixed point, all the coefficients of the OPE can be exactly obtained.

[8-1] General Framework

- Product of two scaling operators, defined at some distance from each other, can be expanded as a linear combination of scaling operators.
- Considering the 3-point correlators and taking into account of the scaling properties of operators, the general form of the OPE coefficients can be fixed up to universal constants.

Product of two is expandable

- Previously, we introduced scaling operators $\{\phi_\mu\}$ as something that spans the space of local operators:

$$\forall Q(\mathbf{x}) \exists q_\mu \left(Q(\mathbf{x}) = \sum_\mu q_\mu \phi_\mu(\mathbf{x}) \right) \quad (1)$$

- At the fixed point, we required that the RGT acts on ϕ_μ as

$$\mathcal{R}_b \phi_\mu(\mathbf{x}) = b^{x_\mu} \phi_\mu(\mathbf{x})$$

- Let us consider the product of two scaling operators, $\phi_\mu(\mathbf{x})\phi_\nu(\mathbf{y})$. This product must appear to be a "local" operator when we view it from a point $\mathbf{z}$ far away from $\mathbf{x}$ and $\mathbf{y}$ (i.e., $|\mathbf{z} - \mathbf{x}| \gg |\mathbf{y} - \mathbf{x}|$).
- Then, we should be able to expand it:

$$\phi_\mu(\mathbf{x})\phi_\nu(\mathbf{y}) = \sum_\alpha C^\alpha_{\mu\nu}(\mathbf{x} - \mathbf{y}) \phi_\alpha\left(\frac{\mathbf{x} + \mathbf{y}}{2}\right)$$

(Equality holds only when viewed from a distant point.)

Three-point correlator (1/2)

- Let us consider three-point correlation function:

$$G_{\mu\nu\lambda}(\mathbf{x},\mathbf{y},\mathbf{z}) \equiv \langle \phi_\mu(\mathbf{x})\phi_\nu(\mathbf{y})\phi_\lambda(\mathbf{z})\rangle$$

- By applying the RGT and then expanding $\phi_\mu\phi_\nu$, we have

$$\begin{aligned} G_{\mu\nu\lambda}(\acute{\mathbf{x}},\acute{\mathbf{y}},\acute{\mathbf{z}}) &= b^{x_\mu+x_\nu+x_\lambda} G_{\mu\nu\lambda}(\mathbf{x},\mathbf{y},\mathbf{z}) \\ &= b^{x_\lambda+x_\mu+x_\nu} \sum_\alpha C^\alpha_{\mu\nu}(\mathbf{x}-\mathbf{y}) G_{\alpha\lambda}\left(\frac{\mathbf{x}+\mathbf{y}}{2},\mathbf{z}\right) \end{aligned} \quad (2)$$

- By reversing the order of the operations, we have

$$\begin{aligned} G_{\mu\nu\lambda}(\acute{\mathbf{x}},\acute{\mathbf{y}},\acute{\mathbf{z}}) &= \sum_\alpha C^\alpha_{\mu\nu}(\acute{\mathbf{x}}-\acute{\mathbf{y}}) G_{\alpha\lambda}\left(\frac{\acute{\mathbf{x}}+\acute{\mathbf{y}}}{2},\acute{\mathbf{z}}\right) \\ &= \sum_\alpha C^\alpha_{\mu\nu}(\acute{\mathbf{x}}-\acute{\mathbf{y}}) b^{x_\alpha+x_\lambda} G_{\alpha\lambda}\left(\frac{\mathbf{x}+\mathbf{y}}{2},\mathbf{z}\right) \end{aligned} \quad (3)$$

Three-point correlator (2/2)

- Comparing (2) and (3), we conclude

$$C^{\alpha}_{\mu\nu}(\mathbf{r}) = \frac{C^{\alpha}_{\mu\nu}\left(\frac{\mathbf{r}}{b}\right)}{b^{x_\mu + x_\nu - x_\alpha}}$$

This leads to

$$\exists c^{\alpha}_{\mu\nu} \left(C^{\alpha}_{\mu\nu}(r) = \frac{c^{\alpha}_{\mu\nu}}{r^{x_\mu + x_\nu - x_\lambda}} \right).$$

Therefore, we have the operator-product expansion:

$$\phi_\mu(\mathbf{x})\phi_\nu(\mathbf{y}) = \sum_\alpha \frac{c^{\alpha}_{\mu\nu}}{r^{x_\mu + x_\nu - x_\lambda}} \phi_\alpha(\mathbf{x}) \qquad \text{(OPE)}$$

Universality

- By normalizing the scaling operators so that

$$\lim_{|\mathbf{x}-\mathbf{y}|\to\infty} |\mathbf{x}-\mathbf{y}|^{2x_\mu} \langle \phi_\mu(\mathbf{x})\phi_\nu(\mathbf{y})\rangle = 1$$

  the OPE coefficient $c_{\mu\nu}^{\alpha}$ can be fixed (and become universal quantities).
- We assume that thus fixed OPE coefficients $c_{\mu\nu}^{\alpha}$ are universal, and characterizing property of the fixed-point, together with the scaling dimensions, x_μ. In other words, they do not depend on the details of the system, but depend only on the symmetry, the space dimension, etc. (This assumption of universality is similar to the assumption of very existence of the fixed-point of the RGT. It is at least supported by several exactly solvable cases.)

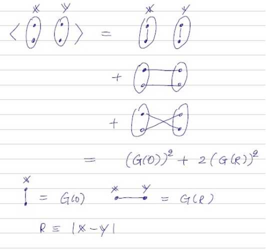
[8-2] OPE at the Gaussian fixed point

- The scaling operators at the Gaussian fixed point can be obtained through the normal order product: $\phi_n \equiv [\![\phi^n]\!]$.
- We can compute exact OPE coefficients of the gaussian fixed point.

A hint for scaling operators — Wick's theorem

- Consider the operator $(\phi(\mathbf{x}))^2$ and its correlation function.

$$
\begin{aligned}
\langle \phi^2(\mathbf{x})\phi^2(\mathbf{y})\rangle &= \langle \underset{1}{\phi(\mathbf{x})}\,\underset{2}{\phi(\mathbf{x})}\,\underset{3}{\phi(\mathbf{y})}\,\underset{4}{\phi(\mathbf{y})}\rangle \\
&= \langle \underset{1}{\phi(\mathbf{x})}\,\underset{2}{\phi(\mathbf{x})}\rangle\langle \underset{3}{\phi(\mathbf{y})}\,\underset{4}{\phi(\mathbf{y})}\rangle \\
&+ \langle \underset{1}{\phi(\mathbf{x})}\,\underset{3}{\phi(\mathbf{y})}\rangle\langle \underset{2}{\phi(\mathbf{x})}\,\underset{4}{\phi(\mathbf{y})}\rangle \\
&+ \langle \underset{1}{\phi(\mathbf{x})}\,\underset{4}{\phi(\mathbf{y})}\rangle\langle \underset{2}{\phi(\mathbf{x})}\,\underset{3}{\phi(\mathbf{y})}\rangle \qquad (4) \\
&= G^2(0) + 2G^2(r)
\end{aligned}
$$



where $r \equiv |\mathbf{x} - \mathbf{y}|$ and

$$G(r) \sim \frac{1}{r^{2x}} \quad \text{where} \quad x \equiv \frac{d-2}{2}$$

Scaling operators

What are scaling operators at the Gaussian fixed point?

- If the constant term $G(0)^2$ in

$$\langle \phi^2(\mathbf{x})\phi^2(\mathbf{y})\rangle = G(0)^2 + 2G(r)^2$$

were absent, $\phi^2(\mathbf{x})$ would be regarded as a scaling operator.

- This observation leads us to define

$$\phi_2(\mathbf{x}) \equiv \phi(\mathbf{x})^2 - \langle \phi(\mathbf{x})^2 \rangle,$$

which has the two-point correlator

$$\begin{aligned}\langle \phi_2(\mathbf{x})\phi_2(\mathbf{y})\rangle &= \langle (\phi^2(\mathbf{x}) - G(0))(\phi^2(\mathbf{y}) - G(0))\rangle \\ &= \langle \phi^2(\mathbf{x})\phi^2(\mathbf{y})\rangle - G(0)^2 = 2G(r)^2 = \frac{2}{r^{4x}}\end{aligned}$$

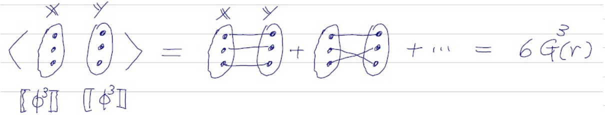
- Therefore, ϕ_2 is the scaling operator with the dimension $x_2 \equiv 2x$.

Normal-ordered operator

- The key to finding general scaling operators is to eliminate the diagrams with "internal connections" such as the first term in (4).
- Therefore, it would be convenient to introduce a symbol $[\![\cdots]\!]$ as

$$[\![A(\mathbf{x})]\!] \equiv A(\mathbf{x}) - \begin{pmatrix}\text{All terms represented by}\\ \text{diagrams with internal}\\ \text{connections}\end{pmatrix}$$

  The operator thus defined is called "normal-ordered."
- When considering correlations among normal-ordered operators, by definition, we can forget about the internal lines. Therefore, 2-point correlators do not have constant terms, which makes the normal-ordered operator $[\![\phi^n]\!]$ a scaling operator. For example,



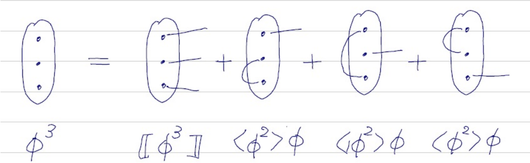
Scaling operators $\phi_2 \equiv [\![\phi^2]\!]$ and $\phi_3 \equiv [\![\phi^3]\!]$

- For ϕ^2, as we have seen already

$$\phi_2 \equiv [\![\phi^2]\!] = \phi^2 - \langle \phi^2 \rangle$$

- For ϕ^3, from the diagram below, we obtain

$$\phi^3 = [\![\phi^3]\!] + 3\langle \phi^2 \rangle \phi$$



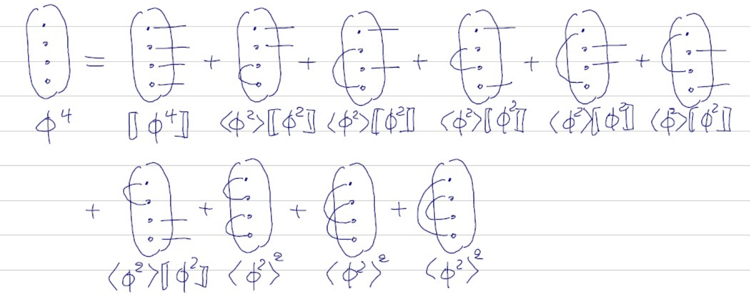
Therefore,

$$\phi_3 \equiv [\![\phi^3]\!] = \phi^3 - 3G(0)\phi$$

Scaling operator $\phi_4 \equiv [\![\phi^4]\!]$

- For ϕ^4, again from the diagram, we obtain

$$\phi^4 = [\![\phi^4]\!] + 6\langle\phi^2\rangle[\![\phi^2]\!] + 3\langle\phi^2\rangle^2$$



Therefore,

$$\begin{aligned}\phi_4 = [\![\phi^4]\!] &= \phi^4 - 6G(0)\phi_2 + 3G(0)^2 \\ &= \phi^4 - 6G(0)\phi^2 - 3G(0)^2\end{aligned}$$

Scaling operators of Gaussian fixed-point

- To summarize, the scaling operators of Gaussian fixed point are

$$\phi_n \equiv [\![\phi^n]\!]$$

- For the standard normalization, consider

$$\langle \phi_n(\mathbf{x})\phi_n(\mathbf{y})\rangle = \sum_{\substack{\text{all connection}\\ \text{patterns}}} \langle \phi(\mathbf{x})\phi(\mathbf{y})\rangle^n = N! G^n(r) = \frac{N!}{r^{2nx}}.$$

Therefore, $\hat{\phi}_n \equiv \frac{1}{\sqrt{N!}}\phi_n$ is the normalized scaling operator.

