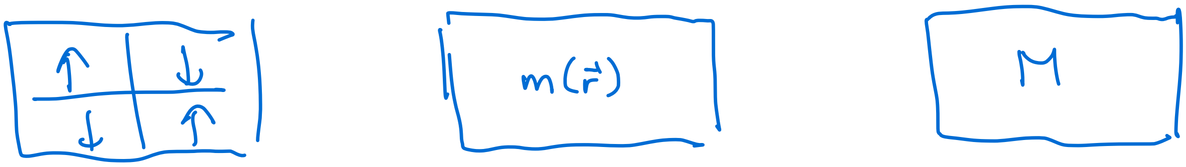
Lecture 4: Statistical fields

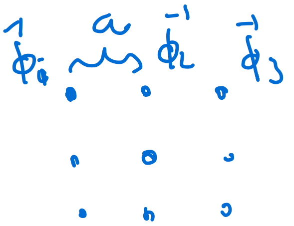
Microscopic scale $\longrightarrow$ Mesoscopic scale $\longrightarrow$ Macroscopic scale.



E.g. theory for observables on mesoscopic scale: $\mathcal{Z} = \int \mathcal{D}\vec{\phi}\; e^{-\beta F_L[\vec{\phi}]}$.

$\vec{\phi}$ is called an <u>order parameter</u>. A functional integral should be interpreted as:

$$\int \mathcal{D}\vec{\phi}\; W[\vec{\phi}(\vec{r}), \partial_\alpha \vec{\phi}(\vec{r}), \dots] = \lim_{\mathcal{N}\to\infty} \prod_{i=1}^{\mathcal{N}} \int d\vec{\phi}_i\; W\left[\vec{\phi}_i(\vec{r}), \frac{\vec{\phi}_{i_\alpha+1} - \vec{\phi}_{i_\alpha}}{a}, \dots\right]$$



$\xrightarrow{\mathcal{N}\to\infty}$ $\vec{\phi}(\vec{r})$

Existence of functional integrals $\Leftarrow$ in physics we have microscopic length scale a.

$F_L[\vec{\phi}]$ can be constructed using phenomenologically on the basis of symmetry arguments:

We write: $F_L[\vec{\phi}] = \int d^d\vec{r}\; f_L(\underbrace{\vec{\phi}, \nabla\vec{\phi}, \nabla^2\vec{\phi}}_{\text{short-range interactions}}, \dots)$

No explicit $\vec{r}$ dependence (system is homogeneous)

- $f_L(\vec{\phi}, \dots)$ must satisfy symmetries of the underlying microscopic Hamiltonian since $\vec{\phi}$ is typically derived from microscopic degrees of freedom.
- f_L is analytic and is expanded in terms of a polynomial.
- Stability.

Saddle-point approximation: $\int \mathcal{D}\vec{\phi}\; \underbrace{e^{-\beta F_L[\vec{\phi}]}}_{\text{analytic}} \approx \underbrace{e^{-\beta \min_{\vec{\phi}} F_L[\vec{\phi}]}}_{\text{can be non-analytic!}}$.

$F_L[\vec{\phi}]$ is an example of a <u>functional</u>. How do we compute $\min_{\vec{\phi}} F_L[\vec{\phi}]$?

Mathematical intermezzo: Functionals (pragmatic view)

Function: e.g. $f: \mathbb{R} \to \mathbb{R}$ given by $x \mapsto f(x)$. $x \in \mathbb{R}$, $f(x) \in \mathbb{R}$.

Functional: $\mathcal{F}: X \to \mathbb{R}$. given by $f \mapsto \mathcal{F}[f]$ $f \in X$. $\mathcal{F}[f] \in \mathbb{R}$.

function space.

Functional depends on a function $f(x)$ $a < x < b$.

It can be regarded as a continuous version of a function of several variables, ie $F(y_1, y_2, \ldots, y_N)$ with $y_1 = f(x_1)$ etc.

