Advanced Statistical Physics

Lecture Notes

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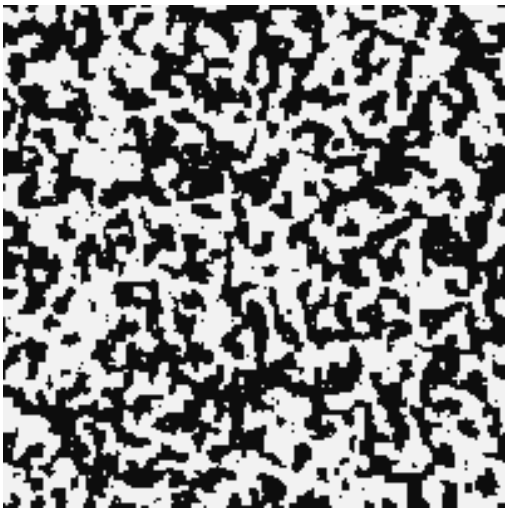

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Lecture 01: Introduction and Van der Waal's Equation of State

What we will discuss here in mainly the equilibrium physics of phase transitions which is both interesting and intriguing. Phase transitions are generally the result of the collective behaviour of interacting particles which produce some change in the thermodynamics of the system. For interaction between particles, we require a *pair potential*, which describes the behaviour of the interaction. One of such potentials is the celebrated *Lennard-Jones* potential (LJP) which goes as:

$$u(r) = \varepsilon_0 \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right]$$

where $r = |\mathbf{r}_i - \mathbf{r}_j|$ is the interparticle distance. This is used as a model for intermolecular interactions in many systems. Another "lesser" realistic (but simpler to handle) model can be described by the potential,

$$u(r) = \begin{cases} \infty & r < r_0 \\ -\varepsilon_0 \left(\frac{r_0}{r}\right)^6 & r > r_0 \end{cases}$$

The above potential tells that the minimum possible separation between molecules is r_0, since $u(r)$ blows up below $r = r_0$. Hence the particles act as *hard spheres* (spheres which cannot penetrate each other) of radius $\frac{r_0}{2}$. For $r > r_0$, $u(r) \sim r^{-6}$ which implies *dipolar interactions*.

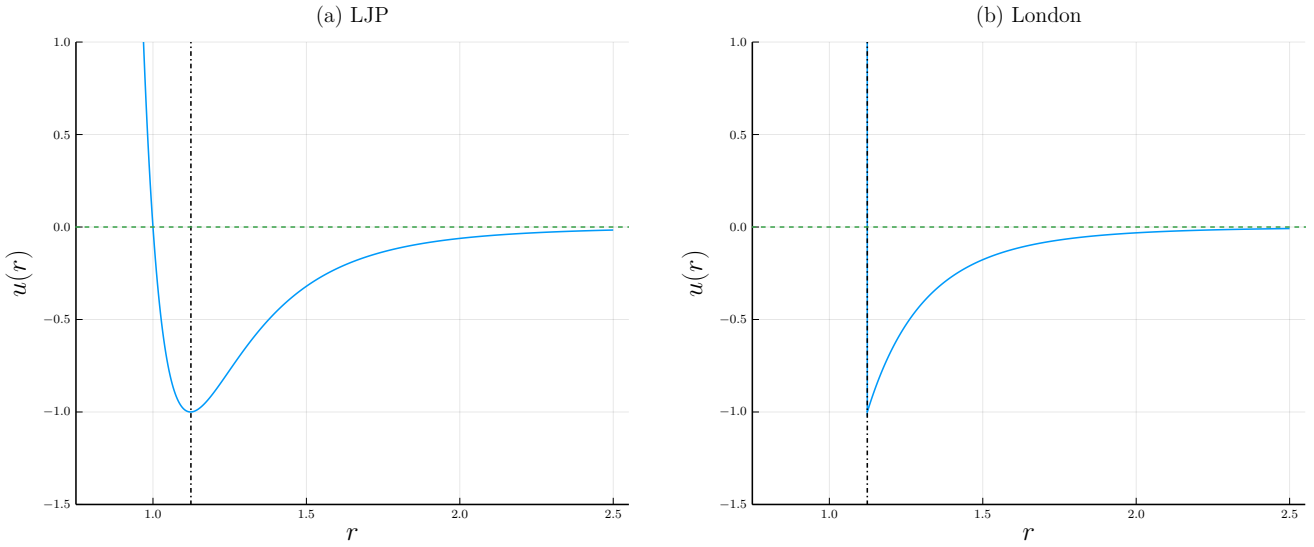


Figure 1: Interaction potentials. (a) Lennard-Jones potential. The vertical line denotes the r at which minima occurs (b) London dispersion potential.

Note that these interactions are mostly *power-law* interactions, $u(r) \sim r^{-s}$. Let d be the dimension of the space in which we are working. Then, it can be shown or motivated that if $s \leq d$, then the interaction is long-ranged which is not ideal for us. Extensivity can break down and some other issues (like negative specific heat) may occur in this case. One such example is that of gravitational systems where $u(r) \sim \frac{1}{r}$. If $s > d$ then the interaction is short-ranged. Since $u(r)$ blows up when $r = 0$, in general, it is advisable to impose a hard core repulsion (like in the London force) which ensures that everything stays okay, since interactions act only after $r > r_0$!