- The scaling dimension is obviously

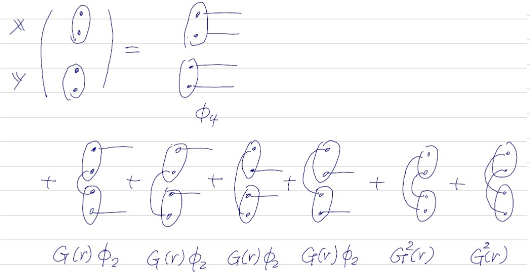
$$x_n \equiv nx = n(d-2)/2$$

- The scaling operators are orthogonal to each other

$$\langle \hat{\phi}_m(\mathbf{x})\hat{\phi}_n(\mathbf{y})\rangle = \frac{\delta_{mn}}{r^{2x_m}}$$

Expansion of $\phi_2(\mathbf{x})\phi_2(\mathbf{y})$

- Consider product of two operators $\phi_2(\mathbf{x})\phi_2(\mathbf{y})$.



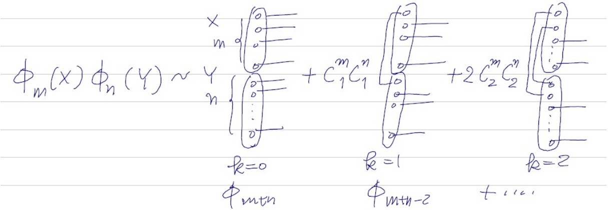
From this diagram, we obtain

$$\phi_2(\mathbf{x})\phi_2(\mathbf{y}) \sim \phi_4\left(\frac{\mathbf{x}+\mathbf{y}}{2}\right) + 4\langle\phi(\mathbf{x})\phi(\mathbf{y})\rangle\phi(\mathbf{x})\phi(\mathbf{y}) + 2\langle\phi(\mathbf{x})\phi(\mathbf{y})\rangle^2$$

$$= \phi_4\left(\frac{\mathbf{x}+\mathbf{y}}{2}\right) + 4G(r)\phi_2\left(\frac{\mathbf{x}+\mathbf{y}}{2}\right) + 2G^2(r).$$

OPE of Gaussian fixed-point

- We can generalize the product $\phi_2\phi_2$ to general two operators.



$$\phi_m(\mathbf{x})\phi_n(\mathbf{y}) \sim \sum_{k=0}^{(m+n)/2} \binom{m}{k}\binom{n}{k} k!\, G^k(r)\phi_{m+n-2k}\left(\frac{\mathbf{x}+\mathbf{y}}{2}\right)$$

$$= \sum_l \frac{c_{mn}^l}{|\mathbf{x}-\mathbf{y}|^{x_m+x_n-x_l}}\phi_l\left(\frac{\mathbf{x}+\mathbf{y}}{2}\right)$$

$$\left(c_{mn}^l = \binom{m}{k}\binom{n}{k}k! \quad \left(k \equiv \frac{m+n-l}{2}\right)\right)$$

Summary

- Generally, we can expand the product of the two scaling operators in terms of scaling operators (OPE), which takes the form

$$\phi_m(\mathbf{x})\phi_n(\mathbf{y}) = \sum_l \frac{c^l_{mn}}{|\mathbf{x}-\mathbf{y}|^{x_m+x_n-x_l}} \phi_l\left(\frac{\mathbf{x}+\mathbf{y}}{2}\right).$$

- The constants c^l_{mn} are universal quantities (provided that the scaling operators are properly normalized).
- For the Gaussian model, the scaling operator can be explicitly defined by the normal-ordering as $\phi_n \equiv [\![\phi^n]\!]$, and its scaling dimension is $x_n \equiv nx = n(d-2)/2$.
- The OPE at the Gaussian fixed-point is characterized by

$$c^l_{mn} = \binom{m}{k}\binom{n}{k} k! \quad \left(k \equiv \frac{m+n-l}{2}\right)$$

Exercise

- For the Gaussian model, obtain ϕ_5 in terms of ϕ^k $(k = 1, 2, 3, \cdots)$, following the same argument as in the lecture.

Lecture 9: Perturbative Renormalization Group

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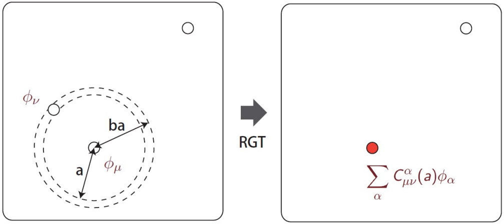
June 17, 2019

In this lecture, we see ...

- When there is a fixed point and we know its OPE, by a perturbative argument, we can derive a set of equations describing RG flow around it. (Then, we can study the behavior of other fixed points in its vicinity, as we will discuss in the next lecture.)
- We can obtain the renormalized Hamiltonian up to the 2nd order (or more if we try harder) in the case of GFP, which is the lowest non-trivial order.

[9-1] General perturbative RG

- We decompose the field operator into the high-frequency component and the low-frequency component.
- Tracing out the high-fruquency component, followed by rescaling, yields the RG flow equations.
- In the RGT from the scale a to ab ($b = 1 + \delta$), the product of two scaling operators within the distance of a, gives rise to new perturbative terms through OPE, which contributes non-linear terms in the RG flow equation.



Expanding the Hamiltonian around a fixed point

- Consider some fixed-point Hamiltonian, $\mathcal{H}_a^*$, with short-distant cut-off (lattice constant) a, and consider a general Hamiltonian expressed in terms of the scaling-operators at $\mathcal{H}_a^*$:

$$\mathcal{H}_a \equiv \mathcal{H}_a^* + \Delta\mathcal{H}_a \qquad \left(\Delta\mathcal{H}_a \equiv \sum_{\alpha} g_\alpha \int_a d\mathbf{x}\, \phi_\alpha(\mathbf{x}) \right)$$

where ϕ_α is the scaling operator at $\mathcal{H}^*$ with the dimension x_α.

$$\phi_\alpha(\mathbf{x}) \;\to\; \acute{\phi}_\alpha(\acute{\mathbf{x}}) = \mathcal{R}_b \phi_\alpha(\mathbf{x}) = b^{x_\alpha} \phi_\alpha(\mathbf{x})$$

RGT to the expansion

- Let us carry out the general program of RG: (i) partial trace, and (ii) rescaling.
- We introduce the ultra-violet cut-off in the form of the restriction on the integral region in (i) that no two operators cannot be within the mutual distance a.
- By the partial trace, we will shift the cut-off length a to $\acute{a} \equiv e^{\lambda} a \approx (1+\lambda)a$.
- Then, the partial trace is equivalent to application of the OPE to every pair of operators that come within the mutual distance of $\acute{a}$, and taking the summation with respect to the relative position of the two (This yields the factor $V_d(\acute{a}^d - a^d) \approx V_d d\lambda a^d$, where V_d is the volume of unit sphere.).

The partial trace (0th order term)

- By denoting the partial trace by $\mathrm{Tr}\,'$, the perturbative expansion becomes

$$\mathrm{Tr}\,' e^{-\mathcal{H}_a^* - \Delta\mathcal{H}_a} = \mathrm{Tr}\,' \left\{ e^{-\mathcal{H}_a^*} \left(1 - \Delta\mathcal{H}_a + \frac{1}{2}(\Delta\mathcal{H}_a)^2 - \cdots \right) \right\}$$

$$\left(\equiv e^{-\tilde{\mathcal{H}}_{ab}(\phi^l)} \right)$$

- We define Z_h and $\tilde{\mathcal{H}}_{ab}^*$ by

$$\text{(0th order term)} = \mathrm{Tr}\,' e^{-\mathcal{H}_a^*(\phi)} = Z_h \times e^{-\tilde{\mathcal{H}}_{ab}^*(\phi^l)}. \tag{1}$$

where the superscript l in ϕ^l is symbolic and reminder of the restriction that two operators cannot come closer than $\acute{a}$. (We also demand that $\tilde{\mathcal{H}}_{ab}^*$ will become back to $\mathcal{H}_a^*$ after the rescaling, because $\mathcal{H}_a^*$ is the fixed-point Hamiltonian.)

The partial trace (1st order term)

$$e^{-\tilde{\mathcal{H}}_a} = \mathrm{Tr}'\left\{e^{-\mathcal{H}_a^*}\left(1 - \Delta\mathcal{H}_a + \frac{1}{2}(\Delta\mathcal{H}_a)^2 - \cdots\right)\right\} \qquad \left(\Delta\mathcal{H}_a \equiv \sum_\alpha g_\alpha \int_a d\mathbf{x}\,\phi_\alpha(\mathbf{x})\right)$$

- Because of the absense of interaction, the 1st order term is easy:

$$\begin{aligned}
(\text{1st-order term}) &= -\mathrm{Tr}'e^{-\mathcal{H}_a^*(\phi)} \sum_\alpha g_\alpha \int_a d\mathbf{x}\,\phi_\alpha(\mathbf{x}) \\
&\overset{(*)}{=} -Z_h e^{-\tilde{\mathcal{H}}_{ab}^*(\phi')} \sum_\alpha g_\alpha \int_{ab} d\mathbf{x}\,\phi'_\alpha(\mathbf{x}) \\
&= -Z_h e^{-\tilde{\mathcal{H}}_{ab}^*(\phi')} \Delta\mathcal{H}_{ab}(\phi')
\end{aligned} \qquad (2)$$

In $(*)$, we have used

$$\mathrm{Tr}'\left[e^{-\mathcal{H}_a^*(\phi)} Q(\phi)\right] = Z_h e^{-\tilde{\mathcal{H}}_{ab}^*(\phi')} Q(\phi')$$

The partial trace (2nd order term)

$$e^{-\tilde{\mathcal{H}}_a} = \mathop{\mathrm{Tr}}_{\phi^h} \left\{ e^{-\mathcal{H}_a^*} \left(1 - \Delta\mathcal{H}_a + \frac{1}{2}(\Delta\mathcal{H}_a)^2 - \cdots \right) \right\} \qquad \left(\Delta\mathcal{H}_a \equiv \sum_\alpha g_\alpha \int_a d\mathbf{x}\, \phi_\alpha(\mathbf{x}) \right)$$

- For the 2nd-order term, we use OPE:

