Lecture 3: ϕ^4 Theory

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Statistical Mechanics I: Lecture 3

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In this lecture we see ...

- The mean-field theory discussed in the previous section does not tell us about the spatial correlation because the variational Hamiltonian has trivial spatial structure, i.e., zero correlation among fluctuations in spins at different locations.
- In this lecture, starting from the Ising model, we derive the ϕ^4 model. While it inherits the same essential properties from the Ising model, it is defined with continuous degrees of freedom in contrast to the Ising spins.
- The advantage of the continuous degrees of freedom is that they allow as to define a variational Hamiltonian that has non-trivial spatial structure, which will be exploited in the next lecture.

ϕ^4 field theory

- We first see a very "hand-waving" derivation of the ϕ^4 field theory using the coarse-graining, starting from the Ising model.
- 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 particular, we expect, the 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.



Coarse-graining

- Let us consider the Ising model on the *d*-dimensional hyper-cubic lattice. (Hereafter, we use symbols like *x* and *y*, instead of *i* and *j*, to specify lattice points.)
- Divide the whole lattice into cells of size ab, where a is the lattice constant and b ≫ 1, and denote the cell located at X as Ω_b(X).
- Consider the "cell average" of spins $S_X \equiv \left(\frac{1}{b}\right)^d \sum_{x \in \Omega_b(X)} S_x$
- Consider the coarse-grained Hamiltonian $\mathcal{\tilde{H}}$ defined as

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

where $\phi \equiv \{\phi_X\}$, $S \equiv \{S_x\}$, and $\Delta(S|\phi) (=0,1)$ takes 1 if and only if $\phi_X = S_X$ at every X.

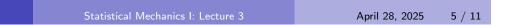
• Generally, the function $\tilde{\mathcal{H}}(\phi)$ is a very complicated one. So, we try to construct its simple approximation by intuition.

An intuitive approximation of $\tilde{\mathcal{H}}$

- $\tilde{\mathcal{H}}$ must have two parts: a single-cell part reflecting the physics inside each cell and a multiple-cell part for inter-cell interactions.
- The single-cell part itself consists of two parts: the energy and the entropy. The internal energy tends to align spins parallel to each other, giving rise to $-\phi^2$ term in $\tilde{\mathcal{H}}$, while the internal entropy favors $\phi \sim 0$ state, producing the terms like $+\phi^2$ and $+\phi^4$.
- For the multiple-cell part, since the total energy should be larger for large spatial inhomogeneity. It would be represented by terms like $(\nabla \phi)^2$, etc, while the odd order terms like $\nabla \phi$ should not appear because of the symmetry of the system.
- Putting these together and including the Zeeman term,

$$\tilde{\mathcal{H}}(\boldsymbol{\phi}) = \sum_{\boldsymbol{X}} \left(\rho |\nabla \phi|^2 + t \phi^2 + u \phi^4 - h \phi \right)$$

 $(\rho, u > 0.$ The sign of t depends on the temperature.)



Derivation by the Hubbard-Stratonovich transformation

$$Z_{\text{lsing}} = \sum_{S} e^{K \sum_{(\boldsymbol{x}, \boldsymbol{x}')} S_{\boldsymbol{x}} S_{\boldsymbol{x}'}} \propto \sum_{S} e^{\frac{K}{2} S^{\mathsf{T}} C S} \begin{pmatrix} c & (|\boldsymbol{x} - \boldsymbol{x}'| = 0) \\ 1 & (|\boldsymbol{x} - \boldsymbol{x}'| = a) \\ 0 & (\text{otherwise}) \end{pmatrix}$$

(... c must be large enough to make C positive definite. Otherwise, it's arbitrary.)
$$\sum_{S} \int_{S} |c| e^{-\frac{1}{2}} dt \sum_{S} |c|^{-1} dt + dt^{\mathsf{T}} S$$