1.1. Van der Waal's gas

Let us see an example of this using the Van der Waal's equation which is a correction to the ideal gas equation $PV = Nk_{\mathrm{B}}T$ and successfully explains the condensation process of gases.

We will work in canonical ensemble here. The *canonical partition function* is written as,

$$\mathcal{Z}(N, V, T) = \frac{1}{N!} \int \prod_i \left(\frac{\mathrm{d}^3 p_i \, \mathrm{d}^3 q_i}{h^3} \right) e^{-\beta \mathcal{H}}$$

where $\mathcal{H}$ is the Hamiltonian of the system. The $N!$ factor has been put to include the indistinguishability of the particles and h^3 factor has been put to make the phase space volume dimensionless. The Hamiltonian consists, as usual, of a kinetic and a pair potential part.

$$\mathcal{H} = \sum_i \frac{p_i^2}{2m} + \frac{1}{2}\sum_{i\neq j} u(|\mathbf{q}_i - \mathbf{q}_j|)$$

The momentum integral can be carried out nicely since this is essentially a Gaussian integral. Using independence of the kinetic terms we get,

$$\mathcal{Z}_{\text{p}} = \left[\int \frac{\mathrm{d}^3 p}{h^3}\ e^{-\beta p^2/2m}\right]^N = \left[\frac{4\pi}{h^3}\int_0^\infty p^2 e^{-\beta p^2/2m}\ \mathrm{d}p\right]^N = \left[\frac{2\pi m k_{\text{B}} T}{h^2}\right]^{3N/2}$$

Defining the thermal wavelength $\lambda_{\text{T}} = {}^{h}/_{\sqrt{2\pi m k_{\text{B}} T}}$, we have

$$\mathcal{Z} = \frac{1}{N!\lambda_{\text{T}}^{3N}} \int \prod_i \mathrm{d}^3 q_i\ e^{-\beta U(\{\mathbf{q}_i\})}$$

where $U(\{\mathbf{q}_i\})$ denotes the interaction term in the Hamiltonian. Tackling this part is extremely hard, since the interactions are between pair of particles, hence independence cannot be assumed.

1.2. Uniform Density Approximation

One of the most popular ways to deal with interactions is through *perturbation*, however, perturbations are generally taken to be *continuous* and hence, non-analyticity (an important aspect of phase transitions) cannot be effectively captured. We will use the method of *mean-field approximation*, which treats the interactions as an "effective potential" which can be found out self-consistently. To simplify our calculations, let us define the number density of the gas, in terms of the delta function,

$$n(\mathbf{q}) = \sum_{i=1}^{N}\ \delta^{(3)}(\mathbf{q} - \mathbf{q}_i) \tag{1}$$

Then the interaction term becomes,

$$\begin{aligned}
2U &= \sum_i \sum_{j\neq i} u(|\mathbf{q}_i - \mathbf{q}_j|) \\
&= \sum_i \sum_{j\neq i} \int \mathrm{d}^3 q_1\ \delta^{(3)}(\mathbf{q}_1 - \mathbf{q}_i)\cdot u(|\mathbf{q}_1 - \mathbf{q}_j|) \\
&= \sum_i \sum_{j\neq i} \int \mathrm{d}^3 q_1\ \delta^{(3)}(\mathbf{q}_1 - \mathbf{q}_i)\cdot \int \mathrm{d}q_2\ \delta^{(3)}(\mathbf{q}_2 - \mathbf{q}_j)\cdot u(|\mathbf{q}_1 - \mathbf{q}_2|) \\
&= \int \mathrm{d}^3 q_1 \mathrm{d}q_2\ \sum_i \sum_{j\neq i} \delta^{(3)}(\mathbf{q}_1 - \mathbf{q}_i)\cdot\ \delta^{(3)}(\mathbf{q}_2 - \mathbf{q}_j)\cdot u(|\mathbf{q}_1 - \mathbf{q}_2|) \\
&= \int \mathrm{d}^3 q_1 \mathrm{d}q_2\ n(\mathbf{q}_1) n(\mathbf{q}_2) u(|\mathbf{q}_1 - \mathbf{q}_2|)
\end{aligned}$$

We will use a heavily *unmotivated* approximation where we will treat the density to be uniform, independent of the spatial coordinate, that is, $n(\mathbf{r}) \equiv n$ Then,

$$U = \frac{n^2}{2}\int \mathrm{d}^3 q_1 \mathrm{d}^3 q_2\ u(|\mathbf{q}_1 - \mathbf{q}_2|)$$

Let us define the variables $\mathbf{R} = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)$ and $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ from which we have $\mathbf{r}_1 = \mathbf{R} + \frac{\mathbf{r}}{2}$ and $\mathbf{r}_2 = \mathbf{R} - \frac{\mathbf{r}}{2}$. The Jacobian of this transformation can be written as,

$$\mathbf{J} \equiv \frac{\partial(\mathbf{r}_1, \mathbf{r}_2)}{\partial \mathbf{R}, \mathbf{r}} = \begin{pmatrix} \mathbb{1} & \frac{1}{2}\mathbb{1} \\ \mathbb{1} & -\frac{1}{2}\mathbb{1} \end{pmatrix} \implies J = \det(\mathbf{J}) = -1$$