(2nd-order term)

$$= \frac{1}{2} \sum_{\alpha\beta} g_\alpha g_\beta \,\mathrm{Tr}' \left(e^{-\tilde{\mathcal{H}}_a^*} \int_a d\mathbf{x} d\mathbf{y}\, \phi_\alpha(\mathbf{x})\phi_\beta(\mathbf{y}) \right)$$

$$\mathrm{Tr}' \left(e^{-\tilde{\mathcal{H}}_a^*} \int_a d\mathbf{x} d\mathbf{y}\, \phi_\alpha(\mathbf{x})\phi_\beta(\mathbf{y}) \right) \Big/ \mathrm{Tr}' \left(e^{-\tilde{\mathcal{H}}_a^*} \right)$$

$$= \int_{|\mathbf{x}-\mathbf{y}|>ab} d\mathbf{x} d\mathbf{y}\, \phi_\alpha^l(\mathbf{x})\phi_\beta^l(\mathbf{y}) + \int_{a<|\mathbf{x}-\mathbf{y}|<ab} d\mathbf{x} d\mathbf{y}\, \phi_\alpha(\mathbf{x})\phi_\beta(\mathbf{y})$$

$$\approx \underbrace{\int_{ab} d\mathbf{x} d\mathbf{y}\, \phi_\alpha^l(\mathbf{x})\phi_\beta^l(\mathbf{y})}_{\text{"trivial term"}} + \underbrace{\int_{a<|\mathbf{x}-\mathbf{y}|<ab} d\mathbf{x} d\mathbf{y}\, \phi_\alpha(\mathbf{x})\phi_\beta(\mathbf{y})}_{\text{"collision term"}}$$

OPE for the collesion term

- For the collision term, we use OPE:

$$
\begin{aligned}
&\int_{a<|\mathbf{x}-\mathbf{y}|<ab} d\mathbf{x}d\mathbf{y}\,\phi_\alpha(\mathbf{x})\phi_\beta(\mathbf{y}) \\
&\quad\approx \int_{a<|\mathbf{x}-\mathbf{y}|<ab} d\mathbf{x}d\mathbf{y}\,\sum_\mu \frac{c_{\alpha\beta}^{\mu}}{a^{x_\alpha+x_\beta-x_\gamma}}\phi_\mu^l(\mathbf{x}) \\
&\quad= \int_{ab} d\mathbf{x}\,V_d((ab)^d - a^d)\sum_\mu \frac{c_{\alpha\beta}^{\mu}}{a^{x_\alpha+x_\beta-x_\gamma}}\phi_\mu^l(\mathbf{x}) \\
&\quad= V_d(b^d-1)\sum_\mu c_{\alpha\beta}^{\mu} a^{y_\alpha+y_\beta-y_\mu}\int_{ab} d\mathbf{x}\,\phi_\mu^l(\mathbf{x})
\end{aligned}
$$

The 2nd order term

- Putting together, the 2nd order term becomes

(2nd-order term)

$$= Z_h e^{-\tilde{\mathcal{H}}^*_{ab}} \frac{1}{2} \sum_{\alpha\beta} g_\alpha g_\beta \left\{ \int_{ab} d\mathbf{x} d\mathbf{y}\, \phi^l_\alpha(\mathbf{x}) \phi^l_\beta(\mathbf{y}) \right.$$

$$\left. + V_d (b^d - 1) \sum_\mu c^\mu_{\alpha\beta} a^{y_\alpha + y_\beta - y_\mu} \int_{ab} d\mathbf{x}\, \phi^l_\mu(\mathbf{x}) \right\}$$

$$= Z_h e^{-\tilde{\mathcal{H}}^*_{ab}} \left(\frac{1}{2} (\Delta \mathcal{H}_{ab}(\phi^l))^2 - \Delta \mathcal{H}^{(\mathrm{int})}_{ab} \right)$$

where

$$\Delta \mathcal{H}^{(\mathrm{int})}_{ab} \equiv -\frac{1}{2} \sum_{\alpha\beta\mu} g_\alpha g_\beta V_d (b^d - 1) \sum_\mu c^\mu_{\alpha\beta} a^{y_\alpha + y_\beta - y_\mu} \int_{ab} d\mathbf{x}\, \phi^l_\mu(\mathbf{x})$$

Summary of partial trace

- Finally, the partial trace results in

$$\mathrm{Tr}\,' e^{-\mathcal{H}^*_a(\phi)-\Delta\mathcal{H}_a(\phi)} \approx Z_h e^{-\tilde{\mathcal{H}}^*_{ab}(\phi^l)-\Delta\mathcal{H}_{ab}(\phi^l)-\Delta\mathcal{H}^{(\mathrm{int})}_{ab}(\phi^l)}$$

- Therefore, our Hamiltonian after the partial trace is

$$\begin{aligned}\tilde{\mathcal{H}}_{ab}(\phi^l) &= \tilde{\mathcal{H}}^*_{ab}(\phi^l) + \Delta\mathcal{H}_{ab}(\phi^l) + \Delta\mathcal{H}^{(\mathrm{int})}_{ab}(\phi^l) \\ &= \tilde{\mathcal{H}}^*_{ab}(\phi^l) + \sum_\mu g_\mu \int_{ab} d\mathbf{x}\,\phi^l_\mu(\mathbf{x}) \\ &\quad - \frac{1}{2}\sum_{\mu\alpha\beta} g_\alpha g_\beta V_d(b^d-1)c^\mu_{\alpha\beta}a^{y_\alpha+y_\beta-y_\mu}\int_{ab} d\mathbf{x}\,\phi^l_\mu(\mathbf{x}) \\ &= \tilde{\mathcal{H}}^*_{ab}(\phi^l) + \sum_\mu \tilde{g}_\mu \int_{ab} d\mathbf{x}\,\phi^l_\mu(\mathbf{x})\end{aligned}$$

where $\tilde{g}_\mu \equiv g_\mu - \frac{1}{2}\sum_{\mu\alpha\beta} g_\alpha g_\beta V_d(b^d-1)c^\mu_{\alpha\beta}a^{y_\alpha+y_\beta-y_\mu}$

Rescaling

- By $\acute{\mathbf{x}} \equiv b^{-1}\mathbf{x}$ and $\acute{\phi}_\mu(\acute{\mathbf{x}}) \equiv b^{x_\mu}\phi^l_\mu(\mathbf{x})$,

$$\acute{\mathcal{H}}_a(\acute{\phi}) = \mathcal{H}^*_a(\acute{\phi}) + \sum_\mu \tilde{g}_\mu \int_a d\acute{\mathbf{x}}\, b^{y_\mu}\acute{\phi}_\mu(\acute{\mathbf{x}})$$

$$\Rightarrow \quad \acute{g}_\mu = b^{y_\mu}\tilde{g}_\mu = b^{y_\mu}\left(g_\mu - \frac{1}{2}\sum_{\alpha\beta} c^\mu_{\alpha\beta} g_\alpha g_\beta V_d (b^d - 1) a^{y_\alpha + y_\beta - y_\mu} \right).$$

- By absorbing the factor $\frac{d}{2}V_d a^{y_\mu}$ in the definition of g_μ and $\acute{g}_\mu$,,

$$\acute{g}_\mu = b^{y_\mu} \times \left(g_\mu - \sum_{\alpha\beta} c^\mu_{\alpha\beta} g_\alpha g_\beta \frac{(b^d - 1)}{d} \right)$$

- By rewriting this equation using $\lambda \equiv \log b$, we finally obtain

$$\frac{dg_\mu}{d\lambda} = y_\mu g_\mu - \sum_{\alpha\beta} c^\mu_{\alpha\beta} g_\alpha g_\beta + O(g^3)$$

[9-2] Perturbative RG around GFP

- The criticality of the Ising model in $d > 4$ is controled by the Gaussian fixed-point, though the critical behavior is modified by the dangerously irrelevant field.
- For $d < 4$, the Gaussian fixed-point is not stable w.r.t. the scaling operator ϕ_4. This motivates us to look for another fixed point by examining the perturbative RG flow around the Gaussian fixed point.

Critical property of the Ising model above 4-dimensions

- Consider the ϕ^4 model.

$$\mathcal{H} = \int d\mathbf{x} \left(|\nabla \phi|^2 + t\phi^2 + u\phi^4 - h\phi \right)$$

- Let us consider the ϕ^2 and ϕ^4 terms as the perturbation to the Gaussian fixed point (GFP). Then, it is natural to express the Hamiltonian in terms of scaling operators at the GFP.

$$\mathcal{H} = \int d\mathbf{x} \left(|\nabla \phi|^2 + t\phi_2 + u\phi_4 - h\phi \right)$$

- The scaling eigenvalues for these terms are

$$x_2 = 2x = d - 2 \;\Rightarrow\; y_2 = d - x_2 = 2$$
$$x_4 = 4x = 2(d-2) \;\Rightarrow\; y_4 = d - x_4 = 4 - d.$$

- Since ϕ_4 is irrelevant if $d > 4$, the critical behavior of the ϕ^4 model (and therefore the Ising model as well) is described by the GFP.

Dangerous irrelevant operator for $d > 4$

- According to the general argument (see Lecture 7), the spontaneous magnetization should have the singularity like

$$m \propto L^{-d+y_h} = L^{-x_h} \propto (t^{-\frac{1}{y_t}})^{-x_h} = t^{\frac{d-2}{4}}. \quad \text{(wrong)}$$

- However, we saw that the mean-field theory correctly describes the critical behavior for $d > 4$ (Ginzburg criterion), which means that

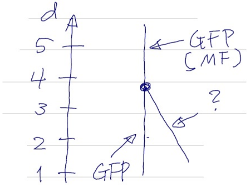
$$m \propto t^{\frac{1}{2}}. \quad \text{(correct)}$$

- This apparent contradiction comes from the nature of the irrelevant field u. Specifically, since the ϕ^4 model at or below the critical point ($t \leq 0$) is not well-defined when $u = 0$, we cannot simply put $u = 0$ in the scaling form as we did in the general argument.

Perturbative RG around GFP

- We have derived the general RG flow equation around a fixed-point.

$$\frac{dg_\mu}{d\lambda} = y_\mu g_\mu - \sum_{\alpha\beta} c^\mu_{\alpha\beta} g_\alpha g_\beta \qquad (3)$$



- If we apply this to GFP, we immediately notice that, for $d > 4$, there is only one relevant field t, implying that the GFP is the controling fixed point.
- Even below four dimensions, we may be able to obtain a new fixed point from (3) if it is near the GFP.
- In other words, we may try to find g_μ that makes the r.h.s. of (3) zero and deduce its properties from (3). (Next lexture)

Summary

- We have derived a set of equations describing RG flow around a given fixed point.
- We can obtain the renormalized Hamiltonian up to the 2nd order (or more if we try harder) in the case of GFP, which is the lowest non-trivial order.
- Above four dimensions, the critical point is controled by the Gaussian fixed point.
- However, the dangerously irrelevant field, u, modifies the critical behaviors to mean-field like.
- Below four dimensions, the critical point is not controled by the Gaussian fixed point because u becomes relevant.
- We may be able to find the "true" fixed point by analyzing the RG flow equation. (Next lecture)

Exercise

- We saw an apparent contradiction between the general scaling argument and the mean-field behaviors expected from the Ginzburg criterion. Think of a scaling form of the singular part of the free energy that obeys the scaling properties expected from the general argument, and, at the same time, produces the correct mean-field critical behaviors.

Lecture 10: ϵ-expansion and Wilson-Fisher fixed point

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In this lecture, we see ...