$$\propto \sum_{S} \int D\psi \, e^{-\frac{1}{2K} \psi^{\mathsf{T}} C^{-1} \psi + \psi^{\mathsf{T}} S} \quad \dots \text{ HS transformation}$$
$$= \int D\psi \, e^{-\frac{1}{2K} \psi^{\mathsf{T}} C^{-1} \psi + \sum_{x} \log \cosh \psi_{x}} \quad \dots \text{ trace over } S$$
$$\propto \int D\phi \, e^{-\left(\frac{K}{2} \phi^{\mathsf{T}} C^{-1} \phi - \sum_{x} \log \cosh(K \phi_{x})\right)} \quad \dots \quad \phi \equiv K^{-1} \psi$$
$$= \int D\phi \, e^{-\mathcal{H}_{\mathsf{HS}}(\phi)}$$

$$\Rightarrow \quad \mathcal{H}_{\mathsf{HS}}(\boldsymbol{\phi}) = \frac{K}{2} \boldsymbol{\phi}^{\mathsf{T}} C^{-1} \boldsymbol{\phi} - \sum_{\boldsymbol{x}} \log \cosh(K \phi_{\boldsymbol{x}})$$

Relevant part of \mathcal{H}_{HS}

$$\mathcal{H}_{\mathsf{HS}}(\boldsymbol{\phi}) = \frac{K}{2} \boldsymbol{\phi}^{\mathsf{T}} C^{-1} \boldsymbol{\phi} - \sum_{\boldsymbol{x}} \log \cosh(K \phi_{\boldsymbol{x}})$$

For the first term, we see $C^{-1} = (cI + \Gamma)^{-1} = \frac{1}{c} \left(I - \frac{\Gamma}{c} + \cdots \right)$ where Γ is the connectivity matrix. Since Γ 's largest eigenvalue is z, the series converges exponentially for c > z. So, it may not be so bad to neglect non-linear terms:

$$\boldsymbol{\phi}^{\mathsf{T}} C^{-1} \boldsymbol{\phi} \approx \frac{1}{c} \boldsymbol{\phi}^{\mathsf{T}} \left(I - \frac{\Gamma}{c} \right) \boldsymbol{\phi} = \sum_{\boldsymbol{x}} \left(\frac{c-z}{c^2} \phi_{\boldsymbol{x}}^2 + \frac{1}{c^2} (\nabla \phi_{\boldsymbol{x}})^2 \right) \text{ (see supplement)}$$

For the log-cosh term, by expending it w.r.t. $K (\log \cosh(x) \approx x^2/2 - x^4/12)$, we obtain \mathcal{H}_{ϕ^4} as the relevant part of \mathcal{H}_{HS} (with $\rho \equiv \frac{K}{2c^2}$, $t \equiv \frac{K}{2}(\frac{c-z}{c^2} - K)$, $u \equiv \frac{K^4}{12}$):

$$\mathcal{H}_{\mathsf{HS}} \approx \mathcal{H}_{\phi^4} \equiv \sum_{\boldsymbol{x}} \left(\rho(\nabla \phi)^2 + t\phi^2 + u\phi^4 \right) \tag{1}$$

Note that t plays the role of the temperature, because it changes sign from positive to negative as the temperature decreases. Though the expansions used here may not be justified by the smallness of variables, they are justified by the renormalization group arguments as we see later.

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Supplement: Hubbard-Stratonovich transformation

For an arbitrary positive definite symmetric matrix A and a vector B, we can show the following,

$$\int D\psi \, e^{-\frac{1}{2} \sum_{x,x'} A_{x,x'} \psi_x \psi_{x'} + \sum_r B_r \psi_x} \\ = \int D\psi \, e^{-\frac{1}{2} \psi^{\mathsf{T}} A \psi + B^{\mathsf{T}} \psi} \\ = \int D\xi |A|^{-1/2} e^{-\frac{1}{2} \xi^{\mathsf{T}} \xi + \eta^{\mathsf{T}} \xi} \quad (\xi \equiv A^{1/2} \psi, \ \eta \equiv A^{-1/2} B) \\ = \int D\xi |A|^{-1/2} e^{-\frac{1}{2} (\xi - \eta)^2 + \frac{1}{2} (\eta)^2} \\ = (2\pi)^{\frac{N}{2}} |A|^{-1/2} e^{\frac{1}{2} (\eta)^2} = (2\pi)^{\frac{N}{2}} |A|^{-1/2} e^{\frac{1}{2} B^{\mathsf{T}} A^{-1} B}$$

