

Part IV Mean Field Theory

Once you have a lot of models
flow theories, we of course have to
develop a systematic way to treat and
study it's properties.

Following the course, we are particularly
interesting in phase transitions and
ordered phases. Ordered states are well
described by inserting a new state
variable, the order parameter.

Mean field theory is an approximation
to the thermodynamic properties of a
system based on treating the order parameter
as spatially uniform.

• A good idea is

- Spatial fluctuations don't matter

- The range of interactions is infinity.

Nevertheless, if we're getting good
predictions in systems with high spatial
dimensions.

These are among formulations of Mean field theory

- Von der Woods Equation of State (1933)
- Molecular field, Weiss (1906)
- Bragg, Williams Ising (1934)
- * London Phenomenological Theory (1937)

London theory, is a functional power series expansion in terms of the order parameter for the transition of interest and assumes that this is small. The free energy is determined based on the nature of the broken symmetry of the ordered phase. - Ginzburg-Landau method of the fluctuation and is a power full method on the vicinity of a second order phase transition.

* Some Facts About Phase Transitions

• No order of high $T_c \rightarrow \langle \phi \rangle = 0$

• The critical temperature, order sets so that $\langle \phi \rangle \neq 0$ $T < T_c$

If $\langle \phi \rangle$ rises continuously from zero - Second Order

• Entropy is always continuous

§ IV.1 London Theory

The most powerful argument in use of London theory is the mathematical simplicity in the sense that under the simple assumption that the order parameter is small near T_c , it gives a wealth of information about phase transitions.

As we already know, equilibrium thermodynamics is completely determined by the function $F[T, \langle \phi; \pi \rangle]$, where $\langle \phi; \pi \rangle$ is the local order parameter and F is our free energy.

The simplest form of the function of F can take is:

$$F = \int d^d x f(T, \langle \phi; \pi \rangle) + \int d^d x \frac{1}{2} c [\nabla \langle \phi; \pi \rangle]^2 \quad (\text{IV.1.1})$$

f = free energy density

∇ = derivatives from spatial uniformity.

c , is a phenomenological constant with units energy \times (length)^{2-d}, i.e. $\langle \phi \rangle$ is unitless f is expanded in power series in $\langle \phi \rangle$

Based on continuous groups. The simplest one is the two dimensional orthogonal group O_2 of rotations. A two 2D vector is represented with a complex number, O_2 is isomorphic with $U(1)$ we will adopt this as our model of a dynamics of a system with an easy phase of magnetization.

2.1 Continuous Symmetry

2. The XY Model

All coefficient can be regarded as functions of T , and the coefficient of the functions order is parities on the equilibrium state isn't bounded in $\langle \phi(x) \rangle$

$$f(T, \langle \phi \rangle) = \frac{1}{2} n \langle \phi \rangle^2 - n \langle \phi \rangle^3 + n \langle \phi \rangle^4 + \dots \quad (\text{IV.1.3})$$

it implies no linear terms in $\langle \phi(x) \rangle$, so that:

$$h = \frac{\partial f}{\partial \langle \phi \rangle} \quad (\text{IV.1.2})$$

Above T_c , $\langle \phi \rangle$ must be zero when it's conjugate field is zero. $\langle \phi \rangle$ and h are related by:

2.2 XY Model

This model has $O(2)$ symmetry and describes a nearest neighbor ferromagnet of classical planar spins $\vec{S} = (S_x, S_y)$ on a d-dimensional hypercubic lattice.

$$H = -J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j = -J \sum_{\langle ij \rangle} (S_i^x S_j^x + S_i^y S_j^y) \quad (\text{IV.2.1})$$

($J > 0$), (interaction under rotation)

In the low temperature limit, we assume that almost all spins are ordered in the same direction. Rotating the system by certain angles variables $\vec{S} = (S \cos \theta, S \sin \theta)$

$$H = -J \sum_{\langle ij \rangle} S^2 \{ \cos(\theta_i - \theta_j) + \sin(\theta_i) \sin(\theta_j) \}$$

$$= -J S^2 \sum_{\langle ij \rangle} \cos[\theta_i - \theta_j] \quad (\text{IV.2.2})$$

In low T $|\theta_i - \theta_j| < 2\pi$ ground state

$$H \approx -J S^2 \sum_{\langle ij \rangle} \cos[\theta_i - \theta_j] \approx -\frac{JN}{2} S^2 + \frac{J}{2} \sum_{\langle ij \rangle} (\theta_i - \theta_j)^2 \equiv E_{\text{eff}} \quad (\text{IV.2.3})$$

doing the functional prescription for sum of ions and integrals

$$\sum_{i=1}^N \int dx^{(i)}$$

and we have to note that this integral is d -dimensional, so we have to keep in the original dimension, so we need a gradient expansion

the non-constant term gives:

$$H_N = \int dx^d |D\theta(x)|^2$$

that is the gradient form of London functional. This is also a Gaussian mean field theory.