Using the new variables, the integral becomes,

$$U = \frac{n^2}{2}\int \mathrm{d}^3R\ \mathrm{d}^3r\ u(r) = \frac{n^2V}{2}\int_{r_0}^{\infty}\mathrm{d}^3r\ u(r) = \frac{N^2}{2V}\int \mathrm{d}^3r\ u(r)$$

where we have used $n = {}^N\!/_V$ and r_0 is the hard-core cutoff. Now, assume a power-law interaction for $r > r_0$, $u(r) = -\varepsilon_0\big(\frac{r_0}{r}\big)^s$ using which we get,

$$U = -\frac{\varepsilon_0 N^2}{2V}\cdot r_0^s\int_{r_0}^{\infty}4\pi r^2\mathrm{d}r\ \frac{1}{r^s} = -\frac{4\pi\varepsilon_0 N^2 r_0^s}{2V(3-s)}\ r^{3-s}\Big|_{r_0}^{\infty}$$

As we can see, U is finite only when $3 - s < 0 \implies s > 3$ where 3 was our spatial dimension. Assuming $s > 3$, we have $r^{3-s} \to 0$ and we have

$$U = \frac{4\pi\varepsilon_0 N^2 r_0^s}{2V(3-s)}r_0^{3-s} = -\frac{4\pi\varepsilon_0 N^2 r_0^3}{2V(s-3)} = -\frac{aN^2}{V} \qquad \text{where,}\ \ a \equiv \frac{2\pi\varepsilon_0 r_0^3}{s-3}$$

We get an 'effective' interaction potential using the *uniform density approximation*. From here, the partion function now becomes,

$$\mathcal{Z} = \frac{e^{\beta aN^2/V}}{N!\lambda_{\mathrm{T}}^{3N}}\int\prod \mathrm{d}q_i$$

Now, the integral is simply not equal to V^N, since we have assumed a hard-sphere gas and each particle has some finite volume. Assume that each particle occupies a small volume ω, which cannot be occupied by the other particles. If one particle occupies volume say V, then the second particle can occupy $V-\omega$, the third occupies $V - 2\omega$ and so on. Then the integral will be just,

$$\begin{aligned}\int\prod \mathrm{d}q_i \equiv \prod_{i=0}^{N-1}(V - i\omega) &\approx \prod(V - j\omega)(V - (N-j)\omega)\\ &= \prod V^2\Big(1 - \frac{j\omega}{V}\Big)\Big(1 - \frac{(N-j)\omega}{V}\Big)\\ &\approx V^N\prod\Big[1 - \frac{(j+N-j)\omega}{V} + \mathcal{O}((\omega/V)^2)\Big]\\ &\approx V^N\Big[1 - \frac{N\omega}{V}\Big]^{N/2} = \Big[V\Big(1 - \frac{N\omega}{V}\Big)^{1/2}\Big]^N\end{aligned}$$

where we have made the product over $\approx N/2$ pairs. Now, assume $N\omega \ll V$ from which we can use the approximation $(1+x)^n \approx 1 + nx$ to get,

$$\Big[V\Big(1 - \frac{N\omega}{V}\Big)^{1/2}\Big]^N \approx \Big[V\Big(1 - \frac{N\omega}{2V}\Big)\Big]^N = \Big[V - \frac{N\omega}{2}\Big]^N$$

We see that the available volume is reduced by a factor of $N\omega/2$. This was the final step and we can now write the partition function,

$$\boxed{\mathcal{Z}(N,V,T) = \frac{e^{\beta aN^2/V}}{N!\lambda_{\mathrm{T}}^{3N}}\Big[V - \frac{N\omega}{2}\Big]^N} \tag{2}$$

The free energy can be obtained from the partition function using $F = -k_{\mathrm{B}}T\ln\mathcal{Z}$,

$$F = -\cancel{k_{\mathrm{B}}T}\cancel{\beta}\frac{aN^2}{V} - Nk_{\mathrm{B}}T\ln\Big[V - \frac{N\omega}{2}\Big] + c(N,T)$$

and from here, we can find the pressure $P = -\left(\frac{\partial F}{\partial V}\right)_{N,T}$

$$P = -\frac{aN^2}{V^2} + \frac{Nk_{\mathrm{B}}T}{\left(V - \frac{N\omega}{2}\right)} \implies \boxed{\left(P + \frac{aN^2}{V^2}\right)(V - Nb) = Nk_{\mathrm{B}}T} \tag{3}$$

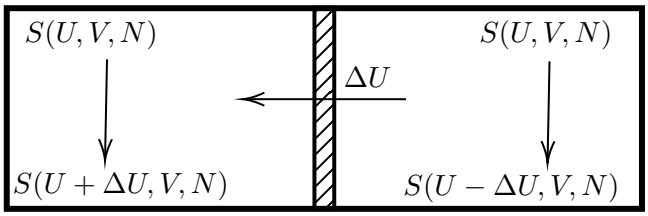
This is the Van der Waal's equation, where we have defined $b = \omega/2$. This can be written in an alternate form using the number of moles, $\mathfrak{n} = N/N_{\mathrm{A}}$ where N_{A} is the Avogadro's number:

$$\left(P + \frac{a'\mathfrak{n}^2}{V^2}\right)(V - \mathfrak{n}b') = \mathfrak{n}RT \iff \left(P + \frac{a'}{v_m^2}\right)(v_m - b') = RT$$