- By applying the perturbative RG to GFP, we will find a new fixed point near the GFP. (Wilson-Fisher fixed point (WFFP))
- By replacing the GFP and the WFFP by their multi-component counterparts, we can obtain the ϵ-expansion of the universality classes of the XY model ($n = 2$) and of the Heisenberg model ($n = 3$).

[10-1] Wilson-Fisher fixed point

- By inspecting the RG flow equation around GFP, we can obtain an $\epsilon(\equiv 4 - d)$ dependent fixed point and its scaling properties to the first order in ϵ (ϵ-expansion).
- From this result one can obtain the lowest order approximation to the Wilson-Fisher fixed point, which is suppose to (exactly) describe the Ising universality class in dimensions $2 < d < 4$.

RG flow equation around GFP

- Now, we are ready to actually compute the RG flow around the GFP searching for a new fixed point for the ϕ^4 model.

- Our tool is the RG flow equation around a fixed point.

$$\frac{dg_n}{d\lambda} = y_n g_n - \sum_{lm} c^n_{lm} g_l g_m + O(g^3) \quad (\lambda \equiv \log b) \tag{1}$$

- For the GFP, we already know

$$\phi_n \equiv [\![\phi^n]\!], \quad y_n = d - x_n, \quad x_n = nx = \frac{n}{2}(d-2)$$
$$c^n_{lm} \equiv \binom{l}{k}\binom{m}{k} k! \quad \left(k \equiv \frac{l+m-n}{2}\right) \tag{2}$$

The Z_2 symmetry

- Let us focus on the relevant fields at the GFP:

$$h \equiv g_1, \quad t \equiv g_2, \quad v \equiv g_3, \quad u \equiv g_4$$

- Note that (1) and (2) ensures that when we start with even fields only, odd fields are not generated by the RGT.
- In addition, we know that the critical point of the Ising model possesses the symmetry with respect to $S \leftrightarrow -S$.
- Therefore, we expect that the fixed point representing the Ising criticality should be found in the "even parity" manifold, i.e., $h = v = 0$.

ϵ-expansion

- In terms of the remaining fields, t and u, the flow equations are

$$\frac{dt}{d\lambda} = y_t t - c^t_{tt} t^2 - 2c^t_{tu} tu - c^t_{uu} u^2 + O(g^3) \qquad (3)$$

$$\frac{du}{d\lambda} = y_u u - c^u_{tt} t^2 - 2c^u_{tu} tu - c^u_{uu} u^2 + O(g^3) \qquad (4)$$

with $y_t = 2$ and $y_u = 4 - d \equiv \epsilon$.

- Hereafter, we regard ϵ as a small quantity.

- Let (t^*, u^*) be the non-trivial solution to the fixed-point equation, i.e., they are not zero and make the RHSs of (3) and (4) zero.

- By considering the order in ϵ, we see $t^* = O(\epsilon^2)$ and $u^* = O(\epsilon)$.
  ($\because$ By perturbation assuption, both u^* and t^* are small. Then, in (3), the only term that can possibly be the same order as t is u^2. Therefore, $t^* \sim {u^*}^2$. With this in mind, inspecting (4) we see that ϵu must be comparable to u^2, so $u^* \sim O(\epsilon)$.)

Wilson-Fisher fixed point

- Now, only keeping the terms that can make difference, we obtain

$$\frac{dt}{d\lambda} = 2t - 96u^2 - 24tu \quad (\equiv A) \tag{5}$$

$$\frac{du}{d\lambda} = \epsilon u - 72u^2 - 16tu \quad (\equiv B) \tag{6}$$

$$\left(c^t_{uu} = \binom{4}{3}\binom{4}{3} 3! = 96, \quad c^u_{uu} = \binom{4}{2}\binom{4}{2} 2! = 72, \quad \text{etc.} \right)$$

- Then, the fixed point is

$$(t^*, u^*) = \left(\frac{\epsilon^2}{108}, \frac{\epsilon}{72} \right) \tag{7}$$

- We regard this as the lowest order approximation to the new fixed point that we've been seeking for. (Wilson-Fisher fixed point (WFFP))

Linearization around the WFFP

- To obtain the scaling properties of the WFFP, we need to re-expand the series-expansion around the WFFP.
- So, let us define

$$\Delta u \equiv u - u^*$$
$$\Delta t \equiv t - t^*$$

and recast (5) and (6) in the form $\frac{d}{d\lambda}\begin{pmatrix}\Delta t \\ \Delta u\end{pmatrix} = Y \begin{pmatrix}\Delta t \\ \Delta u\end{pmatrix}$.

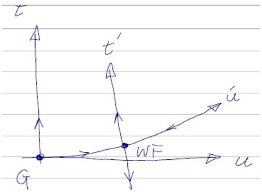
- Obviously, the matrix Y can be obtained as

$$Y \equiv \begin{pmatrix} \frac{\partial A}{\partial t} & \frac{\partial A}{\partial u} \\ \frac{\partial B}{\partial t} & \frac{\partial B}{\partial u} \end{pmatrix}_{\Delta t = \Delta u = 0} = \begin{pmatrix} 2 - 24u^* & -192u^* \\ -16u^* & \epsilon - 144u^* \end{pmatrix}$$
$$= \begin{pmatrix} 2 - \frac{1}{3}\epsilon & -\frac{8}{3}\epsilon \\ -\frac{2}{9}\epsilon & -\epsilon \end{pmatrix}.$$

Scaling properties of the WFFP

- Thus, the linearized RG flow equation around the new fixed point is

$$\frac{d}{d\lambda}\begin{pmatrix}\Delta t\\ \Delta u\end{pmatrix} = \begin{pmatrix}2-\frac{1}{3}\epsilon & -\frac{8}{3}\epsilon\\ -\frac{2}{9}\epsilon & -\epsilon\end{pmatrix}\begin{pmatrix}\Delta t\\ \Delta u\end{pmatrix}.$$



- Since the off-diagonal elements do not contribute to the eigenvalues to $O(\epsilon)$,

$$y_u^{\mathrm{WF}} = -\epsilon \quad \text{and} \quad y_t^{\mathrm{WF}} = 2 - \frac{\epsilon}{3}$$

- The "t-like" scaling field is relevant.

$$y_t^{\mathrm{3DWF}} \approx 1.666\cdots \quad \left(y_t^{\mathrm{3DIsing}} \approx 1.59,\right)$$

$$y_t^{\mathrm{2DWF}} \approx 1.333\cdots \quad \left(y_t^{\mathrm{2DIsing}} = 1\right)$$

Scaling eigenvalue of h at WFFP

- Writing down the RG flow equation for h, which has been neglected so far,

$$\frac{dh}{d\lambda} = y_h h - 2c_{th}^h th + (u^2 h\text{-term}) = \frac{d+2}{2}h - 4th + \cdots$$
$$\approx \left(\frac{d+2}{2} - 4t^* + \cdots \right) h$$

- Therefore, $y_h^{\mathrm{WF}} = \dfrac{d+2}{2} + O(\epsilon^2)$. In other words,

$$\eta^{\mathrm{WF}} = 2x_h^{\mathrm{WF}} - d + 2 = d + 2 - 2y_h^{\mathrm{WF}} = 0 + O(\epsilon^2).$$

This should be compared with

$$\eta^{\mathrm{3dIsing}} = 0.022(3) \quad \text{and} \quad \eta^{\mathrm{2dIsing}} = 0.25$$

Irrelevancy of other operators

- Even if some field is irrelevant at the GFP, it may turn relevant at the WFFP. If so, it alters the final destination of the RG flow, in which case the WFFP is not the contoring FP.
- The RG flow equation for g_n around the GFP is

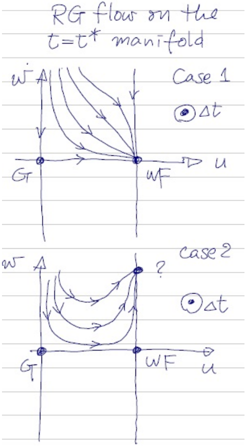
$$\frac{dg_n}{d\lambda} = \left(d - \frac{n}{2}(d-2)\right) g_n - 12n(n-1)ug_n,$$

- Remembering that $u^* = \epsilon/72$,

$$y_n^{\mathrm{WF}} = \left(d - \frac{n}{2}(d-2)\right) - 12n(n-1)\frac{4-d}{72}$$

- For $n \geq 6$, we have negative y_n:

$$y_n^{\mathrm{WF}} = \frac{18-2n-n^2}{6}\ (d=3), \frac{6+n-n^2}{3}\ (d=2).$$



[10-2] $O(n)$ models

- To apply the perturbative RG to the XY (O(2)) and the Heisenberg (O(3)) models we will introduce the multi-component ϕ^4 model.
- We can then construct the RG flow equation as before.

Multi-component ϕ^4 model

- Let us apply the perturbative RG to the XY (O(2)) or the Heisenberg (O(3)) models.
- To follow the same line of argument as before, we need something analogous to the ϕ^4 model to start with.
- So, let us consider multi-component field

$$\boldsymbol{\phi}(\mathbf{x}) \equiv \left(\phi^1(\mathbf{x}), \phi^2(\mathbf{x}), \cdots, \phi^n(\mathbf{x})\right)^{\mathsf{T}}$$

  and the multi-component ϕ^4 model:

$$\mathcal{H} \equiv \int d\mathbf{x} \left(|\nabla\boldsymbol{\phi}|^2 + t\boldsymbol{\phi}^2 + u(\boldsymbol{\phi}^2)^2 - h\phi^1\right)$$

- If $t = u = h = 0$, the n-components are independent and each represents a Gaussian fixed point. Therefore, it is a fixed point for the new Hamiltonian. (We call this fixed point the GFP, too.)

Correlation functions

- To get familiarized with the new model, let us consider $\langle \phi^2(\mathbf{x})\phi^2(\mathbf{y})\rangle_{\mathrm{GFP}}$.
- Since we can use Wick's theorem for the multi-component GFP,

$$
\begin{aligned}
&\langle \phi^2(\mathbf{x})\phi^2(\mathbf{y})\rangle \\
&\quad = \langle \phi^\alpha(\mathbf{x})\phi^\alpha(\mathbf{x})\phi^\beta(\mathbf{y})\phi^\beta(\mathbf{y})\rangle \quad \text{(Einstein's convention)} \\
&\quad = \langle \phi^\alpha(\mathbf{x})\phi^\alpha(\mathbf{x})\rangle\langle \phi^\beta(\mathbf{y})\phi^\beta(\mathbf{y})\rangle \\
&\qquad + 2\langle \phi^\alpha(\mathbf{x})\phi^\beta(\mathbf{y})\rangle\langle \phi^\alpha(\mathbf{x})\phi^\beta(\mathbf{y})\rangle \\
&\quad = n^2 G^2(0) + 2nG^2(r)
\end{aligned}
$$

where $r \equiv |\mathbf{x} - \mathbf{y}|$ and $G(r) \equiv \langle \phi^1(\mathbf{x})\phi^1(\mathbf{y})\rangle \approx r^{-2x}$ as usual.