the $\langle \phi \rangle$ model is symmetric under a rotation, in this sense it's only a function of:

$$\langle \phi \rangle^2 = \sum_{l=1}^n \langle \phi^l \rangle^2$$

~~$\chi^2(x, x') = \int_{x_1}^{x_2} \sqrt{2m(V(x) - E)} dx$~~

due to small deviations we have to include the gradient term:

$$\chi^2(x, x') = \int_{x_1}^{x_2} \sqrt{2m(V(x) - E)} dx$$

Now, we seek for the response of the system of small perturbations in the order parameter. We already know how to do by basic equilibrium thermodynamics.

$$\delta \langle \phi \rangle = \left(\frac{\partial \langle \phi \rangle}{\partial \mu} \right)^{1/2} \delta \mu$$

$$\text{Zero field } -h_i = 0 \quad \langle \phi \rangle = 0, \quad T > T_c$$

$$h_i = \frac{\partial F}{\partial \langle \phi \rangle} = (h + 4\mu \langle \phi \rangle^2) \langle \phi \rangle$$

and the equation of state:

$$\int (T, \langle \phi \rangle) = \frac{1}{2} h \langle \phi \rangle^2 + \mu \langle \phi \rangle^2$$

the London free energy:

(11)

$$\langle \phi_j | x | \phi_j \rangle - \langle \phi_j | x | \phi_j \rangle = \langle \phi_j | x | \phi_j \rangle - \langle \phi_j | x | \phi_j \rangle$$

use where

$$x_{ij}^{-1} = T_{ij}$$

The generalized autocorrelation is related to the correlation function:

$$x_{ij}^{-1}(\phi) = \frac{\partial \phi_j}{\partial \phi_i} = (H + \mu x + \frac{1}{2} \phi_j^2 + c \phi_j^2) \phi_j + \delta \phi_j \phi_j$$

$$\frac{\partial \phi_j}{\partial \phi_i} = \mu \phi_j + \mu \langle \phi_j^2 \rangle \phi_j + c \phi_j^2$$

~~The non-local correlation function:~~

$$f = \frac{1}{2} \mu (\phi_1^2 + \phi_2^2) + \mu (\phi_1^2 + \phi_2^2) + \frac{1}{2} c (\phi_1^2 + \phi_2^2)$$

force:

It is more convenient work on Fourier

$$\left. \begin{aligned} \chi_{I'}^T &= M + 4u \langle \phi \rangle + c q^2 \\ \chi_{II'}^T &= M + 2u \langle \phi \rangle + c q^2 \end{aligned} \right\} \begin{aligned} & q^2 \\ & \text{if } T \perp c \end{aligned}$$

using this fact, we can see that:

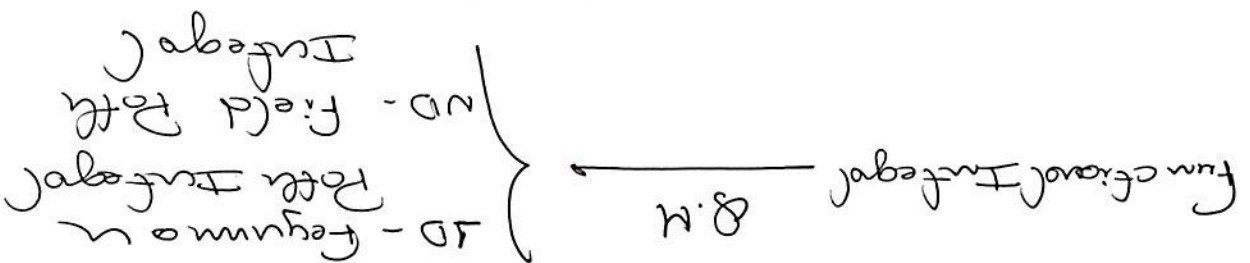
$$\left. \begin{aligned} g_I &= \langle \phi_{I'}(x) | \phi_{I'}(x) \rangle - \langle \phi_I(x) | \langle \phi_{I'}(x) \rangle \\ g_{II} &= \langle \phi_{II'}(x) | \phi_{II'}(x) \rangle - \langle \phi_{II}(x) | \langle \phi_{II'}(x) \rangle \end{aligned} \right\}$$

$$g_{II'}(x, x') = g_{II}(x, x') e_i e_j + g_I(x, x') (\delta_{ij} - e_i e_j)$$

We will select a preferential direction, as we need to break the correlation function. This can be done as follows:

3. Mean Field Theory and Functional Integrals

There is a classical version to field theoretical methods applied to condensates and matter systems:



We can do a mean field theory from this formalism.