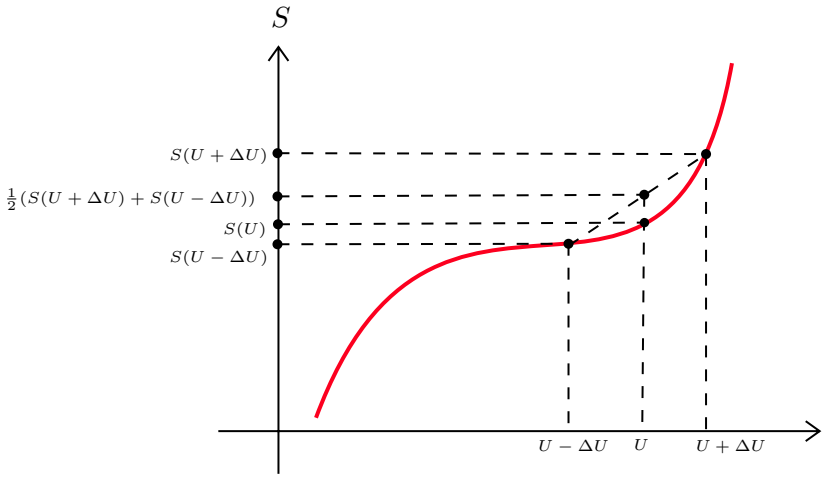
where $a' = N_{\mathrm{A}}^2 a$ and $b' = bN_{\mathrm{A}}$ and v_m is the molar volume.

Lecture 02: Stability of Thermodynamic Systems

We will discuss about the conditions under which the system in consideration is stable. This will in turn help us to understand *phase transitions* which are consequences of instability!



Consider two identical subsystems, with entropies $S(U, V, N)$, separated by an adiabatic wall. Suppose we remove an amount of energy ΔU from the first subsystem and transfer it to the second, the total energy changes from $2S(U, V, N)$ to $S(U + \Delta U) + S(U - \Delta U, V, N)$. Suppose that the entropy of the system looked something like in the diagram below.



Then, the resultant entropy after this transfer would be greater than the initial entropy. This would lead to inhomogenities in the system. Within one subsystem, there would be an uneven re-distribution of energy within different regions. This loss of homogenity indicates a *phase separation*!

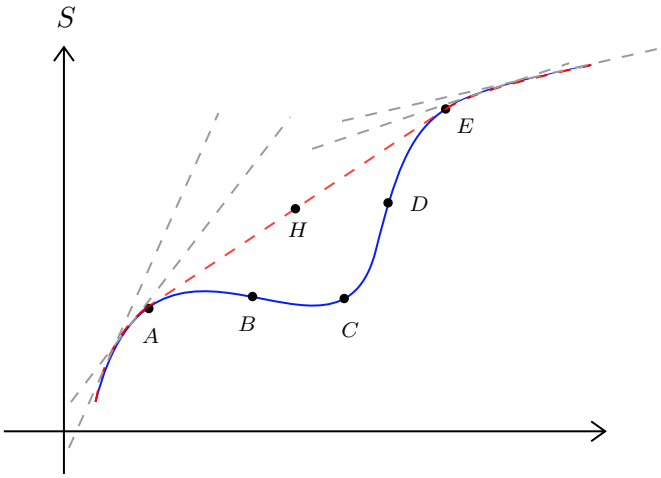
Thus the stability condition is the *concavity of entropy*, that is,

$$S(U - \Delta U, V, N) + S(U + \Delta U, V, N) \leq 2S(U) \tag{4}$$

Taylor expansion of the left hand side leads to the condition (under the limit $\Delta U \to 0$)

$$\boxed{\left(\frac{\partial^2 S}{\partial U^2}\right)_{V,N} \leq 0} \tag{5}$$

This implies that the curvature of the entropy should be downwards! It might happen that we obtain a 'locally convex' entropy curve from some calculation or from experimental data, which does not obey concavity.



This *convex intruder* cannot describe the equilibrium state and we have to obtain the *stable thermodynamic fundamental equation* from this curve. To do that, we construct all the *superior tangents*, that is, tangents which are above this curve. Now, within the family of tangents, there will be one line which will touch the curve at two places.

In the diagram, tangent at any point after A (but before E) will cross the curve. Now, the tangent at A will touch the curve at E. If it had not touched, it would have either intersected the curve or gone above E (If it has intersected the curve, then the tangent at A should not have been considered at all since we are considering only superior tangents. If it had gone over E, this means that there must be some points after A, where this touching will occur. In any case, what we want to say is that, there will be a 'common tangent' at points A and E).

Now, take the envelope of this family of tangents and this will be the fundamental thermodynamic equation that describes the equilibirum states.

Any point on the straight line denotes a phase-separated state, where part of the system is in state A and another part is in E. This happens because of the convex curve of entropy, which creates an inhomogenity.

Note that in the region AB and DE, entropy is still concave, hence these are called *metastable* or locally stable states. These states satisfy Eq.(5) but does not satisfy Eq.(4) while the region BCD satisfy neither condition.