Diagramatic representation

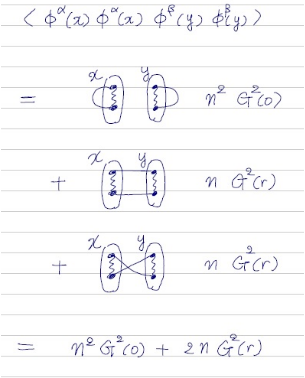
- We have seen that

$$\langle \phi^2(\mathbf{x})\phi^2(\mathbf{y})\rangle = n^2 G^2(0) + 2nG^2(r)$$

- Compared with the previous case of $n = 1$, the difference is the factors n^2 and n.
- For a given pattern of Wick paring, draw the diagram like the one in the right:

wavy lines	$\leftrightarrow$	repeated indices
regular lines	$\leftrightarrow$	Wick paring

- To the term represented by a diagram with g loops, we assign the factor n^g.



Scaling operator ϕ_2

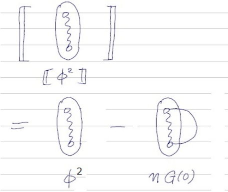
- As before, we can define the normal-order product, $\llbracket \cdots \rrbracket$, as the operator that we obtain after removing all contributions from the diagrams with inner connections.
- For example,

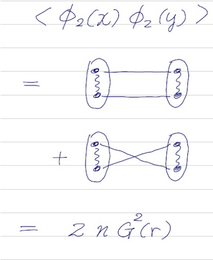
$$\phi_2 \equiv \left\llbracket \phi^2 \right\rrbracket = \phi^2 - nG^2(0)$$

- For the correlator of two ϕ_2s, we have

$$\langle \phi_2(\mathbf{x})\phi_2(\mathbf{y})\rangle = 2nG^2(r)$$

(See the diagram on the right.)





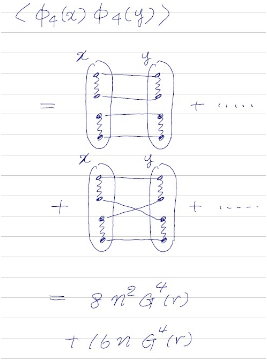
Scaling operator ϕ_4

- Similarly, we define ϕ_4 as

$$\phi_4(\mathbf{x}) \equiv \left[\!\left[\left(\phi^2(\mathbf{x})\right)^2 \right]\!\right]$$

- Then, the correlator becomes

$$\begin{aligned}
&\langle \phi_4(\mathbf{x})\phi_4(\mathbf{y})\rangle \\
&\quad = (\text{Two-loop terms}) \\
&\qquad + (\text{One-loop terms}) \\
&\quad = 8n^2 G^4(r) + 16nG^4(r) \\
&\quad = (8n^2 + 16n)G^4(r)
\end{aligned}$$



$c^u_{tt}, c^t_{tt}, c^u_{tu}, c^t_{tu}$ for $O(n)$ GFP

- First, let us expand $\phi_2(\mathbf{x})\phi_2(\mathbf{y})$.

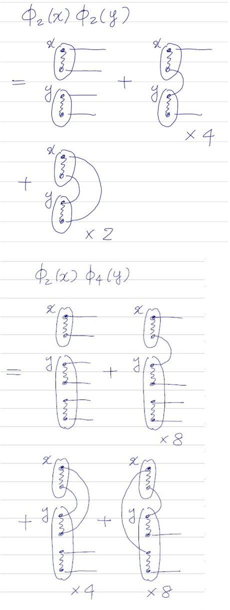
$$\phi_2(\mathbf{x})\phi_2(\mathbf{y}) \approx \phi_4(\mathbf{x}) + 4G(r)\phi_2(\mathbf{x}) + \cdots .$$

Thus, we obtain $c^u_{tt} = 1$ and $c^t_{tt} = 4$.

- For $\phi_2(\mathbf{x})\phi_4(\mathbf{y})$, we obtain

$$\begin{aligned}\phi_2(\mathbf{x})\phi_4(\mathbf{y}) &= \phi_6(\mathbf{x}) + 8G(r)\phi_4(\mathbf{x}) \\ &\quad + 4nG^2(r)\phi_2(\mathbf{x}) + 8G^2(r)\phi_2(\mathbf{x}) \\ &= \phi_6 + 8G\phi_4 + (4n+8)G^2\phi_2 + \cdots .\end{aligned}$$

We obtain $c^u_{tu} = 8$ and $c^t_{tu} = 4(n+2)$.



Wilson-Fisher FP for $O(n)$ GFP

- The RG flow equation is

$$\begin{cases} \frac{dt}{d\lambda} &= 2t - 32(n+2)u^2 - 8(n+2)tu & \equiv A \\ \frac{du}{d\lambda} &= \epsilon u - 8(n+8)u^2 - 16tu & \equiv B \end{cases}$$

$$\Rightarrow \ (t^*, u^*) = \left(\frac{\epsilon^2}{4(n+8)^2}, \frac{\epsilon}{8(n+8)} \right)$$

- The flow equation for t around WFFP is

$$\frac{dt}{d\lambda} = (2 - 8(n+2)u^*)t \quad \Rightarrow \quad y_t^{\mathrm{WF}} = 2 - \frac{n+2}{n+8}\epsilon$$

- For h, we have

$$\frac{dh}{d\lambda} = (y_h^{\mathrm{G}} + O(\epsilon^2))h = \frac{d+2}{2}h$$

$$\Rightarrow \quad y_h^{\mathrm{WF}} = \frac{d+2}{2} = 3 - \frac{\epsilon}{2}$$

ϵ-expansion summary

		Ising ($n=1$)		XY ($n=2$)		Heisenberg ($n=3$)	
		ϵ-exp.	true	ϵ-exp.	true	ϵ-exp.	true
4D	y_t	2	2	2	2	2	2
	y_h	3	3	3	3	3	3
3D	y_t	1.67	1.59	1.60	1.49	1.55	1.41
	y_h	2.5	2.48	2.5	2.48	2.5	2.49
2D	y_t	1.33	1	1.20	—	1.09	—
	y_h	2.0	1.875	2.0	—	2.0	—

Summary

- By applying the perturbative RG to GFP, we have found a new fixed point near the GFP. (Wilson-Fisher fixed point (WFFP))
- We can apply the same perturbative argument to the n-component field ϕ, resulting in the ϵ-expansion of the universality classes of the XY model ($n = 2$) and of the Heisenberg model ($n = 3$). In 3D, the estimates of scaling dimesnions were surprisingly good, whereas even in 2D, they are not so far from the correct values.

Homework

- Obtain the OPE of $\phi_u(\mathbf{x})\phi_u(\mathbf{y})$ at the GFP, and show that

$$c_{uu}^{u} = 8(n+8) \quad \text{and} \quad c_{uu}^{t} = 32(n+2)$$

Lecture 11: Magnetic Anisotropies

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July 1, 2019

In this lecture, we see ...

- It is not only $O(n)$ models that we can study by considering the multiple-component field. We can deal with anisotropies as well.

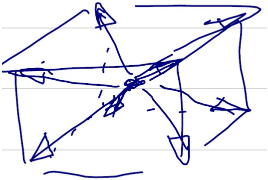
[11-1] Cubic anisotropy

- Real magnetic systems can never be truely isotropic because spins are coupled with orbital degrees of freedom that are subject to the influence of the lattice.
- In the case of the cubic lattice, for example, the localized spins feel the anisotropy field that has the same symmetry as the cubic lattice.

$$v\left((S_i^x)^4 + (S_i^y)^4 + (S_i^z)^4\right)$$

Decoupled Ising fixed point

- To understand why this term represents the effect of the cubic lattice, consider the case where $v \to \infty$. In this limit, the spin has to point to one of the corners of the unit cell (cube).
- Note that in this limit, the system becomes 3 decoupled Ising models. We will find a fixed point corresponding to this limit.



Scaling operators

- For the ϵ-expansion of the systems with the cubic symmetry, we consider $[\![\cdots]\!]$ of each term in the Hamiltonian.
- t-operator:

$$\phi_t \equiv \sum_\alpha [\![\phi^\alpha(\mathbf{x})\phi^\alpha(\mathbf{x})]\!]$$

- u-operator:

$$\phi_u \equiv \sum_{\alpha\beta} \left[\!\!\left[\phi^\alpha(\mathbf{x})\phi^\alpha(\mathbf{x})\phi^\beta(\mathbf{x})\phi^\beta(\mathbf{x})\right]\!\!\right]$$

- v-operator:

$$\phi_v \equiv \sum_\alpha [\![\phi^\alpha(\mathbf{x})\phi^\alpha(\mathbf{x})\phi^\alpha(\mathbf{x})\phi^\alpha(\mathbf{x})]\!]$$

OPE

- $\phi_t \phi_u \approx \cdots + 8\phi_u + 4(n+2)\phi_t + \cdots$

$$c_{tu}^t = 4(n+2), \quad c_{tu}^u = 8, \quad c_{tu}^v = 0$$

- $\phi_t \phi_v \approx \cdots + 8\phi_v + 12\phi_t + \cdots$

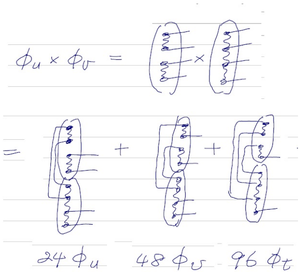
$$c_{tv}^t = 12, \quad c_{tv}^u = 0, \quad c_{tv}^v = 8$$

- $\phi_u \phi_v \approx \cdots + 24\phi_u + 48\phi_v + 96\phi_t + \cdots$

$$c_{uv}^t = 96, \quad c_{uv}^u = 24, \quad c_{uv}^v = 48$$

- $\phi_v \phi_v \approx \cdots + 72\phi_v + 96\phi_t + \cdots$

$$c_{vv}^t = 96, \quad c_{vv}^u = 0, \quad c_{vv}^v = 72$$



RG flow equation

- Keeping in mind that $u = O(\epsilon)$ and $t = O(\epsilon^2)$, as before, the part of the RG flow equation necessary for the lowest order discussion is

$$\begin{cases} \frac{dt}{d\lambda} & = A \equiv \quad 2t - 8(n+2)tu - 24tv + \cdots \\ \frac{du}{d\lambda} & = B \equiv \quad \epsilon u - 8(n+8)u^2 - 48uv + \cdots \\ \frac{dv}{d\lambda} & = C \equiv \quad \epsilon v - 96uv - 72v^2 + \cdots \end{cases}$$

  Note that we have omitted the terms, such as tu in B and u^2 in A, that would not contribute to y_t, y_u, y_v at the non-Gaussian FPs.

