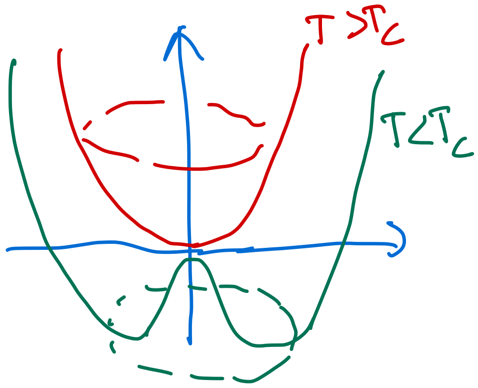
Lecture 5: Correlations in Gaussian approximation.

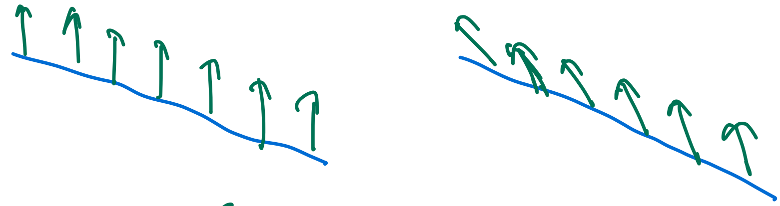
Partition function: $$Z = \int \mathcal{D}\vec{\phi}\, e^{-\beta F_L[\vec{\phi}]} \quad (*)$$

functional integral

When $F_L[\vec{\phi}]$ has discrete symmetry $\rightarrow$ domain walls
continuous symmetry $\rightarrow$ Goldstone modes / bosons

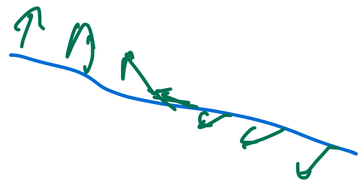


Intuition for goldstone modes



same energy

But there exists excitations that look like



that cost little energy by stretching the winding over longer and longer distances.

Examples
- Phase fluctuations in superfluids.
- Phonons
- Magnons.
- Schlieren texture in nematic liquid crystals.

Take for example $O(3)$ model:

$$F_L[\vec{m}] = \int d^d\vec{r} \left[\frac{K}{2} |\nabla \vec{m}|^2 + \frac{a}{2} |\vec{m}|^2 + \frac{b}{4} |\vec{m}|^4 \right]$$

and write $\vec{m} = m_0 (\cos\phi \sin\theta, \sin\phi \sin\theta, \cos\theta)$ $\quad \phi \in [0, 2\pi)$, $\theta \in [0, \pi)$

Then $$F_L[\vec{m}] = \int d^d\vec{r} \left[\frac{K}{2} |\nabla m_0|^2 + \frac{a}{2} m_0^2 + \frac{b}{4} m_0^4 + \frac{K}{2} m_0^2 \left[(\nabla\theta)^2 + \sin^2\theta (\nabla\phi)^2 \right] + \dots \right.$$

Two Goldstone modes. θ and ϕ and they interact.

Generally let's take effective Hamiltonian / Landau free energy that is invariant under symmetry group $\mathcal{G}$. Suppose $\mathcal{G}$ is spontaneously broken to H. Then the manifold of ground states is $\mathcal{G}/H$ and $\#\text{goldstones} = \dim \mathcal{G} - \dim H$.

<u>Example</u> O(N) model. $\mathcal{G} = O(N)$, $H = O(N-1)$

Ground state manifold: $\dfrac{O(N)}{O(N-1)} = S^{N-1}$

$\Rightarrow N-1$ goldstone modes.

This is consistent, since $\dim(O(N)) = \frac{1}{2}N(N-1)$

(Recall $O(N) = \{A \in \mathbb{R}^{N\times N} \mid A^T A = I\}$ $\rightarrow$ $N(N+1)/2$ constraints.)