NOTE:

A generic condition for stability is given by $\delta P \delta V \leq 0$ where δP and δV represent a small deviation from the equilibrium value. We can write,

$$0 \geq \delta V \left[\left.\frac{\partial P}{\partial V}\right|_T \delta V + \frac{1}{2}\left.\frac{\partial^2 P}{\partial V^2}\right|_T (\delta V)^2 + \frac{1}{6}\left.\frac{\partial^3 P}{\partial V^3}\right|_T (\delta V)^3 + \dots \right] \tag{6}$$

The first term has $(\delta V)^2$ which is always positive. Hence to make this term negative, we need

$$\left.\frac{\partial P}{\partial V}\right|_T \leq 0$$

Suppose that $\left.\frac{\partial P}{\partial V}\right|_T = 0$. Then the second term has $(\delta V)^3$ and irrespective of what sign $\left.\frac{\partial^2 P}{\partial V^2}\right|_T$ has, δV can always be chosen to make the overall term positive. Hence the only option we have is that

$$\left.\frac{\partial^2 P}{\partial V^2}\right|_T = 0$$

Similar to the first term, we have the third term as,

$$\frac{\partial^3 P}{\partial V^3}\Big|_T \leq 0$$

These define the stability conditions for our thermodynamic system.

2.1. Stability Relations for Potentials

We will now discuss what are the consequence of stability on the thermodynamic potentials, F and G. We will use the fact that for a mechanically stable system, the *specific heat* and the *isothermal compressibility* must be positive for all temperatures. It can be motivated since compressibility and specific heat are related to number and energy fluctuations, σ_{N} and σ_{E} respectively, both of which are positive.

From appendix A, we see that $S = -\left(\frac{\partial F}{\partial T}\right)_{V,N}$ from which we get:

$$\left(\frac{\partial^2 F}{\partial T^2}\right)_{V,N} = -\left(\frac{\partial S}{\partial T}\right)_{V,N} = -\frac{1}{T}C_v \leq 0$$

Similarly, we can use $S = -\left(\frac{\partial G}{\partial T}\right)_{P,N}$ from which we get:

$$\left(\frac{\partial^2 G}{\partial T^2}\right)_{P,N} = -\left(\frac{\partial S}{\partial T}\right)_{P,N} = -\frac{1}{T}C_p \leq 0$$

From this, we infer that $G(T,P,N)$ and $F(T,V,N)$ are concave functions of temperature. Apart from temperature, since F depends on V and G depends on P, let us check for pressure and volume too. We note that $V = \left(\frac{\partial G}{\partial P}\right)_{T,N}$ and $P = -\left(\frac{\partial F}{\partial V}\right)_{T,N}$

$$\begin{aligned}\left(\frac{\partial^2 G}{\partial P^2}\right)_{T,N} &= \left(\frac{\partial V}{\partial P}\right)_{T,N} = -V\mathcal{K}_{\mathrm{T}} \leq 0 \\ \left(\frac{\partial^2 F}{\partial V^2}\right)_{T,N} &= -\left(\frac{\partial P}{\partial V}\right)_{P,N} = \frac{1}{V\mathcal{K}_{\mathrm{T}}} \geq 0\end{aligned} \tag{7}$$

where we have appropriately used the definitions of isothermal compressibility and heat capacity. Using this, we find that G is a concave function of pressure and F is a convex function of volume. From the above expressions in Eq 7, we can also write

$$\left(\frac{\partial^2 G}{\partial P^2}\right)_{T,N} = -\left\{\left(\frac{\partial^2 F}{\partial V^2}\right)_{T,N}\right\}^{-1} \tag{8}$$

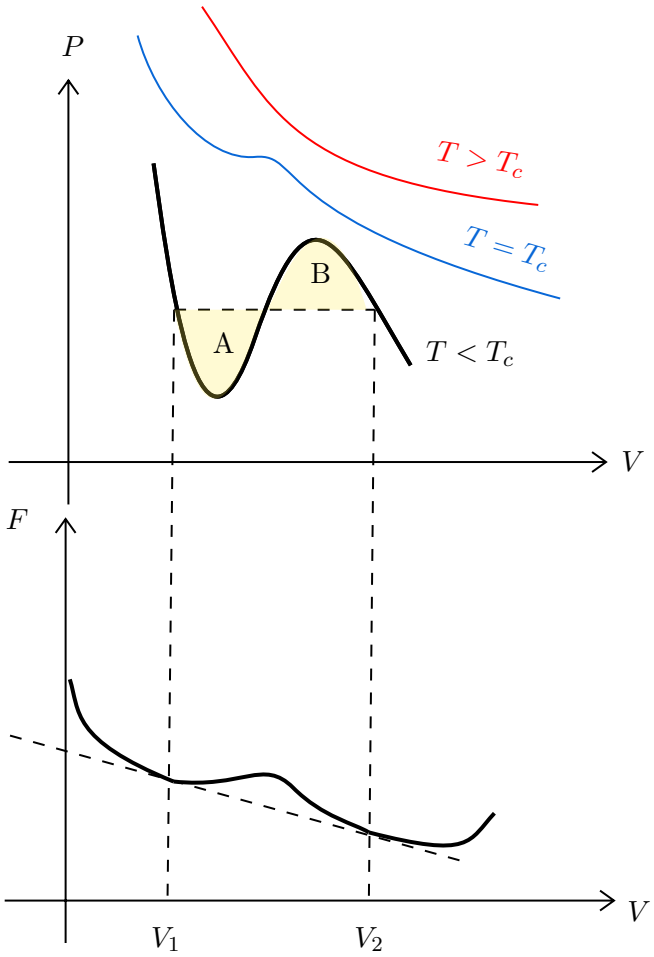
2.2. Stability Analysis of Van der waal's solutions