- We have four fixed points:
  1. [G] $(t, u, v) = (0, 0, 0)$
  2. [WF] $(t, u, v) = (t^*_{\mathrm{WF}}, u^*_{\mathrm{WF}}, 0)$
  3. [DI] $(t, u, v) = (t^*_{\mathrm{DI}}, 0, v^*_{\mathrm{DI}})$ ("decoupled Ising FP")
  4. [C] $(t, u, v) = (t^*_{\mathrm{C}}, u^*_{\mathrm{C}}, v^*_{\mathrm{C}})$ ("cubic FP")

Linearization

- In all cases, we have the same form of the linearized RG flow eqs. in terms of $\Delta\mathbf{u} \equiv (t - t^*, u - u^*, v - v^*)^{\mathrm{T}}$:

$$\frac{d\Delta\mathbf{u}}{d\lambda} = Y\Delta\mathbf{u}$$

$$\text{where} \quad Y \equiv \left(\begin{array}{ccc} \frac{\partial A}{\partial t} & \frac{\partial A}{\partial u} & \frac{\partial A}{\partial v} \\ \frac{\partial B}{\partial t} & \frac{\partial B}{\partial u} & \frac{\partial B}{\partial v} \\ \frac{\partial C}{\partial t} & \frac{\partial C}{\partial u} & \frac{\partial C}{\partial v} \end{array} \right)_{t^*,u^*,v^*}$$

$$\equiv \left(\begin{array}{ccc} 2 - 8(n+2)u^* - 24v^* & O(\epsilon) & O(\epsilon) \\ O(\epsilon) & \epsilon - 16(n+8)u^* - 48v^* & -48u^* \\ O(\epsilon) & -96v^* & \epsilon - 96u^* - 144v^* \end{array} \right)$$

- The lower-right 2×2 sub-matrix is important:

$$\frac{\partial(B,C)}{\partial(u,v)} = \left(\begin{array}{cc} \epsilon - 16(n+8)u^* - 48v^* & -48u^* \\ -96v^* & \epsilon - 96u^* - 144v^* \end{array} \right)$$

"WF" $\cdots$ $O(n)$ Wilson-Fisher FP

- Within the manifold of $v = 0$, obviously, all results will be the same as before:

$$t^*_{\mathrm{WF}} = \frac{\epsilon^2}{4(n+8)^2} \quad \text{and} \quad u^*_{\mathrm{WF}} = \frac{\epsilon}{8(n+8)} \; .$$

- The (u, v)-part of the Y matrix becomes

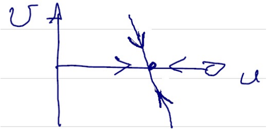
$$\frac{\partial(B, C)}{\partial(u, v)} = \epsilon \times \begin{pmatrix} -1 & -\frac{6}{n+8} \\ 0 & \frac{n-4}{n+8} \end{pmatrix}$$

- The eigenvalues and eigenvectors are

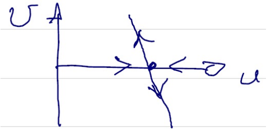
$$y_u^{\mathrm{WF}} \equiv -\epsilon \cdots \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad y_v^{\mathrm{WF}} = \frac{n-4}{n+8}\epsilon \cdots \begin{pmatrix} -1 \\ \frac{n+2}{3} \end{pmatrix}$$

- Therefore, we have $n_c \approx 4$ and the WFFP is stable if $n < n_c$.

Case 1: $n < n_c$



Case 2: $n > n_c$



"DI" $\cdots$ Decoupled Ising fixed point

- Remembering the RG flow equation for v, we find a FP with $u^* = 0$:

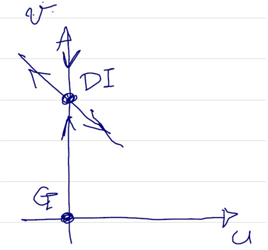
$$(u^*_{\mathrm{DI}}, v^*_{\mathrm{DI}}) = \left(0, \frac{\epsilon}{72}\right).$$

- The (u,v)-part of the Y matrix becomes

$$\frac{\partial(B,C)}{\partial(u,v)} = \begin{pmatrix} \epsilon - 48v^* & 0 \\ -96v^* & \epsilon - 144v^* \end{pmatrix}$$
$$= \epsilon \cdot \begin{pmatrix} 1/3 & 0 \\ -4/3 & -1 \end{pmatrix}$$

- The eigenvalues and eigenvectors are

$$y^{\mathrm{DI}}_u = \frac{\epsilon}{3} \cdots \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \quad y^{\mathrm{DI}}_t = -\epsilon \cdots \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$



"C" $\cdots$ Cubic fixed point

- Assuming $u, v = O(\epsilon)$ and $t = O(\epsilon^2)$,

$$(u_C^*, v_C^*) = \left(\frac{\epsilon}{24n}, \frac{(n-4)\epsilon}{72n} \right).$$

- The (u, v)-part of the Y matrix becomes

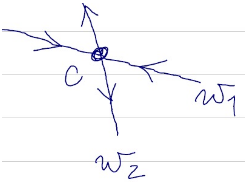
$$\frac{\partial(B, C)}{\partial(u, v)} = -\frac{\epsilon}{3n} \cdot \begin{pmatrix} n+8 & 6 \\ 4(n-4) & 3(n-4) \end{pmatrix}$$

- The eigenvalues and eigenvectors are

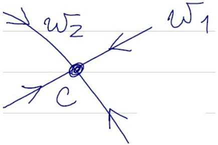
$$y_{w_1}^C = -\epsilon \quad \cdots \begin{pmatrix} 3 \\ n-4 \end{pmatrix},$$

$$y_{w_2}^C = -\frac{n-4}{3n}\epsilon \quad \cdots \begin{pmatrix} 1 \\ -2 \end{pmatrix}$$

Case 1: $n < n_c$



Case 2: $n > n_c$



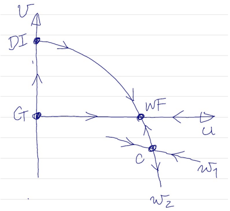
Global structure of RG flow

- Putting together, we can draw the RG flow diagram including the 4 fixed points.

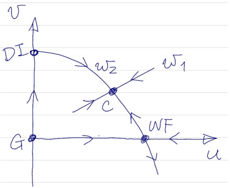
	$n < n_c$ $u^* > 0, v^* < 0$	$n > n_c$ $u^* > 0, v^* > 0$
G	$y_u > 0, y_v > 0$	$y_u > 0, y_v > 0$
WF	$y_u < 0, y_v < 0$	$y_u < 0, y_v > 0$
DI	$y_u > 0, y_v < 0$	$y_u > 0, y_v < 0$
C	$y_{w_1} < 0, y_{w_1} > 0$	$y_{w_2} < 0, y_{w_2} < 0$

- Depending on whether $n < n_c$ or $n > n_c$ we can draw two types of the diagram.
- So, after all the cubic anisotropy is irrelevant for real magnetic systems?

Case 1: $n < n_c$



Case 2: $n > n_c$



Nature of the transition in real magnets

- The value for n_c seems to be close to 3 in 3D. So, there has been a long-standing controversy about the nature of the ferromagnetic transition under the cubic anisotropy.
- According to [Varnashev: PRB 61 14660 (2000)] $n_c(d = 3) < 3$, or more specifically $n_c(d = 3) = 2.89(2)$.
- For general discussion see [Calabrese et al: arXiv:cond-mat/0509415].

Summary

- By representing the cubic anisotropy by the term $v \sum_\alpha (\phi_i^\alpha)^4$, we have constructed a field theory that may explain the effect of the lattice anisotropy on the spin systems that is otherwise symmetric.
- The ϵ-expansion of the ϕ^4 model with the v term produces a new fixed point. (Cubic fixed point)
- The cubic fixed point is stable for $n > n_c$ whereas it is unstable for $n < n_c$, where $n_c = 4 + O(\epsilon)$.
- According to a more sophisticated numerical estimate, n_c in 3D is slightly below 3, which suggests that we cannot simply neglect the cubic anisotropy in 3D.
- However, the critical region may be narrow in real systems due to smallness of the cubic anisotropy field and the proximity of n_c to 3.

Homework (submit your report at the next lecture)

- Consider the critical point of the Heisenberg model. Discuss the effect of the uniaxial symmetry breaking-field that is represented by adding the term

$$-D\left[(S_i^z)^2 - \frac{1}{2}((S_i^x)^2 + (S_i^y)^2)\right]$$

to the isotropic Hamiltonian, i.e., the regular Heisenberg model. (Consider the scaling dimension of the scaling operator that corresponds to the above operator, and obtain its scaling dimension at the Wilson-Fisher fixed point for $n = 3$, to the lowest order in ϵ.)

Lecture 12: Berezinskii-Kosterlitz-Thouless transition

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July 8, 2019

[12-1] XY model in two dimensions

- In two dimensions, continuous spin models cannot have magnetically ordered state. (Mermin-Wagner theorem)
- The XY model, however, has a strange type of phase transition that does not break the symmetry. (BKT transition)
- We can understand this transition by mapping the model into the Coulomb gas model. In this mapping, the spin vortices in the XY model corresponds to charges.
- By a RGT, we obtain Kosteritz's RG flow equation, that predicts special characters of the BKT transition.

Mermin-Wagner theorem

Theorem 1 (Mermin-Wagner(1966))

In two dimensions, if the system has a continuous symmetry (represnted by a compact connected Lie group), it cannot be spontaneously broken at any finite temperature. [Pfister, Commun. Math. Phys. 79 181 (1981).]

- Consider the XY model in two dimensions:

$$\mathcal{H} = -K \sum_{(ij)} \mathbf{S}_i \cdot \mathbf{S}_j = -K \sum_{(ij)} \cos(\theta_i - \theta_j)$$

  where $\mathbf{S}_i \equiv (\cos\theta_i, \sin\theta_i)^{\mathsf{T}}$.

- The XY model has the $U(1)$ symmetry with respect to the transformation $\theta_i \to \theta_i + \alpha$.
- Does the theorem prohibit the phase transition in the XY model?

Berezinskii-Kosterlitz-Thouless transition

- A theoretical proposal of a new type of phase transition without spontaneous symmetry breaking. (Berezinskii (1971), Kosterlitz-Thouless (1973))
- Later the predicted transition was discovered in a thin film experiment of superfluid He4. (Bishop-Reppy (1978))

Vortices

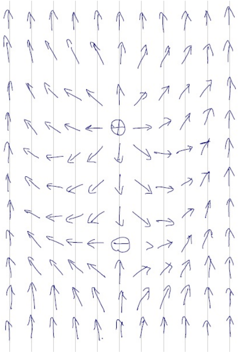
- A typical configuration of 2-component spins near or below the transition temperature consists of a smooth texture with vortices.
- The smooth texture allows the approximation,

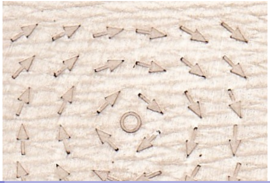
$$\cos(\theta_i - \theta_j) \approx 1 - \frac{1}{2} \left| \mathbf{r}_{ij} \cdot \nabla\theta \right|^2$$

- Therefore, we expect that the Hamiltonian is

$$\mathcal{H} = -Ka^d \sum_{(ij)} \cos(\theta_i - \theta_j)$$
$$\approx \frac{K}{2} \int d\mathbf{x} \left| \nabla\theta \right|^2 + \mu N_{\mathrm{v}}$$

where N_{v} is the total number of vortices.





Stationary configuration and fluctuation around it

- Here we introduce a new field variable ϕ that is the deviation of θ from its stationary solution Θ for a given vortex configurations:

$$\theta = \Theta + \phi.$$

- The configuration Θ is determined by the stationary condition, and it is a harmonic function.

$$0 = \delta E = \frac{K}{2} \int d\mathbf{x} \left\{ |\nabla(\Theta + \delta\Theta)|^2 - |\nabla\Theta|^2 \right\}$$
$$= K \int d\mathbf{x}\, \nabla\Theta \cdot \nabla\delta\Theta = -K \int d\mathbf{x}\, \triangle\Theta\delta\Theta$$

$$\Rightarrow \ \triangle\Theta = 0 \quad \text{(Except at vortices)}$$

- Note that Θ can be uniquely determined by the vortex configuration.