Examples:

(i): $F(y_1, y_2, \ldots y_N) = \sum_{i=1}^{N} a_i y_i \longrightarrow F[y] = \int dx\, a(x) f(x)$

(ii) $G(y_1, y_2, \ldots, y_N) = \sum_{i,j}^{} h_{ij} y_i y_j \to G[y] = \int dx \int dx'\, h(x,x') f(x) f(x')$

Differentiation: Take $f(\vec{y})$ with f function of N variables $\vec{y} = (y_1, \ldots, y_N)$.

Then total differential: $df = \sum_{i=1}^{N} \frac{\partial f}{\partial y_i} dy_i = \sum_{i=1}^{N} A_i(\vec{y}) dy_i$

df can be interpreted as: $df = f(y + dy) - f(y)$.

Similarly, for functional $\mathcal{F}[u]$:

$$\delta \mathcal{F}[u] = \mathcal{F}[u + \delta u] - \mathcal{F}[u] = \int dx\, A[u; x]\, \delta u(x).$$

functional derivative.

"$\delta u \to 0$"

$$=: \int dx\, \frac{\delta \mathcal{F}[u]}{\delta u(x)}\, \delta u(x).$$

Note integration boundaries appropriate to particular problem.
Let ϕ be a test function. Then we can also define the functional derivative as

$$\lim_{\epsilon \to 0} \frac{d}{d\epsilon} \mathcal{F}[u+\epsilon\phi] = \int dx \, \frac{\delta \mathcal{F}[u]}{\delta u(x)} \phi(x).$$

We can by above construction also define higher order functional derivatives: We find:

$$\frac{\delta^2 \mathcal{F}[u]}{\delta u(x) \delta u(x')} = \frac{\delta^2 \mathcal{F}[u]}{\delta u(x') \delta u(x)} \quad \text{etc.} \quad \left(\text{compare } \frac{\partial^2 f}{\partial x \partial y} = \frac{\partial^2 f}{\partial y \partial x} \right)$$

Functional Taylor expansion.

Suppose we expand around a given function $u_0(x)$:

$$\mathcal{F}[u] = \mathcal{F}[u_0] + \int dx \left. \frac{\delta \mathcal{F}}{\delta u(x)} \right|_{u=u_0} [u(x) - u_0(x)]$$

$$+ \frac{1}{2} \int dx \int dx' \underbrace{\left. \frac{\delta^2 \mathcal{F}}{\delta u(x) \delta u(x')} \right|_{u=u_0}}_{\text{just functions of } x \text{ and } x' \ldots} [u(x) - u_0(x)][u(x') - u_0(x')] + \ldots$$

Chain rule: $\mathcal{F}$ functional of u, depends solely on v, which is also functional of u.

$$\frac{\delta \mathcal{F}}{\delta u(x)} = \int dx' \, \frac{\delta \mathcal{F}}{\delta v(x')} \frac{\delta v(x')}{\delta u(x)}.$$

(End of intermezzo).

In language of functional derivatives: $\min_{\vec{\phi}} \mathcal{F}_L[\vec{\phi}] = \mathcal{F}_L[\langle \vec{\phi} \rangle]$

where $\left. \dfrac{\delta \mathcal{F}_L}{\delta \vec{\phi}(\vec{r})} \right|_{\vec{\phi} = \langle \vec{\phi} \rangle} = 0.$

Lets take example: $F_L[\vec{\phi}] = \int d\vec{r} \left[\frac{K}{2} |\nabla \vec{\phi}|^2 + \frac{a}{2} |\vec{\phi}(\vec{r})|^2 + \frac{b}{4} |\vec{\phi}(\vec{r})|^4 \right].$

Take variations $\vec{\phi} \rightarrow \vec{\phi} + \delta\vec{\phi}$ So what is $\delta F_L[\vec{\phi}]$?