Recall the Van der Waal's equation from Eq (3),

$$\left(P + \frac{aN^2}{V^2}\right)(V - Nb) = Nk_{\mathrm{B}}T$$

At high temperature, the P vs. V curves at constant temperature (*isotherm*) follows the usual ideal-gas curve. However, there exists a critical temperature T_{c} (which can be found out from the equation), such that, for $T < T_{\mathrm{c}}$, there always exist a region, where the slope $\frac{\partial P}{\partial V}$ is positive. Since $\mathcal{K}_{\mathrm{T}} = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_{N,T}$, this implies a negative compressibility, which, as motivated before, is *unphysical*.

This leads to a breakdown of the theory and Maxwell subsequently proposed an *ad hoc* remedy, similar in line to the construction of superior tangents that we noted earlier.



Consider the diagram above. Here, for a subcritical temperature, we see a region between V_1 and V_2 where the slope is positive. This region corresponds to the *concave intruder* (since free energy is a convex function of volume) in the free energy plot. Similarly as before, we replaced the concave part with a straight line denoting the commong tangent. This corresponds to joining the region between V_1 and V_2 in the P-V plot with a straight horizontal line. It can also be shown that the horizontal line is at just such a value of the pressure that the areas labelled A and B are equal and hence this construction is also called *equal-area* construction.

Lecture 03: First Order Phase Transition

Let us now see some qualitative aspect of phase transition. Each phase transition can be viewed as a result of the failure of the stability criteria. We will see some characteristic aspects of first order phase transition[1]. However, let us first note some geometric interpretation of the thermodynamic potentials.

3.1. Geometric Interpretation of Potentials

We will consider the relation $G = F + PV$ which can be obtained from the Legendre transform of the internal energy.

[1] In modern language, these are called *abrupt phase transition*

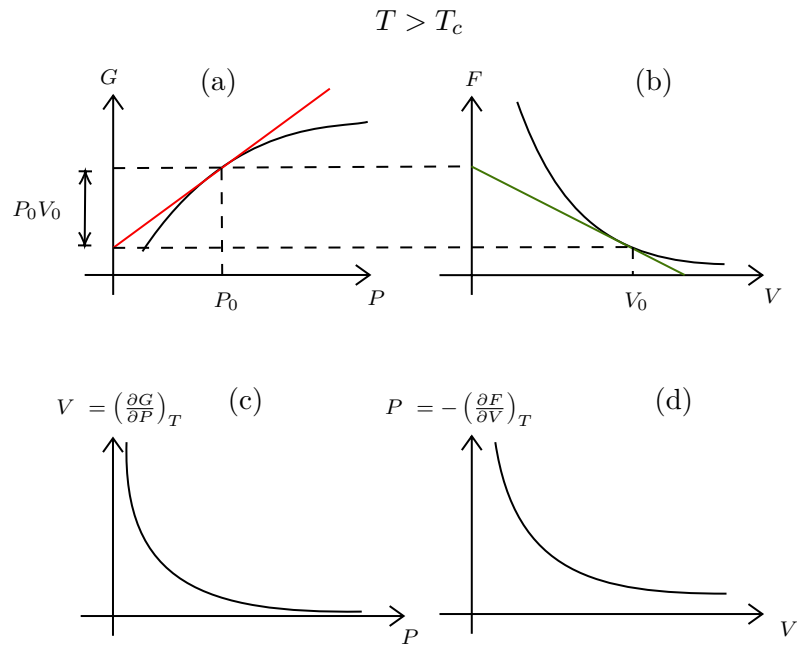


Figure 2: Relation between G and F. (a) Variation of Gibbs potential with pressure at a temperature $T > T_c$ (b) Corresponding plot of Helmholtz potential with V (c) and (d) denotes the P-V diagrams constructed from these potentials

In the above figure, observe the plot of G vs. P, which is smooth. We draw the tangent line at a $P = P_0$ and this intercepts the y-axis somewhere. The equation of the tangent is $G = PV + c$ as $V = \left(\frac{\partial G}{\partial P}\right)_{T,N}$ and it passes through the point (P_0, G_0). Thus we have,

$$G_0 = P_0V_0 + c \implies c = G_0 - P_0V_0$$

The tangent has an intercept of $G_0 - P_0V_0$ and so the remaining length as shown by the arrow in is Fig.2 (a) is $G_0 - (G_0 - P_0V_0) = P_0V_0$. From the length of the intercept of the tangent, we can obtain the Helmholtz potential for this value of P_0. We also obtain the volume from the slope of the tangent. The corresponding F vs. V graph has been plotted using these values. Also, plotted are the V vs. P graph (using the slope of the tangent of the Gibbs potential) and the P vs. V graph (using the slope of the tangent of the Helmholtz potential). This is the case for $T > T_c$. Now let us see the case when $T < T_c$ and the phase transition has occurred. We will see this with respect to the Van der Waal's equation.