Vortex/fluctuation separation

- Using Θ, we can separate the vortices from the Gaussian fluctuation:

$$\mathcal{H} = \frac{K}{2} \int d\mathbf{x}\ |\nabla(\Theta + \phi)|^2 + \mu N_{\rm v} = \mathcal{H}_{\rm v} + \mathcal{H}_{\rm G}.$$

where

$$\mathcal{H}_{\rm v} \equiv \frac{K}{2} \int d\mathbf{x}\ |\nabla\Theta|^2 + \mu N_{\rm v}$$
$$\mathcal{H}_{\rm G} \equiv \frac{K}{2} \int d\mathbf{x}\ |\nabla\phi|^2$$

(Note that the term $\nabla\phi \cdot \nabla\Theta$ does not contribute because of the stationary condition for Θ.)

Vortex field Ω

- Since Θ is a harmonic function, another harmonic function Ω must exist such that $\dfrac{\partial \Omega}{\partial x} = -\dfrac{\partial \Theta}{\partial y}$, and $\dfrac{\partial \Omega}{\partial y} = \dfrac{\partial \Theta}{\partial x}$.
- Suppose a region Γ that includes a vortex.

$$I \equiv \oint_{\partial \Gamma} d\mathbf{l} \cdot \nabla \Theta = 2\pi q \quad (q = \pm 1, \pm 2, \cdots)$$

- Since $d\mathbf{l} \cdot \nabla \Theta = -d\mathbf{n} \cdot \nabla \Omega$,

$$\int_{\Gamma} d\mathbf{x} \, \triangle \Omega = \int_{\partial \Gamma} d\mathbf{n}(\mathbf{x}) \cdot \nabla \Omega = -I = -2\pi q \quad (\because \text{Gauss' theorem})$$

- Remembering that $\triangle \Omega = 0$ almost everywhere,

$$\triangle \Omega = -\sum_i 2\pi q_i \delta(\mathbf{x} - \mathbf{x}_i) = -2\pi \rho_{\mathrm{v}}(\mathbf{x})$$

Coulomb gas (1)

- Using Green's function, $G(\mathbf{x})$, that satisfies $\triangle G(\mathbf{x}) = -\delta(\mathbf{x})$, we can express Ω as

$$\Omega(\mathbf{x}) = 2\pi \int d\mathbf{y} G(\mathbf{x}-\mathbf{y})\rho_{\rm v}(\mathbf{y}).$$

- The vortex part in $\mathcal{H}_{\rm v}$ can be reformed as

$$\begin{aligned}
\frac{K}{2}\int d\mathbf{x}\,|\nabla\Theta|^2 &= \frac{K}{2}\int d\mathbf{x}\,|\nabla\Omega|^2 \\
&= -\frac{K}{2}\int d\mathbf{x}\,\Omega\,\triangle\Omega = \pi K \int d\mathbf{x}\,\Omega\rho_{\rm v} \\
&= 2\pi^2 K \int d\mathbf{x}d\mathbf{y}\,G(\mathbf{x}-\mathbf{y})\rho_{\rm v}(\mathbf{x})\rho_{\rm v}(\mathbf{y}) \\
&= 4\pi^2 K \sum_{(ij)} G(\mathbf{x}_i - \mathbf{y}_i) q_i q_j
\end{aligned}$$

Coulomb gas (2)

- Here we introduce the ultra-violet cut-off in the form of the constraint (on the region of the integral with respect to the vortex positions) that **no two vortices can be within the mutual distance of a.**

- Using

$$G(r) \approx -\frac{1}{2\pi} \log r$$

and the charge neutrality condition ($\sum_i q_i = 0$),

$$\mathcal{H}_{\rm v} = -2\pi K \sum_{(ij)} \log \frac{|\mathbf{x}_i - \mathbf{x}_j|}{\Lambda} q_i q_j + \mu N_{\rm v} \quad (\Lambda \text{ is arbutrary})$$

Vortices form a Coulomb-gas.

Grand partition function (J. M. Kosterlitz: J. Phys. C 7 1046 (1974))

- In what follows, we assume that $q_i = \pm 1$ since vortices $|q_i| > 1$ are energetically unfavorable and would not yield dominant contribution.
- $X_N \equiv (\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_N)$ and $Y_N \equiv (\mathbf{y}_1, \mathbf{y}_2, \cdots, \mathbf{y}_N)$ are the positions of positive and negative vortices, respectively.
- Then, the grand partition function is

$$\Xi(\zeta, g) = \sum_N \frac{\zeta^{2N}}{(N!)^2} Z_N^a(g) \quad (\zeta \equiv e^{\mu})$$

$$Z_N^a(g) \equiv \int_{\Omega(a)} dX_N dY_N \, e^{-gV_N(X_N, Y_N)} \quad (g \equiv 2\pi K)$$

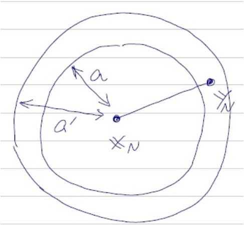
$$\Omega(a) \equiv \{ \ (X_N, Y_N) \mid \text{Any two elements are apart by more than } a \ \}$$

$$V_N(X_N, Y_N) \equiv -\sum_{(ij)} (v(\mathbf{x}_i, \mathbf{x}_j) + v(\mathbf{y}_i, \mathbf{y}_j)) + \sum_{ij} v(\mathbf{x}_i, \mathbf{y}_j)$$

$$v(\mathbf{x}, \mathbf{y}) \equiv \log(|\mathbf{x} - \mathbf{y}|/\Lambda)$$

Partial trace — Increasing the cut-off a

- Following the general program of the RGT, we first want to take the partial trace with respect to the short-scale degrees of freedom.
- We take the partial integral over the region $\Delta\Omega(a) \equiv \Omega(a) - \Omega(\acute{a})$ where $\acute{a} \equiv (1+\lambda)a$.
- The region consists of 3 components:



$$\Delta\Omega(a) \approx \sum_{ij} \Omega_{ij}^{+-}(\acute{a}) + \sum_{(ij)} (\Omega_{ij}^{++}(\acute{a}) + \Omega_{ij}^{--}(\acute{a}))$$

$$\Omega_{ij}^{+-}(\acute{a}) \equiv \{\ (X_N, Y_N) \in \Omega(a) \mid$$

All pairs are separated by more than $\acute{a}$,

except $a < |\mathbf{x}_i - \mathbf{y}_j| < \acute{a}$. $\}$

$$\Omega_{ij}^{++}(\acute{a}) \equiv \cdots$$

Partial trace — Dipole-mediated interaction

The contribution from Ω^{+-} should be dominant.

$$Z_N^a - Z_N^{\acute{a}} \approx \sum_{ij} \int_{\Omega_{ij}^{+-}(\acute{a})} dX_N dY_N \, e^{-gV_N} = N^2 \int_{\Omega_{NN}^{+-}(\acute{a})} dX_N dY_N \, e^{-gV_N}$$

$$= N^2 \int_{\Omega(\acute{a})} dX_{N-1} dY_{N-1} \, e^{-gV_{N-1}} \int_{a<|\mathbf{x}_N-\mathbf{y}_N|<\acute{a}} d\mathbf{x}_N d\mathbf{y}_N \; e^{-g\sum_i [\Delta v(\mathbf{x}_i) - \Delta v(\mathbf{y}_i)]}$$

$$(\Delta v(\mathbf{x}_i) \equiv v(\mathbf{x}_i, \mathbf{x}_N) - v(\mathbf{x}_i, \mathbf{y}_N))$$

$$\approx N^2 \int_{\Omega(\acute{a})} dX_{N-1} dY_{N-1} \, e^{-gV_{N-1}}$$

$$\times \int_{a<|\mathbf{x}_N-\mathbf{y}_N|<\acute{a}} d\mathbf{x}_N d\mathbf{y}_N \left\{ 1 + \frac{g^2}{2} \left(\sum_{i=1}^{N-1} (\Delta v(\mathbf{x}_i) - \Delta v(\mathbf{y}_i)) \right)^2 \right\}$$

$$\underset{(*)}{\approx} N^2 \int_{\Omega(\acute{a})} dX_{N-1} dY_{N-1} \, e^{-gV_{N-1}} \times \left(\cancel{2\pi a^2 \lambda L^2} + 4\pi^2 a^4 \lambda g^2 V_{N-1} \right)$$

(contribution to the regular part is omitted)

Partial trace — Screening effect

$$\Xi(\zeta, g) = \sum_N \frac{\zeta^{2N}}{(N!)^2} Z_N^a(g)$$

$$\approx \sum_N \frac{\zeta^{2N}}{(N!)^2} \left(Z_N^{\acute{a}}(g) + N^2 \int_{\Omega(\acute{a})} dX_{N-1} dY_{N-1}\, e^{-gV_{N-1}} \gamma g^2 \lambda V_{N-1} \right)$$

$$(\gamma \equiv 4\pi^2 a^4;\ (N-1) \to N)$$

$$= \sum_N \frac{\zeta^{2N}}{(N!)^2} \int_{\Omega(\acute{a})} dX_N dY_N\, e^{-gV_N} \left(1 + \gamma g^2 \lambda \zeta^2 V_N\right)$$

$$\approx \sum_N \frac{\zeta^{2N}}{(N!)^2} \int_{\Omega(\acute{a})} dX_N dY_N\, e^{-(g - \gamma g^2 \lambda \zeta^2) V_N}$$

The 2nd order perturbation screens the Coulomb interaction

Rescaling of the interaction

We rescale the length so that $\acute{a}$ comes back to a.

$$\acute{\mathbf{x}}_i = \frac{a}{\acute{a}} \mathbf{x}_i = e^{-\lambda} \mathbf{x}_i$$

By this replacement, the interaction becomes

$$\begin{aligned}
& V_N(X_N, Y_N) \\
&= -\sum_{(ij)} \left(\log \frac{\mathbf{x}_i - \mathbf{x}_j}{\Lambda} + \log \frac{\mathbf{y}_i - \mathbf{y}_j}{\Lambda} \right) + \sum_{ij} \log \frac{\mathbf{x}_i - \mathbf{y}_j}{\Lambda} \\
&= -\sum_{(ij)} \left(\log \frac{(\acute{\mathbf{x}}_i - \acute{\mathbf{x}}_j)}{\Lambda} + \log \frac{(\acute{\mathbf{y}}_i - \acute{\mathbf{y}}_j)}{\Lambda} + 2\lambda \right) + \sum_{ij} \left(\log \frac{(\acute{\mathbf{x}}_i - \acute{\mathbf{y}}_j)}{\Lambda} + \lambda \right) \\
&= V_N(\acute{X}_N, \acute{Y}_N) + (-N(N-1) + N^2)\lambda \\
&= V_N(\acute{X}_N, \acute{Y}_N) + N\lambda
\end{aligned}$$