$$\delta F_L[\vec{\phi}] = \int d\vec{r} \left[K \nabla \vec{\phi}(\vec{r}) \cdot \delta \nabla \vec{\phi}(\vec{r}) + a \vec{\phi}(\vec{r}) \cdot \delta\vec{\phi}(\vec{r}) + b |\vec{\phi}(\vec{r})|^2 \vec{\phi}(\vec{r}) \cdot \delta\vec{\phi}(\vec{r}) \right]$$

$$= \text{boundary term} + \int d\vec{r} \, \underbrace{\left[-K \nabla^2 \vec{\phi}(\vec{r}) + a \vec{\phi}(\vec{r}) + b |\vec{\phi}(\vec{r})|^2 \vec{\phi}(\vec{r}) \right]}_{\equiv \frac{\delta F_L[\vec{\phi}]}{\delta \phi(\vec{r})}} \cdot \delta\vec{\phi}(\vec{r})$$

So field configuration that minimizes $F_L[\vec{\phi}]$ is determined by the differential equation: $K \nabla^2 \vec{\phi}(\vec{r}) = a \vec{\phi}(\vec{r}) + b |\vec{\phi}(\vec{r})|^2 \vec{\phi}(\vec{r})$ (*).

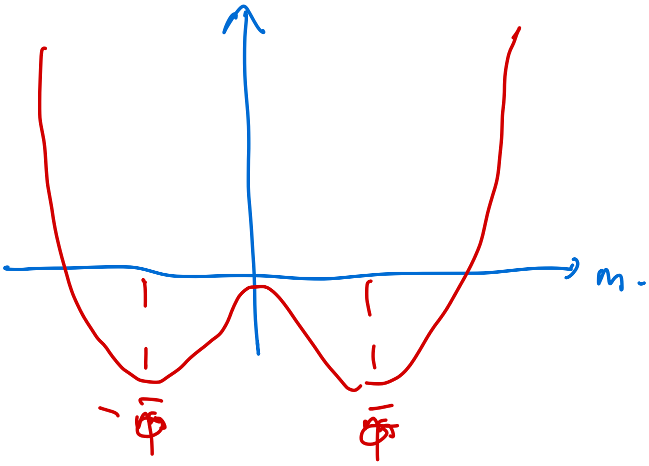
"energy penalty for having interfaces" (+ boundary conditions).

Without special boundary conditions the homogeneous field configuration minimises $F_L[\vec{\phi}]$. (*) is called saddle-point equation/Euler-Lagrange equation

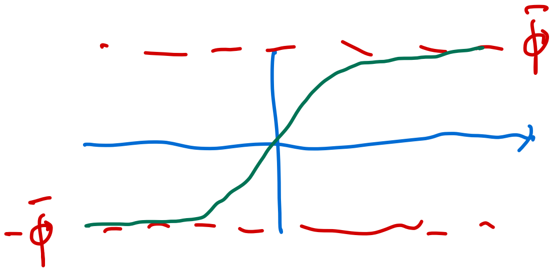
Suppose now that $\vec{\phi}$ is a scalar. ϕ.

Underlying Hamiltonian has a discrete symmetry $\Leftrightarrow F_L[\phi] = F_L[-\phi]$.

Below T_c discrete symmetry is broken and if two such states are formed, they



have to necessarily be seperate by a domain wall. This can be stabilised by suitable boundary conditions.



Free energy cost of having a domain wall $\Rightarrow$ tutorials.