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

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

Supplement: The connectivity matrix Γ and derivatives

In the derivation of the ϕ^4 action, we considered the inverse of $C \equiv cI + \Gamma$, i.e., $C^{-1} = \frac{1}{c} \left(I - \frac{\Gamma}{c} + \cdots \right)$ where Γ is the lattice connectivity matrix

 $\Gamma_{m{x}'m{x}}\equiv \left\{ egin{array}{cc} 1 & ({
m if}\ m{x}'\ {
m and}\ m{x}\ {
m are}\ {
m nearest}\ {
m nearest}\ {
m neighbors}
ight) \ 0 & ({
m othewise}) \end{array}
ight. .$

We used the follwoing formula:

$$\phi^{\mathsf{T}}\Gamma\phi = 2\sum_{(\boldsymbol{x}',\boldsymbol{x})} \phi_{\boldsymbol{x}'}\phi_{\boldsymbol{x}} = \sum_{(\boldsymbol{x}',\boldsymbol{x})} \left(\phi_{\boldsymbol{x}'}^2 + \phi_{\boldsymbol{x}}^2 - (\phi_{\boldsymbol{x}'} - \phi_{\boldsymbol{x}})^2\right)$$
$$= \frac{1}{2}\sum_{\boldsymbol{x},\boldsymbol{\delta}} \left(\phi_{\boldsymbol{x}+\boldsymbol{\delta}}^2 + \phi_{\boldsymbol{x}}^2 - (\phi_{\boldsymbol{x}+\boldsymbol{\delta}} - \phi_{\boldsymbol{x}})^2\right) = \sum_{\boldsymbol{x}} \left(z\phi_{\boldsymbol{x}}^2 - (\nabla\phi_{\boldsymbol{x}})^2\right)$$

where δ is a vector pointing to nearest neighbors, and $\nabla \phi_x$ is the lattice gradient vector. (It would correspond to the regular nabla operator in the limit of fine space discretization.)

What's ϕ ?

Remembering the HS transformation, for any real symmetric matrix A,

$$\begin{split} \langle \mathbf{S}^{\mathsf{T}} A \mathbf{S} \rangle_{\mathsf{lsing}} &= Z_{\mathsf{lsing}}^{-1} \left. \frac{\partial}{\partial \eta} \sum_{\mathbf{S}} e^{\frac{K}{2} \mathbf{S}^{\mathsf{T}} (C + \frac{2\eta}{K} A) \mathbf{S}} \right|_{\eta \to 0} \\ &= Z_{\mathsf{HS}}^{-1} \int D\phi \left. \frac{\partial}{\partial \eta} e^{-\left(\frac{K}{2} \phi^{\mathsf{T}} (C + \frac{2\eta}{K} A)^{-1} \phi - \sum_{\mathbf{x}} \log \cosh(K \phi_{\mathbf{x}})\right)} \right|_{\eta \to 0} \\ &= Z_{\mathsf{HS}}^{-1} \int D\phi \left. \frac{\partial}{\partial \eta} e^{-\left(\frac{K}{2} \phi^{\mathsf{T}} (C^{-1} - \frac{2\eta}{K} C^{-1} A C^{-1}) \phi - \sum_{\mathbf{x}} \log \cosh(K \phi_{\mathbf{x}})\right)} \right|_{\eta \to 0} \\ &= Z_{\mathsf{HS}}^{-1} \int D\phi \left. e^{-\left(\frac{K}{2} \phi^{\mathsf{T}} C^{-1} \phi - \sum_{\mathbf{x}} \log \cosh(K \phi_{\mathbf{x}})\right)} \phi^{\mathsf{T}} C^{-1} A C^{-1} \phi \right|_{\eta \to 0} \\ &= \langle \phi^{\mathsf{T}} C^{-1} A C^{-1} \phi \rangle_{\mathsf{HS}} \end{split}$$

This means that $C^{-1}\phi$ behaves the same way as S. In other words, ϕ_x is $\tilde{S}_x \equiv \sum_{x'} C_{xx'} S_{x'}$, i.e., a weighted sum of spins in a local cluster. (Thus, we have recovered something similar to the hand-waving derivation of the ϕ^4 theory.)

Exercise 3.1: 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 $\phi_1 \equiv \frac{1}{2}(S_1 + S_2)$ 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'.)

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