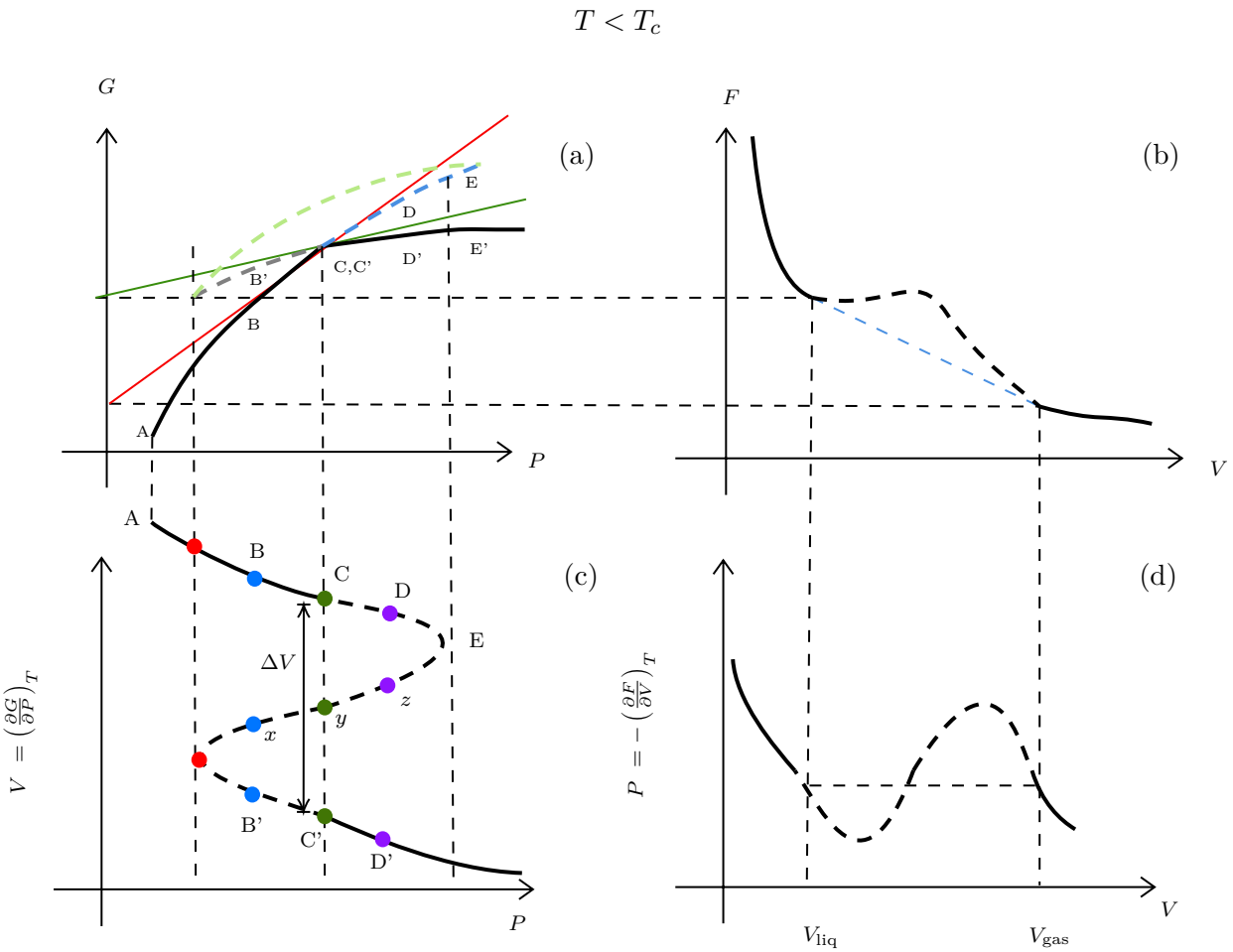


Figure 3: Plot of different quantities for $T < T_c$

In this scenario, G will have a 'kink' for some pressure $P = P_0$, since for first order phase transition, the derivative of the free energy is discontinuous. At this point, $\left(\frac{\partial^2 G}{\partial P^2}\right) \to \infty$ (even though this quantity cannot be defined exactly at $P = P_0$) and using Eq.(8), we get $\left(\frac{\partial F}{\partial V}\right) = 0$. Thus we expect that the corresponding plot of F has a *straight line* portion, as is shown in Fig.3 (b) with a blue dashed line.

Let us now see how the plot of G in (a) is actually constructed. For that, we need the isotherm in (c). Let us start at A and then, integrating we have

$$G(P) - G(P_{\text{A}}) = \int_{P_{\text{A}}}^{P} V \mathrm{d}P$$

and we do this for all values of P. This creates a closed loop kind of plot, since for a single P, we have three values of V. Note that, this disappears for higher temperature since then, Van der Waal's equation consists of only one real and two complex roots.

What happens physically? Let us suppose our system is in a temperature bath and the temperature is fixed. So, consider the isotherm in (c) and start increasing pressure from P_A. The system will follow this isotherm. At P_A, there is a unique volume and thus a unique state of the system. Now, if we increase further, for each pressure, we will get multiple values of volume, so there are different states to choose from.

