Lecture 4: Ornstein-Zernike Formula

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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.
- In the previous lecture, we derived the continuous version of the Ising model, i.e., ϕ^4 model.
- We can apply the GBF variational approximation to the ϕ^4 Hamiltonian, with the variational Hamiltonian that has a non-trivial spatial structure.
- As a result, we obtain the Ornstein-Zernike form for the correlation function.

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 mean-field approximation neglecting the special variance results in the same type of
- 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 ϕ^4 model in the discrete space,

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

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

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

(If you prefer continuous wave numbers, you could instead use $\mathcal{H} = \int \frac{d^d\boldsymbol{k}}{(2\pi)^d} (\rho k^2 + t) \tilde{\phi}^*_{\boldsymbol{k}} \tilde{\phi}_{\boldsymbol{k}} + u \int \frac{d^d\boldsymbol{k}_1 \cdots d^d\boldsymbol{k}_4}{(2\pi)^{4d}} \, \delta\left(\sum_\mu \boldsymbol{k}_\mu\right) \tilde{\phi}_{\boldsymbol{k}_1} \cdots \tilde{\phi}_{\boldsymbol{k}_4} - h\tilde{\phi}_{\boldsymbol{0}}$.)

Supplement: Convention (Fourier transformation)

In this lecture, we use the following conventions:

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

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

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

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

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

For translationally and rotationally symmetric case,

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

GBF variational approximation (1)

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

$$\mathcal{H}_0 \equiv \frac{1}{L^d}\sum_{\boldsymbol{k}} \epsilon_{\boldsymbol{k}} |\phi_{\boldsymbol{k}}|^2 \qquad (2)$$

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

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

$$E_0 = \frac{1}{L^d}\sum_{\boldsymbol{k}} \epsilon_{\boldsymbol{k}}\langle |\phi_{\boldsymbol{k}}|^2\rangle_0 = \sum_{\boldsymbol{k}} \frac{\epsilon_{\boldsymbol{k}}}{L^d}\frac{L^d}{2\epsilon_{\boldsymbol{k}}} = \sum_{\boldsymbol{k}} \frac{1}{2} = \frac{N}{2} \quad \text{“Equipartition”}$$

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

(Additive constants have been omitted.)

GBF variational approximation (2)

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

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

We have used $\langle \phi_{k'} \phi_k \rangle_0 = \delta_{k',-k} \langle |\phi_k|^2 \rangle_0$. In terms of $G_{\boldsymbol{k}} \equiv L^{-d} \langle |\phi_{\boldsymbol{k}}|^2 \rangle_0 = (2\epsilon_{\boldsymbol{k}})^{-1}$, we obtain

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

Thus we have, $\quad f_{\mathsf{v}} \equiv L^{-d} F_{\mathsf{v}} = B + 3uA^2 + \frac{1}{2L^d} \sum_{\boldsymbol{k}} \log \epsilon_{\boldsymbol{k}}, \qquad (3)$

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

Stationary condition

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

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

$\cdots$ Spatial fluctuation shifts the transition point.

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

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

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 $\mathcal{H} = \frac{1}{2}\boldsymbol{\phi}^\mathsf{T} A \boldsymbol{\phi}$ with A being a real positive-definite symmetric 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 $\langle \cdots \rangle \equiv \dfrac{\int D\boldsymbol{\phi}\, e^{-\mathcal{H}(\boldsymbol{\phi})} \ldots}{\int D\boldsymbol{\phi}\, e^{-\mathcal{H}(\boldsymbol{\phi})}}$

Supplement: Proof of Wick's theorem

If we define $\Xi \equiv \int D\boldsymbol{\phi}\, e^{-\frac{1}{2}\boldsymbol{\phi}^\mathsf{T} A\boldsymbol{\phi} + \boldsymbol{\xi}^\mathsf{T}\boldsymbol{\phi}}$, 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 $\Xi \propto e^{\frac{1}{2}\boldsymbol{\xi}^\mathsf{T}\Gamma\boldsymbol{\xi}}$, with $\Gamma \equiv A^{-1}$, which yields