Most of the systems we study are described in terms of lattice models:

$$Z = \sum_c f_c(c_i) + \frac{1}{2} \sum_{i,j} c_{ij} (\phi_i - \phi_j)^2$$

The transition to continuum is made by the following prescription:

$$V_0 \int dx \rightarrow \sum_c f_c(\phi_i) \Rightarrow \int \frac{d^d x}{V_0} f_0(\phi(x))$$

$$\frac{1}{2} \sum_c c_{ij} (\phi_i - \phi_j)^2 = \frac{1}{2} \int \frac{d^d x}{V_0} [d^d x c[\nabla\phi(x)]]^2$$

$$0 = \int d^d x c_{10}$$

functional integrals are an example

to take in account all the configurations to form the field $\phi(x)$ configurations to the constraints:

$$\int D\phi(x) = \lim_{V \rightarrow 0} \frac{1}{V} \int d\phi$$

there is only one exactly soluble case, the generation of the Gaussian integral:

$$\int_{-\infty}^{\infty} dy e^{-\frac{1}{2}cy^2 + \lambda y} = \left(\frac{c}{2\pi}\right)^{-1/2} e^{\lambda^2/2c}$$

doing in this way:

$$\int_{-\infty}^{\infty} \left(\frac{1}{\pi}\right)^{1/2} dy e^{-\frac{1}{2}y^2 + \lambda y} = \left(\frac{c}{2\pi}\right)^{-1/2} e^{\lambda^2/2c}$$

The thermodynamic partition function can be calculated as:

$$Z = \int D\phi(x) e^{-\beta(\mathcal{H} - \int dx h(x)\phi(x))}$$

$h(x)$ is external field or correlation generator.

The continuum limit of the lattice model is of the form:

$$\mathcal{H} = \int dx f[\phi(x)] + \frac{1}{2} \int dx e[\Delta\phi(x)]^2$$

with means:

$$Z = \int \prod \phi e^{-\mathcal{H}[\phi]}$$

We can fix the gaussian identity to solve the partition function of the non-metric fermion

$$\mathcal{H}_0 = \frac{1}{2} \sum_{i,j} \chi_{ij} \phi_i \phi_j$$

form in form:

$$\phi_i = \frac{1}{\sqrt{N}} \sum_j e^{i q \cdot R_j} \phi_j$$

$$\chi(q) = \frac{1}{N} \sum_{j,k} e^{-i q \cdot R_j} \chi_{jk} e^{i q \cdot R_k}$$

Using the basis in that:

$$\langle 0 | \phi \rangle = N^{-1/2} e^{i q \cdot R_0}$$

eigen values:

$$\langle \phi | \mathcal{H} | \phi \rangle = \frac{1}{2} \sum e^{i q \cdot (R_i - R_j)} \chi_{ij} = \chi_0(q) = \chi_0(q)$$

So, the form in form:

$$\phi_i = \phi_j$$

$$\mathcal{H}_0 = \frac{1}{2} \sum_{i,j} \chi_{ij} \phi_i \phi_j$$

and the external term: $\phi_{ext} = \sum_k \phi_k$

in Gaussian integration:

$$I = \int_{-\infty}^{+\infty} dx^n e^{-\frac{1}{2}(x_i A_{ij} x_j + i b_i x_i)}$$

we can diagonalize this by a orthogonal transform:

in vector notation:

$$I = \int dx^n e^{-\frac{1}{2} A_i(x_i + b_i)} \left\{ \begin{array}{l} A_2 = \frac{1}{2} \sum_{ij} x_i A_{ij} x_j \\ \vec{b} \cdot \vec{x} = \sum_j b_j x_j \end{array} \right.$$

one first look to the minimum of the quadratic form

$$\frac{\partial}{\partial x_i} (A_i(x_i) - b_i \cdot x_i) = 0 \Rightarrow \sum_j A_{ij} x_j = b_i$$

$$\text{the solution is } x_j = \sum_i (A^{-1})_{ji} b_i$$

$A \rightarrow$ Green function of the operator A !

Green function = convolution function

change of variable: $x_1 \rightarrow y$

$$x_1 = \sum_j (A^{-1})_{1j} b_j + y; \Rightarrow \underbrace{-A_2(x)}_{-A_2(x) + b_2 \cdot x = w_2(b)} - A_2(y)$$

$$\mathcal{N}_0 = \frac{1}{2} \int d^d x d^d x' n(x, x') \phi(x) \phi(x')$$

field.