Mean-field theory does not describe Goldstone modes (cont. sym.) or domain walls (discrete symmetry). So let's take O(N) model

$$F_L[\vec{\phi}] = \frac{1}{2}\int d^d\vec{r}\left[K|\nabla\vec{\phi}|^2 + a|\vec{\phi}|^2 + \frac{b}{2}|\vec{\phi}|^4\right]$$

with $\mathcal{Z} = \int D\vec{\phi}\, e^{-\beta F_L[\vec{\phi}]}$ Write $\vec{\phi} = \langle\vec{\phi}\rangle + \delta\vec{\phi}$

Then: $$\mathcal{Z} = e^{-\beta F_L[\langle\vec{\phi}\rangle]}\int D\delta\vec{\phi}\, \exp\left[-\frac{\beta K}{2}\int d^d\vec{r}\left\{|\nabla\delta\vec{\phi}|^2 + \xi(T)^{-2}|\delta\vec{\phi}|^2\right\}\right]$$

$$\xi(T) = \begin{cases}\sqrt{\dfrac{K}{|a(T)|}} & T>T_c\\[2ex] \sqrt{\dfrac{K}{2|a(T)|}} & T<T_c\end{cases} \sim |T-T_c|^{-1/2}$$

(Note that this is de facto an application of the functional Taylor expansion)

Recall from last lecture:

$$\mathcal{F}[u] = \mathcal{F}[u_0] + \int dx\, \frac{\delta\mathcal{F}}{\delta u(x)}\bigg|_{u=u_0}[u(x)-u_0(x)]$$
$$+\frac{1}{2}\int dx\int dx'\, \frac{\delta^2\mathcal{F}}{\delta u(x)\delta u(x')}\bigg|_{u=u_0}[u(x)-u_0(x)][u(x')-u_0(x')] + \ldots\ldots$$

The lowest-order correction to MFT is quadratic (why?).

We are interested in computing correlators $\langle \delta\vec{\phi}(\vec{r})\,\delta\vec{\phi}(\vec{r}\,')\rangle$ and to see what are the corrections to the mean-field result. So we need to know how to compute Gaussian functional integrals.

Let us consider a scalar order parameter first. So integrals are of the form:

$$Z[j] = \int \mathcal{D}\phi \, \exp\Big[-\frac{1}{2}\int d^d\vec{r}\int d^d\vec{r}\,'\,\phi(\vec{r})\,G^{-1}(\vec{r},\vec{r}\,')\,\phi(\vec{r}\,') + \int d^d\vec{r}\; j(\vec{r})\,\phi(\vec{r})\Big].$$

(we add on purpose sources which will be clear in a moment).

Note that (see tutorials):

$$Z(\vec{j}) = \int_{-\infty}^{+\infty} dx_1 \cdots \int_{-\infty}^{+\infty} dx_n \; e^{-\frac{1}{2}\vec{x}\cdot\underline{\underline{A}}\cdot\vec{x} + \vec{j}\cdot\vec{x}} = Z(0)\exp\Big(\frac{1}{2}\vec{j}\cdot\underline{\underline{A}}^{-1}\cdot\vec{j}\Big),$$

$$\text{where } Z(0) = \frac{(2\pi)^{n/2}}{\sqrt{\det(\underline{\underline{A}})}} = (2\pi)^{n/2}\exp\Big[-\frac{1}{2}\mathrm{Tr}(\log \underline{\underline{A}})\Big].$$

Furthermore, $\displaystyle \langle x_{i_1}\cdots x_{i_n}\rangle = \frac{1}{Z(\vec{j})}\frac{\partial^n}{\partial j_{i_1}\cdots\partial j_{i_n}} Z(\vec{j})\Big|_{\vec{j}=0}.$

In particular: $$\langle x_i x_j\rangle = \frac{1}{Z(\vec{j})}\frac{\partial^2}{\partial j_i \partial j_j} Z(\vec{j})\Big|_{\vec{j}=0} = A^{-1}_{ij}$$

Note that: $A_{ik}A^{-1}_{kj} = \delta_{ij}$

So now we can generalize to continuous case:

$$Z[j] = Z[0]\exp\Big[\frac{1}{2}\int d^d\vec{r}\int d^d\vec{r}\,'\, j(\vec{r})\,G(\vec{r},\vec{r}\,')\,j(\vec{r}\,')\Big]$$

$$\text{with } Z[0] = \mathcal{N}\sqrt{\det G^{-1}} = \mathcal{N}\exp\Big[-\frac{1}{2}\mathrm{Tr}(\log G^{-1})\Big].$$

$$\text{where } \int d\vec{r}\,''\, G^{-1}(\vec{r},\vec{r}\,'')\,G(\vec{r}\,'',\vec{r}\,') = \delta(\vec{r}-\vec{r}\,')$$

and $\langle \phi(\vec{r})\phi(\vec{r}\,')\rangle = G(\vec{r},\vec{r}\,')$.