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

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

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

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

$$= L^{-d}\sum_{\boldsymbol{k},\boldsymbol{k}'} e^{i\boldsymbol{k}'\boldsymbol{x}'}e^{i\boldsymbol{k}\boldsymbol{x}}\delta_{\boldsymbol{k}'+\boldsymbol{k},\boldsymbol{0}}G_{\boldsymbol{k}} = L^{-d}\sum_{\boldsymbol{k}} e^{-i\boldsymbol{k}(\boldsymbol{x}'-\boldsymbol{x})}\frac{1}{2\epsilon_{\boldsymbol{k}}}$$

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

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

($*$ $\cdots$ see supplement)

Mean-field values of ν and η

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

Mean-field value of ν

For $T > T_c$, $G(r) \propto \frac{1}{r^{\frac{d-1}{2}}}e^{-r/\xi}$, $\xi = \kappa^{-1} \propto \frac{1}{\sqrt{|T - T_c|}}$ $\Rightarrow \nu_{\rm MF} = \frac{1}{2}$

Mean-field value of η

At $T = T_c$, $G(r) \propto \frac{1}{r^{d-2}}$ $\Rightarrow \eta_{\rm MF} = 0$ $\left(G(r) \propto \frac{1}{r^{d-2+\eta}}\right)$

CF: $(\nu, \eta) = \begin{cases} (\ 0.5\ ,\ 0\ )\ (d \geq 4) \\ (\ 0.63002(10)\ ,\ 0.03627(10)\ )\ (d = 3) & (PRB82(2010), 174433) \\ (\ 1\ ,\ 0.25\ )\ (d = 2) \end{cases}$

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

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

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

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

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

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

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

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

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

As before, we have

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

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,

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

- It is, then, a little tedious but not hard to see that (3) is replaced by

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

where $m \equiv \langle \phi_{\boldsymbol{x}} \rangle_0$ and, as before,

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

Gaussian MF approximation below T_c (2)

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

$$t + 6uA + 2um^2 = 0$$

$$\text{or} \quad m^2 = -\frac{t + \sigma}{2u} \quad (\sigma \equiv 6uA) \qquad (5)$$

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

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

Using (5), $\epsilon_{\boldsymbol{k}} = \rho k^2 - 2(t + \sigma) = \rho(k^2 + \acute{\kappa}^2) \quad \left(\acute{\kappa}^2 \equiv \frac{-2(t + \sigma)}{\rho} \right)$

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

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

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

Supplement: Wick's theorem with symmetry-breaking field

For deriving (4), 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 $\delta\phi_{\boldsymbol{x}} \equiv \phi_{\boldsymbol{x}} - \langle\phi_{\boldsymbol{x}}\rangle_0$, not ϕ itself. In the momentum space, by defining $\delta\phi_{\boldsymbol{k}} \equiv \phi_{\boldsymbol{k}} - \bar{\phi}_{\boldsymbol{0}}\delta_{\boldsymbol{k}}$ ($\delta_{\boldsymbol{k}} \equiv \delta_{\boldsymbol{k},\boldsymbol{0}}$, $\bar{\phi}_{\boldsymbol{0}} = L^d m$),

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

Therefore, we obtain

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

Exercise 4.1: In the lecture, in obtaining the OZ form for the correlation function, we employed the variational Hamiltonian that has the form $L^{-d}\sum_{\boldsymbol{k}}\epsilon_{\boldsymbol{k}}|\phi_{\boldsymbol{k}}|^2 - \eta\phi_{\boldsymbol{k}=0}$. What if we used $\mathcal{H}_0 = \lambda\sum_{\boldsymbol{x}}(\phi_{\boldsymbol{x}} - m)^2$ instead? (Here, λ and m are variational parameters.) Obtain the equations of state that relates λ and m to ρ, t and u. For the sake of simplicity, consider the case where $h = 0$.