The continuous limit follows the same path. In fact the continuous limit is something like the coordinate representation of the

$$q_{0i} = \int d^d x' e^{i q \cdot (R_i - R_{i'})} \frac{1}{T} \langle \phi_i \phi_{i'} \rangle$$

$$\chi[T, \nu] = -T \ln Z = -T \ln \int \prod d\phi_i e^{-\beta(\mathcal{H}_0 + \mathcal{H}_{int})} = \frac{1}{2} T \ln [\dots]$$

Once we had the partition function, one can extract the free energy:

In our example: $A = n(q)$

$$I(A, b) = \int_{-\infty}^{+\infty} d^n y e^{-A_2(y)} = \int_{-\infty}^{+\infty} d^n y e^{-\frac{1}{2} y^T A y} e^{-\frac{1}{2} y^T b}$$

end then

$$\mathcal{N}_2(b) = \frac{1}{2} \sum_{i,j=1}^n b_i (A^{-1})_{ij} b_j$$

in quantum mechanics, this is nothing more than the transformation to the field operator:

$$\hat{\psi}(x) = \sum_n \hat{\psi}_n(x) c_n$$

doing the Fourier transform:

$$\phi(x) = \int \frac{d^d q}{(2\pi)^d} e^{i q \cdot x} \phi(q)$$

and then the definition:

$$h(q) = \int \frac{d^d x}{(2\pi)^d} e^{i q(x-x')} h(x|x')$$

we get the ~~same~~ commutation relation:

$$h_0 = \frac{1}{2} \int \frac{d^d q}{(2\pi)^d} h(q) |q|^2$$

the free energy:

$$\mathcal{F} = \frac{1}{2} T V \int \frac{d^d q}{(2\pi)^d} \ln [h(q) v(q)] - \frac{1}{2} \int \frac{d^d x}{(2\pi)^d} \beta g_0(x, x') h(x)$$

More details about Green functions and correlation functions; see: Fetter on Wolfram.

Now we can use this to do mean field?

- Functional Mean Field theory

A field theory from which we can calculate all thermodynamic properties are defined by:

$$Z = \int \mathcal{D}\phi(x) e^{-\mathcal{H} - \int dx h(x)\phi(x)} / \tau$$

once the partition function is known:

(same formulas called - Ginzburg-Landau)

$$\mathcal{H} = \int dx \left[f[\phi(x)] + \frac{1}{2} (dx e [\nabla \phi(x)])^2 \right]$$

From this, we calculate the thermodynamic partition function and its configuration field $F[\phi(x)]$

and sum over that all configuration contributions to Z .

However, is a thing to consider that some higher order contributions more than others

of course, they note the same probability, but maybe one more important.

in fact, the functions integrated are determined by the saddle point of the "action", that is $e^{-\int dx h(x)\phi(x)}$.

- See - Anders Weber section 14 (2nd edition)

The saddle point is determined by:

$$\left. \frac{\delta \mathcal{H}}{\delta \phi(x)} \right|_{\phi(x) = \phi_{sp}(x)} = h(x)$$

The mean field theory for the Ising model consists in approximating the Z only by the saddle point configuration.

$$Z = \int \mathcal{D}\phi \left\{ \exp \left[-\beta \int dx h(x)\phi_{sp}(x) \right] \right\}$$

$$\equiv \int \mathcal{D}\phi \left\{ \exp \left[-\beta \left(\int dx h(x)\phi(x) \right) \right] \right\}$$

Mean field Theory

$$\langle \phi(x) \rangle = \phi_{sp}(x) \rightarrow F_{MF} = \mathcal{H}[\phi_{sp}(x)]$$

$$\int_{-\infty}^{\infty} \psi^* \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \psi dx = E \int_{-\infty}^{\infty} \psi^* \psi dx$$

$$\int_{-\infty}^{\infty} \psi^* \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \psi dx = E \int_{-\infty}^{\infty} \psi^* \psi dx$$

are defined by:

from the stationary wave function, the correlation function

* Gaussian Correlations and Correlation function

Corrections to mean field theory can be studied expansion in power of:

$$\delta\phi(x) = \phi(x) - \langle\phi(x)\rangle \rightarrow \phi(x) = \delta\phi(x) + \langle\phi(x)\rangle$$

by definition $\langle\delta\phi(x)\rangle = 0$

expanding the partition in second order of $\delta\phi(x)$

- functional power series:

$$\Phi[\langle\phi(x)\rangle + \delta\phi(x)] = \Phi[\langle\phi(x)\rangle] + \int dx \frac{\delta\Phi}{\delta\phi(x)} \delta\phi(x) + \frac{1}{2} \int dx dx' \frac{\delta^2\Phi}{\delta\phi(x)\delta\phi(x')} \delta\phi(x)\delta\phi(x')$$

~~the~~ the saddle point is the one who minimizes. the $\delta\phi$, so the first derivative ~~doesn't~~ doesn't exist:

up to order two:

$$2\Phi[\langle\phi(x)\rangle] - \int dx dx' h(x) \langle\phi(x)\rangle + \frac{1}{2} \int dx dx' \delta\phi(x) \delta\phi(x') \delta\phi(x) \delta\phi(x')$$

$g_0(x, x') =$ correlation function