So let us first consider the correlation function of our $\mathbb{Z}_2$ model.

$\Rightarrow \langle \delta\phi(\vec{r})\delta\phi(\vec{r}\,')\rangle = G(\vec{r},\vec{r}\,')$ where

$G^{-1}(\vec{r},\vec{r}\,') = \beta K\left(-\nabla^2 + \xi(T)^{-2}\right)\delta(\vec{r}-\vec{r}\,')$. So how to determine $G(\vec{r},\vec{r}\,')$?

$$\Rightarrow \int d\vec{r}\,'' G^{-1}(\vec{r},\vec{r}\,'')G(\vec{r}\,'',\vec{r}\,') = \int d\vec{r}\,''\,\beta K\left(-\nabla^2 + \xi(T)^{-2}\right)\delta(\vec{r}-\vec{r}\,'')G(\vec{r}\,'',\vec{r}\,')$$

$$\Rightarrow \quad \beta K\left[-\nabla^2 + \xi(T)^{-2}\right]G(\vec{r}-\vec{r}\,') = \delta(\vec{r}-\vec{r}\,')$$

Solve with FT. For finite volume V, we have for our fields:

$$\phi_{\vec{k}} = \int d^d\vec{r}\, e^{-i\vec{k}\cdot\vec{r}}\phi(\vec{r}) \iff \phi(\vec{r}) = \frac{1}{V}\sum_{\vec{k}} e^{i\vec{k}\cdot\vec{r}}\phi_{\vec{k}}.$$

(Recall since we did square gradient, we implicitly set $\phi_{\vec{k}} = 0$ for $|\vec{k}| > \Lambda$ with $\Lambda = \frac{\pi}{a}$).

Since it is finite spatial volume: $\vec{k} = \frac{2\pi}{L}\vec{n}$ $\vec{n}\in\mathbb{Z}^d$ (periodic bcs) with $V = L^d$. So in thermodynamic limit:

$$\phi(\vec{r}) = \int \frac{d^d\vec{k}}{(2\pi)^d} e^{i\vec{k}\cdot\vec{r}}\tilde{\phi}(\vec{k}) \iff \tilde{\phi}(\vec{k}) = \int d^d\vec{k}\, e^{-i\vec{k}\cdot\vec{r}}\phi(\vec{r})$$

So we find $\tilde{G}(\vec{k}) = \dfrac{k_B T}{K}\dfrac{1}{\vec{k}^2 + \xi^{-1}(T)^2}$ Let's check this result in $d=3$.

So $G(\vec{r}) = \dfrac{k_B T}{K}\displaystyle\int \frac{d^3\vec{k}}{(2\pi)^3}\frac{e^{i\vec{k}\cdot\vec{r}}}{\vec{k}^2 + \xi^{-1}(T)^2}$ (see Tutorials).

$$= \frac{k_B T}{4\pi K}\frac{e^{-r/\xi}}{r}. \Rightarrow \langle \delta\phi(\vec{r})\delta\phi(\vec{r}\,')\rangle = \frac{k_B T}{4\pi K}\frac{e^{-|\vec{r}-\vec{r}\,'|/\xi}}{|\vec{r}-\vec{r}\,'|}.$$

ξ is indeed correlation length!

At CP: $G(\vec{r}-\vec{r}\,') \sim \frac{1}{|\vec{r}-\vec{r}\,'|^{d-2+\eta}}$ At MF+Gauss $\Rightarrow$ $\eta=0$! But $\eta = 1/4$ (2D) $\eta \simeq 0.0363$ (3D)

Remarks: • $G(\vec{r})$ is a Green's function. In Field Theory language it is called a propagator or sometimes vertex function.