We apply the GBF inequality $F_{\mathrm{v}} \equiv F_0 + \langle\mathcal{H} - \mathcal{H}_0\rangle_0 \geq F$ to

$$
\mathcal{H} = \sum_{\boldsymbol{x}}(\rho(\nabla\phi)^2 + t\phi^2 + u\phi^4 - h\phi)
$$

and

$$
\mathcal{H}_0 = \lambda\sum_{\boldsymbol{x}}(\phi - m)^2.
$$

For F_0, we have

$$\beta F_0/N = -\log \int d\phi e^{-\lambda(\phi - m)^2} = \frac{1}{2}\log(\lambda/\pi).$$

For calculating $\langle \mathcal{H} \rangle_0$ and $\langle \mathcal{H}_0 \rangle_0$, we apply Wick's theorem to $\langle (\delta\phi)^n \rangle_0$ with $\delta\phi \equiv \phi - m$ and $\langle (\delta\phi)^2 \rangle_0 = 1/(2\lambda)$, to obtain,

$$\begin{aligned}
&\langle \phi \rangle_0 = m, \quad \langle \phi^2 \rangle_0 = \langle (m+\delta\phi)^2 \rangle_0 = m^2 + \langle \delta\phi^2 \rangle_0 = m^2 + \frac{1}{2\lambda}, \\
&\langle \phi^4 \rangle_0 = \langle (m+\delta\phi)^4 \rangle_0 = m^4 + 6m^2 \langle \delta\phi^2 \rangle_0 + \langle \delta\phi^4 \rangle_0 \\
&\qquad = m^4 + 6m^2 \langle \delta\phi^2 \rangle_0 + 3\langle \delta\phi^2 \rangle_0^2 = m^4 + \frac{3m^2}{\lambda} + \frac{3}{4\lambda^2}, \\
&\langle (\nabla\phi)^2 \rangle_0 = \frac{1}{2}\sum_\delta \langle (\phi_{r+\delta} - \phi_r)^2 \rangle_0 = \frac{z}{2}\langle \phi_{r+\delta}^2 + \phi_r^2 - 2\phi_{r+\delta}\phi_r \rangle_0 = \frac{z}{2\lambda} = \frac{d}{\lambda}.
\end{aligned}$$

Then, noting that β is included in the definition of the Hamiltonians and the free energy,

$$\frac{F_v}{N} = \frac{1}{2}\log\frac{\lambda}{\pi} + \left(\frac{d\rho}{\lambda} + \frac{t}{2\lambda} + \frac{3u}{4\lambda^2}\right) + \left(t + \frac{3u}{\lambda}\right)m^2 + um^4 - hm - \frac{1}{2}$$

From the stationary conditions, we obtain the mean-field type behaviors. Specifically, at $h = 0$,

$$\begin{aligned}
&m = 0,\ \lambda = d\rho + t - t_c \quad (t > t_c) \\
&m = \sqrt{(t_c - t)/6u},\ \lambda = d\rho \quad (t < t_c)
\end{aligned}$$

where $t_c \equiv -3u/\lambda$.

The same results can be obtained by working with the wave-number space instead of the real space. We substitute ϕ_k in $\mathcal{H}$ by $\phi_k \equiv \delta\phi_k + mL^d\delta_{k,0}$, and consider $\mathcal{H}_0 \equiv \lambda L^{-d}\sum_k \delta\phi_k$. One thing that needs a careful treatment the discrete nature of "∇". If we simply replace $(\nabla\phi)^2$ by $-k^2|\phi_k|^2$, as we usually do in the wave-number space calculation, the result would be slightl]y different from the real-space calculation (though the difference is merely quantitative, and not so essential). Since ∇ here is the difference rather than the differentiation, to be precise, we must use $\sum_{\alpha=1}^{d} 2(1-\cos k_\alpha)$ in the place of k^2. When we take the average of this term over the wave numbers in the 1st Brillouin zone, the cosine term yields zero, while the constant term yields $2d = z$, which is exactly the same as the coefficient ρ/λ term in the real-space calculation.