Rescaling

Now, we can summarize the RGT as

$$
\begin{aligned}
&\Xi(\zeta, g) \\
&= \sum_N \frac{\zeta^{2N}}{(N!)^2} e^{2dN\lambda} \int_{\Omega(a)} d\acute{X}_N d\acute{Y}_N \, e^{-(g-\gamma g^2\zeta^2\lambda)V_N(\acute{X}_N,\acute{Y}_N)} e^{-gN\lambda} \\
&= \sum_N \frac{1}{(N!)^2} \left(\zeta e^{(d-\frac{g}{2})\lambda}\right)^{2N} \int_{\Omega(a)} dX_N dY_N \, e^{-(g-\gamma g^2\zeta^2\lambda)V_N(X_N,Y_N)} \\
&= \Xi(\acute{\zeta}, \acute{g}) \times e^{(\text{regular term})}
\end{aligned}
$$

where

$$
\zeta' = \zeta e^{\left(d-\frac{g}{2}\right)\lambda} \quad \text{and} \quad g' = g - \gamma g^2 \zeta^2 \lambda
$$

In the form of differential equations,

$$
\frac{d\zeta}{d\lambda} = \left(2 - \frac{g}{2}\right)\zeta \quad \text{and} \quad \frac{dg}{d\lambda} = -\gamma g^2 \zeta^2
$$

RG flow equation

It is convenient to use $x \equiv 2 - g/2$ instead of g, and focus on the vicinity of $x = \zeta = 0$.

$$\frac{d\zeta}{d\lambda} = x\zeta \quad \text{and} \quad \frac{dx}{d\lambda} = -\frac{1}{2}\frac{dg}{d\lambda} \approx 8\gamma\zeta^2$$

We can remove the factor 8γ by defining $y \equiv \sqrt{8\gamma}\zeta$:

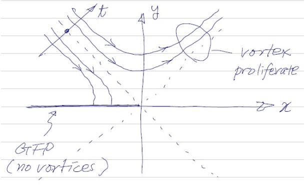
$$\begin{cases} \dfrac{dx}{d\lambda} = y^2 \\ \dfrac{dy}{d\lambda} = xy \end{cases} \qquad \begin{pmatrix} x = 2 - \pi K \\ y = (\text{const}) \times e^{\mu} \end{pmatrix} \qquad \text{(Kosterlitz's RG eq.)}$$

RG flow diagram

- The constant of motion of the RG equation

$$\frac{dx}{d\lambda} = y^2, \quad \frac{dy}{d\lambda} = xy$$

can be given by $t \equiv y^2 - x^2$.



- The value of t depends only on the initial values of the parameter, μ and $K = 1/T$. Schematically, the initial points are located on the t axis.

- There are two cases: $(t < 0)$ y goes to zero (no vortices) and $(t > 0)$ y goes to infinity (vortex proliferation). The separatorix, $t = 0$, corresponds to the BKT transition.

Solution and correlation length

- In the case where $t \equiv y^2 - x^2 > 0$, $\dfrac{dx}{d\lambda} = y^2 = t + x^2$. This equation has the solution $x(\lambda) = \sqrt{t}\tan\left(\sqrt{t}\,(\lambda - \lambda_0)\right)$.
- Note that $x_0 \equiv x(0) \sim -O(1)$, and $x(\log\xi) \sim O(1)$. ($\because$ In the initial state, there is no reason to assume that any one of the parameter is extremely large or small. The same is true for a system with the correlation length of $O(1)$.)
- The first condition means $\tan(\sqrt{t}\lambda_0) \sim \dfrac{1}{\sqrt{t}} \gg 1$, which is satisfied only when $\sqrt{t}\lambda_0 \sim \dfrac{\pi}{2}$, or, $\lambda_0 \sim \dfrac{\pi}{2\sqrt{t}}$.
- The second condition means $\log\xi - \lambda_0 \sim \dfrac{\pi}{2\sqrt{t}}$.
- From these we have

$$\xi \sim e^{\frac{\pi}{\sqrt{t}}} \sim \exp\left(\frac{\mathrm{const}}{\sqrt{T - T_c}}\right). \quad \text{(More divergent than any power-law)}$$

Correlation function below the transition temperature

- When $T < T_c$, the system flows to the vortex free states, i.e., it is asymptotically described by the Gaussian fixed-point Hamiltonian.

- Therefore, the 2-point correlation function is

$$\langle S^x(\mathbf{x})S^x(\mathbf{y}) + S^y(\mathbf{x})S^y(\mathbf{y})\rangle = \langle e^{i(\phi(\mathbf{x})-\phi(\mathbf{y}))}\rangle$$

$$= Z_{\mathrm{G}}^{-1} \int d\phi \, e^{-\frac{K}{2}\int d\mathbf{x}|\nabla\phi|^2 - i\boldsymbol{\omega}\cdot\boldsymbol{\phi}}$$

where $\omega(\mathbf{x}) \equiv 1,\ \omega(\mathbf{y}) \equiv -1$, and $\omega(\mathbf{r}) \equiv 0$ everywhere else.

- The lattice Lapracian is the inverse of the lattice Green function, $G(\mathbf{x},\mathbf{y}) = G(r) \sim -\frac{1}{2\pi}\log r$ +(const) $(r \equiv |\mathbf{x}-\mathbf{y}|)$. Therefore,

$$= Z_{\mathrm{G}}^{-1} \int d\phi \, e^{-\frac{K}{2}\boldsymbol{\phi}^{\mathsf{T}} G^{-1}\boldsymbol{\phi} - i\boldsymbol{\omega}\cdot\boldsymbol{\phi}}$$

$$= e^{-\frac{1}{2K}\boldsymbol{\omega}^{\mathsf{T}} G\boldsymbol{\omega}} = e^{-\frac{1}{K}(G(0)-G(r))} \propto r^{-\frac{1}{2\pi K}}.$$

Universal jump

- Thus, we have obtained the correlation function $\sim r^{-\eta}$ with

$$\eta = \frac{1}{2\pi K} = \frac{k_{\mathrm{B}} T}{2\pi J}.$$

This type of correlation is called “quasi-long-range order”.

- In particular, at the transition point, $K_c \equiv \frac{2}{\pi}$, the exponent takes a universal value, $\eta(K = K_c) = 1/4$.
- In the context of 2D superfluidity, the superfulid density ρ_{s} is, when it is finite, related to K as

$$K = \frac{\hbar^2 \rho_{\mathrm{s}}}{m k_{\mathrm{B}} T}$$

where m is the mass of a constituent particle. Therefore, ρ_{s} has a jump with a universal magnitude at the BKT transition.

Supplement: Screeing by dimers

$$I \equiv \int_{a<|\mathbf{x}_N-\mathbf{y}_N|<á} d\mathbf{x}d\mathbf{y} \sum_{ij} (\Delta v(\mathbf{x}_i) - \Delta v(\mathbf{y}_i))(\Delta v(\mathbf{x}_j) - \Delta v(\mathbf{y}_j))$$

- We use approximation
  $$\Delta v(\mathbf{r}) \equiv \log(\mathbf{r} - \mathbf{x}_N) - \log(\mathbf{r} - \mathbf{y}_N), \approx -\frac{\mathbf{x}_i - \mathbf{x}_N}{|\mathbf{x}_i - \mathbf{x}_N|^2} \cdot \mathbf{d}. \quad (\mathbf{d} \equiv \mathbf{y}_N - \mathbf{x}_N.)$$
- Consider a single term

$$I_{ij} \equiv \int_{a<|\mathbf{x}_N-\mathbf{y}_N|<á} d\mathbf{x}d\mathbf{y} \sum_{ij} \Delta v(\mathbf{x}_i)\Delta v(\mathbf{y}_i)$$

$$\approx \int d\mathbf{x}_N \int_{a<|\mathbf{d}|<á} d\mathbf{d} \left(\frac{\mathbf{x}_i - \mathbf{x}_N}{|\mathbf{x}_i - \mathbf{x}_N|^2} \cdot \mathbf{d} \right) \left(\frac{\mathbf{y}_i - \mathbf{x}_N}{|\mathbf{y}_i - \mathbf{x}_N|^2} \cdot \mathbf{d} \right)$$

$$= 2\pi a^4 \lambda \int d\mathbf{x}_N \frac{\mathbf{x}_i - \mathbf{x}_N}{|\mathbf{x}_i - \mathbf{x}_N|^2} \cdot \frac{\mathbf{y}_i - \mathbf{x}_N}{|\mathbf{y}_i - \mathbf{x}_N|^2}$$

Supplement: Screeing by dimers (2)

$$I_{ij}(\mathbf{x}_i, \mathbf{y}_j) \approx 2\pi a^4 \lambda \int d\mathbf{x}_N \, \frac{\mathbf{x}_i - \mathbf{x}_N}{|\mathbf{x}_i - \mathbf{x}_N|^2} \cdot \frac{\mathbf{y}_i - \mathbf{x}_N}{|\mathbf{y}_i - \mathbf{x}_N|^2}$$

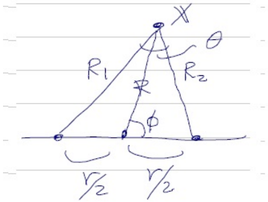
$$\underset{(*)}{\approx} 2\pi \log \frac{L}{|\mathbf{x}_i - \mathbf{y}_j|}$$

$$I = \sum_{ij} (I_{ij}(\mathbf{x}_i, \mathbf{x}_j) + I_{ij}(\mathbf{y}_i, \mathbf{y}_j) - I_{ij}(\mathbf{x}_i, \mathbf{y}_j) - I_{ij}(\mathbf{y}_i, \mathbf{x}_j))$$

$$= 2\pi a^4 \lambda \left[4\pi \left\{ \sum_{(ij)} (v(\mathbf{x}_i, \mathbf{x}_j) + v(\mathbf{y}_i, \mathbf{y}_j)) - \sum_{ij} v(\mathbf{x}_i, \mathbf{y}_j) \right\} \right]$$

$$= 8\pi^2 a^4 \lambda \times V_{N-1}(X_{N-1}, Y_{N-1})$$

Supplement: An integral formula



$$I \equiv \int d\mathbf{x}\, \frac{\cos\theta}{R_1 R_2}$$

$$= \int d\mathbf{x}\, \frac{R^2 - r^2/4}{((\frac{r}{2})^2 + R^2)^2 - r^2 R^2 \cos^2\phi}$$

$$I = \int_0^L dR\, R\, \frac{R^2 - r^2/4}{4}$$

$$\times \int_0^{2\pi} \frac{d\phi}{(r^2/4 + R^2)^2 - r^2 R^2 \cos^2\phi}$$

$$= \int_0^L dR \frac{2\pi R}{R^2 + r^2/4} = \pi \log \frac{L^2 + r^2/4}{r^2/4} \approx 2\pi \log \frac{L}{r}$$

We've used $\displaystyle \int_0^{2\pi} \frac{d\phi}{a + b\cos^2\phi} = \frac{2\pi}{\sqrt{a(a+b)}}$.

Summary

- The XY model is mapped to a composite system of vortices and fluctuations.
- The vortices behave as a 2D Coulomb gas.
- The fluctuations are governed by the massless Gaussian model.
- The RGT to the 2D Coulomb gas yields a set of RG flow equation.
- Above the transition temperature, the correlation length diverges as $\xi \sim \exp(c/\sqrt{T - T_c})$.
- Below the transition temperature, the system flows into the vortex-less Gaussian FP, where the spin-spin correlation obeys power-low with the exponent η varying with temperature.
- Its value is $1/4$ at the transition point. This means the universal jump in the superfluid density.