• We could have used $\int \mathcal{D}\phi = \lim_{N\to\infty} \prod_{i=1}^{N} \int d\phi_i$ and then make coordinate transf. with discrete FT.

Then $\int \mathcal{D}\phi = \prod_{\vec{k}} C \int d\phi_{\vec{k}}\, d\phi^*_{\vec{k}}$ with $\phi^*_{\vec{k}} = \phi_{-\vec{k}}$.

Now (using shorthand notation $\delta\phi = \phi'$):

$$\int \mathcal{D}\phi' \exp\left\{-\frac{\beta K}{2}\int d^d\vec{r}\left[|\nabla\phi'|^2 + \xi^{-2}\phi'^2\right]\right\}$$

$$= \prod_{|\vec{k}|>0} C \int d\phi'_{\vec{k}}\, d\phi'_{\vec{k}}{}^{*} \exp\left\{-\frac{\beta K}{2}\sum_{\vec{k}} \phi^{*\prime}_{\vec{k}}(\vec{k}^2+\xi^{-2})\phi'_{\vec{k}}\right\}.$$

$$\Rightarrow \langle \phi_{\vec{k}}\phi^*_{\vec{k}}\rangle = \frac{k_B T}{K}\frac{1}{\vec{k}^2+\xi^{-2}}$$

But this is like using equipartition theorem !

$\Rightarrow H = \sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}}{2m}$. $\left\langle \frac{p_{i\alpha}^2}{2m}\right\rangle = \frac{1}{2}k_B T.$ $\alpha = x, y, z$. $i = 1, \dots, N$.

(Every quadratic degree of freedom in Hamiltonian receives $\frac{1}{2}k_B T$).

What about free energy?

$$Z = e^{-\beta F_L[\langle\phi\rangle]}\int \mathcal{D}\delta\phi \exp\left[-\frac{\beta K}{2}\int d^d\vec{r}\left\{|\nabla\delta\phi|^2 + \xi(T)^{-2}\delta\phi^2\right\}\right]$$

$$= e^{-\beta F_L[\langle\phi\rangle]}\, e^{-\frac{1}{2}\sum_{\vec{k}} \log\left[\beta K(\vec{k}^2+\xi^{-2})\right]}$$

$$\beta F = \beta F_L[\langle\phi\rangle] + \frac{1}{2}\sum_{\vec{k}} \log\left[\beta K(\vec{k}^2+\xi^{-2})\right].$$ In continuum limit:

with $\beta \Delta F = \beta F - \underbrace{\beta F_{MF}}_{F[\langle\phi\rangle]}$ and $V = L^d$

$$\frac{\beta \Delta F}{V} = \frac{1}{2}\int \frac{d^d\vec{k}}{(2\pi)^d} \log\left[\beta K\left(\vec{k}^2 + \xi^{-2}\right)\right].$$

We find that in the Gaussian approximation, the same result as in mean-field theory (critical exponents, T_c), but the only correction is in the heat capacity. Define $c_V = \frac{C_V}{V}$, then $c_V = -T\,\frac{\partial^2(F/V)}{\partial T^2}$.

Taking the derivative gives two contributions, which are proportional to

$$I_1 = \int_{|\vec{k}|<\Lambda} \frac{d^d\vec{k}}{(2\pi)^d} \frac{1}{(\vec{k}^2+\xi^{-2})^2} \quad \text{and} \quad I_2 = \int_{|\vec{k}|<\Lambda} \frac{d^d\vec{k}}{(2\pi)^d} \frac{1}{\vec{k}^2+\xi^{-2}}.$$

Let us analyze both integrals.

First:

$$I_2 \propto \int_0^\Lambda dk \frac{k^{d-1}}{k^2+\xi^{-2}}$$

Let's do rescaling: $\vec{q} := \xi\vec{k}$

$$\propto \xi^{2-d}\int_0^{\xi\Lambda} dq \frac{q^{d-1}}{1+q^2}$$

Recall at T_c $\xi \to \infty$

$\therefore$ inspect integrand for $q \to 0$ and $q \to \infty$

- For q small and $d \geq 1$ there are no problems with divergence.
- For q large integrand $\sim q^{d-3}$ so for convergence: $d-3<-1$
  $d<2$.