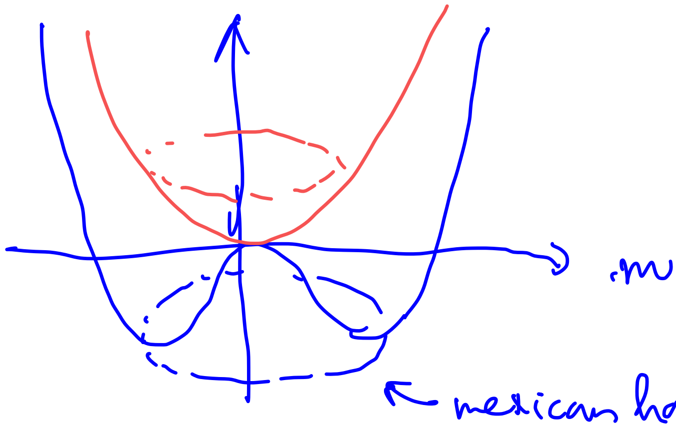
For discrete symmetry breaking, there is no possibility to continuosly deform one ground state in another ground state. What if there is a continuous symmetry? We illustrate this with a two-dimensional vectorial order parameter

$$\vec{m}(\vec{r}) = (m_1(\vec{r}), m_2(\vec{r}))$$ (superfluidity, planar magnets, ...)

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

is now invariant under $\vec{m}(\vec{r}) \longmapsto R\,\vec{m}(\vec{r})$ (rotation in order-parameter space)

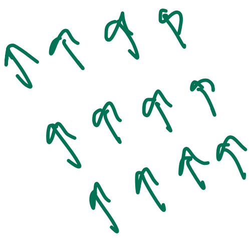
So now.



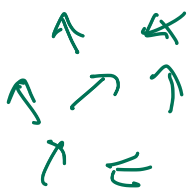
← mexican hat potential.

So we have situation:

$T<T_c$. $\langle \vec{m} \rangle \neq 0$



$T>T_c$.



$\langle \vec{m} \rangle = 0$.

In contrast to Ising case where Hamiltonian (in absence of external magnetic field) is invariant under $\mathbb{Z}_2$ (discrete symmetry)
We have no an "infinite amount" of ground states with equal energy.

If Hamiltonian is invariant under a continuous symmetry

⇒ there are excitations that cost no energy (Goldstone modes.)

So for $T<T_c$ we can infinitesimally homogeneously rotate the system for $T<T_c$.

$\vec{m}(\vec{r}) \longmapsto R(\vec{r})\,\vec{m}(\vec{r})$ are modes that cost little energy.

Examples are phonons, magnons, ...

Minimising (*) sets $|\vec{m}(\vec{r})|$ but not its direction (phase)

So it is useful to do a change of variables from $\vec{m}(\vec{r})$ to $\psi(\vec{r}) \in \mathbb{C}$.

and write $\psi(\vec{r}) = |\psi| e^{i\theta(\vec{r})}$ $\quad$ $|\psi|$ is determined but not $\theta(\vec{r})$.

Take $\theta(\vec{r})$ to be slowly varying function.

Then $F_L[\theta] = \text{const} + \frac{\overline{K}}{2}\int d\vec{r}\,(\nabla\theta)^2.$ $\quad$ Uniform rotations leave $F_L[\theta]$ invariant. ✓

$\overline{K} = K|\psi|^2$

Decomposition in normal modes: $\theta(\vec{r}) = \frac{1}{\sqrt{V}}\sum_{\vec{q}}{}' e^{i\vec{q}\cdot\vec{r}}\,\theta_{\vec{q}}$

$\Rightarrow F_L[\theta] = \text{cst} + \frac{\overline{K}}{2}\sum_{\vec{q}}{}' q^2 |\theta_{\vec{q}}|^2.$

Goldstone modes are slowly varying phase variations. (i.e. long wavelength excitations on top of the ground state).

Is there a systematic way to find: $Z = \int \mathcal{D}\vec{m}\; e^{-\beta F_L[\vec{m}]}$?

Let us illustrate this with the Ising model in a spatially varying external magnetic field.

$$Z = \sum_{\{s_i\}}{}' \exp\left(\beta J \sum_{\langle ij\rangle}{}' s_i s_j + \beta\mu \sum_i{}' H_i s_i\right)$$

Idea: We introduce a fluctuating field m_i that is on average equal to $\langle s_i\rangle$. i.e. $\langle m_i\rangle = \langle s_i\rangle$.