So $$I_2 \propto \begin{cases} \xi^{2-d} & \text{for } d=1 \\ \sim \ln \Lambda\xi & \text{for } d=2 \\ \Lambda^{d-2} & \text{for } d>2 \end{cases}$$

Now let us analyse I_1:

$$I_1 \propto \xi^{4-d} \int_0^{\xi\Lambda} dq \, \frac{q^{d-1}}{(1+q^2)^2} .$$

- At $q \to 0$ again convergent for $d \geq 1$
- At $q \to \infty$ integrand $\sim q^{d-5}$ so integrable at infinity iff $d<4$

$$I_1 \propto \begin{cases} \xi^{4-d} & 1 \leq d < 4 \\ \ln \Lambda\xi & d = 4 \\ \Lambda^{d-4} & d > 4 \end{cases}$$

(Recall $\Lambda \sim \frac{1}{a}$)

Since Λ is a finite scale imposed by a microscopic length scale; leading order divergence at T_c goes like ξ^{4-d} $1 \leq d \leq 4$.

and $\xi \sim |T-T_c|^{-\nu}$ $\nu = 1/2$

So $\Delta c_v \sim |T-T_c|^{\nu(4-d)} = |T-T_c|^{-(2-d/2)}$ for $1 \leq d < 4$.

$\nu = \frac{1}{2}$ (MF)

α first correction to MF.

For $d \geqslant 4$ we find that Δc_v is a constant.

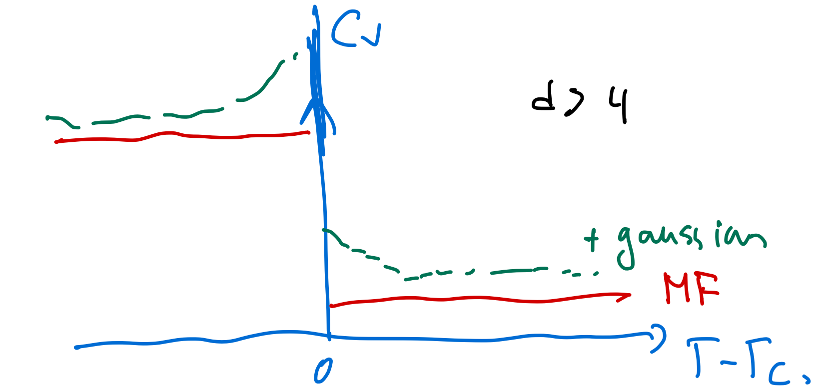
So recall $C_v \sim |T-T_c|^{-\alpha}$

In MF theory $\alpha = 0$ (discontinuity)

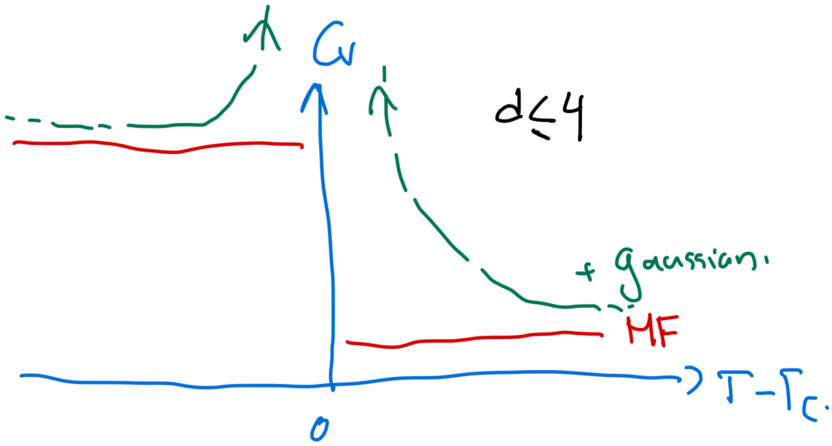
with Gaussian correction $\alpha = 2 - \frac{d}{2}$ $d<4$.

$\alpha = 0$ $d \geqslant 4$.

Critical exponents are unaffected for $d \geqslant 4$. This is called the upper critical dimension ($d_u = 4$)



Still discontinuous, critical exponent is unaffected.



Heat capacity diverges at critical point!