Define $h_i = \beta \mu H_i$ and $K_{ij} = \begin{cases} J & \text{for } i,j \text{ NN} \\ 0 & \text{otherwise.} \end{cases}$

Then: $$\mathcal{Z} = \sum_{\{s_i\}} \exp\Big[\underbrace{\tfrac{1}{2}\sum_{i,j} s_i K_{ij} s_j}_{} + \sum_i h_i s_i\Big].$$

this is the term that gives problems
⇒ goal is to decouple this term.

We have the following exact identity:

$$\exp\Big[\tfrac{1}{2}\sum_{i,j} s_i K_{ij} s_j\Big] = \underset{\text{const.}}{C} \int \prod_{i=1}^{N} dm_i \exp\Big[-\tfrac{1}{2}\sum_{i,j} m_i K_{ij}^{-1} m_j + \sum_i s_i m_i\Big]$$

Insertion in partition function gives:

$$\mathcal{Z} = C \int \prod_{i=1}^{N} dm_i \exp\Big(-\tfrac{1}{2}\sum_{i,j} m_i K_{ij}^{-1} m_j\Big) \sum_{\{s_i\}} \exp\Big[\sum_i (m_i + h_i) s_i\Big].$$

This procedure is called the Hubbard-Stratonovich transformation.

each spin feels a fluctuating magnetic field $m_i + h_i$.

The sum over spins can now be performed:

$$\mathcal{Z} \propto \Big(\prod_{i=1}^{N} \int dm_i\Big) \exp\big[-\beta F_L(\{m_i\})\big]. \quad (**)$$

with

$$\beta F_L(\{m_i\}) = \tfrac{1}{2}\sum_{i,j} m_i K_{ij}^{-1} m_j - \sum_i \ln\cosh(m_i + h_i).$$

It is convenient to do a similarity transformation: $m_i = \sum_j K_{ij} \tilde{m}_j$.
The Jacobian in (**) will give an extra constant.

Then

$$\beta F_L(\{m_i\}) = \frac{1}{2}\sum_{i,j} \tilde{m}_i K_{ij} \tilde{m}_j - \sum_i \ln\cosh\left(\sum_j K_{ij}\tilde{m}_j + h_i\right)$$

Now note that in continuum limit (e.g. three spatial dimensions):

$$\sum_{i,j} \tilde{m}_i K_{ij} \tilde{m}_j \sim \int \frac{d\vec{k}}{(2\pi)^3}\, \hat{m}(\vec{k})\, \hat{K}(k)\, \hat{m}(\vec{k})$$

where $\hat{m}(\vec{k}) = \hat{m}(-\vec{k})$ since m_i is real.

We find for cubic lattice:

$$\tilde{K}(\vec{k}) = K \sum_{\alpha=x,y,z} \cos(k_\alpha a) = \frac{1}{2}K\left(2 - a^2 k^2 + \mathcal{O}(k^4)\right)$$

in real space gives square gradients!

We take the continuum limit: $a \to 0$, $N \to \infty$

and expanding $\ln\cosh$ gives:

$$\beta F_L[m] = \frac{1}{2}\int d\vec{r}\, \left\{ K|\nabla m(\vec{r})|^2 + a(T)\, m(\vec{r})^2 + \frac{b}{2} m(\vec{r})^4 + \ldots - h(\vec{r})\, m(\vec{r}) \right\}.$$

with $\mathcal{Z} = \int \mathcal{D}m\, e^{-\beta F_L[m]}$. (We obtained this earlier just by using symmetry arguments!!)

Note that it is straightforward to generalize the above procedure to other models with continuous microscopic degrees of freedom; e.g.

$$H = -J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j \quad \text{(classical Heisenberg model)}$$

Note: $\vec{S}_i \longrightarrow \underline{\underline{R}} \cdot \vec{S}_i$ leaves H invariant.

Rotation matrix