Consider the blue points (all having same P but different V). Of these, the state x is unstable and hence the system has two states B and B' to choose from. The state chosen is the one with the minimum value of G which is determined from panel (a). As clearly seen, the physical state chosen is B. Increasing pressure further, we get to C where the kink is there.

On increasing further, we see that the state chosen is D' since this has lesser value of G. The blue and

gray dashed lines in (a) denote the branch of G with higher value of G and thus, is not chosen. The green dashed line represent the unstable region where the states, say x, y or z lies. We see that in (c), no state from the dashed region is selected and hence after C, there is a volume jump, denoted by ΔV. The physical isotherm is thus the one created from the Maxwell equal area construction (as discussed before) and the straight line in the isotherm denotes the *coexistence* of two phases.

The points C and C' are determined by the condition that $G(P_c) = G(P_{c'})$ and hence, $\int_{P_c}^{P_{c'}} V \mathrm{d}P = 0$, which proves that the areas divided by the line segment are indeed equal.

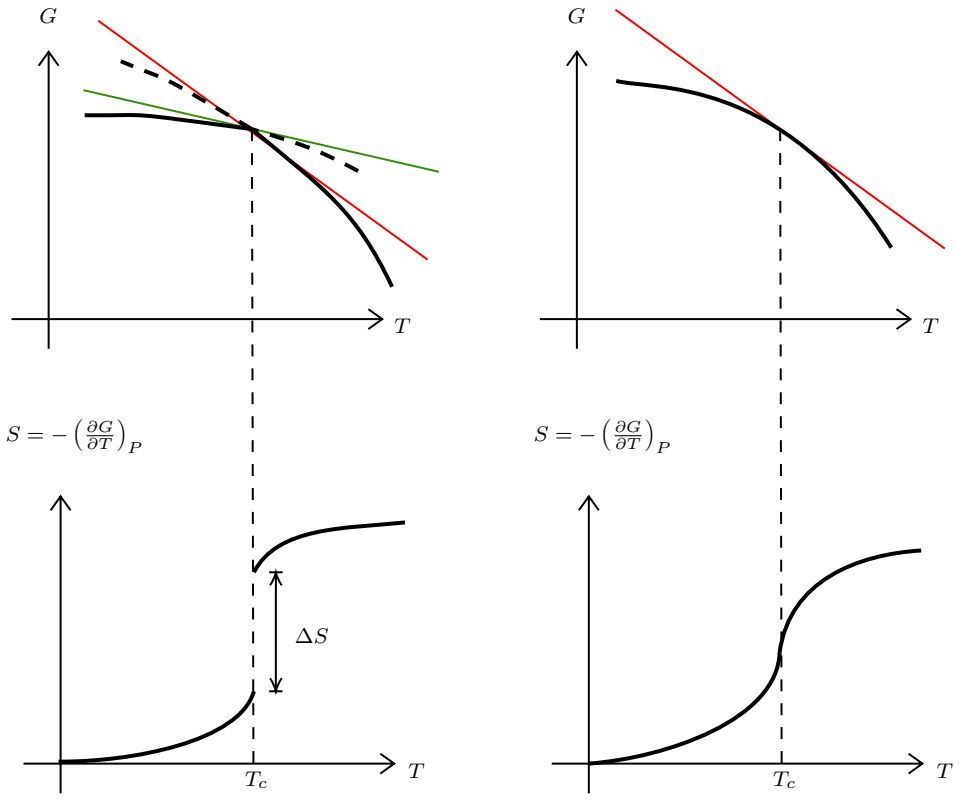


Figure 4: The left column shows the variation of G and S with temperature for first order phase transition, clearly showing an entropy discontinuity. The right column shows this for a higher order phase transition.

There is also an entropy change associated with phase transitions. For first order phase transitions, there is an abrupt entropy jump since entropy is defined as $S = -\left(\frac{\partial G}{\partial T}\right)_P$ and G has a 'kink', making it non-differentiable at the critical point. This entropy jump is associated with the latent heat $L = T_c \Delta S$. For higher order phase transitions, where G is smooth (but some higher order derivative is discontinuous), there is no latent heat since S is continuous. However, the specific heat $C \sim \frac{\mathrm{d}S}{\mathrm{d}T}$ diverges at the critical point.

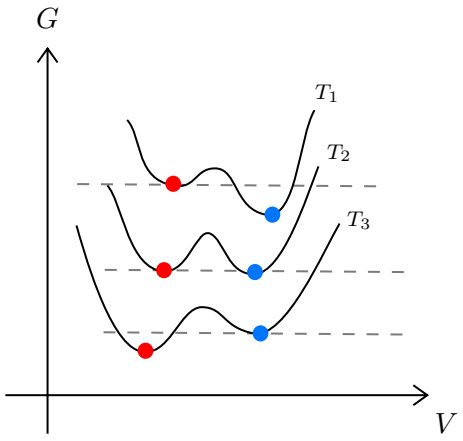


Figure 5: G vs. V plots for different temperatures.

From the previous analysis, we saw that in some interval, we had three values of volume for each pressure (out of which one was unphysical). A physical scenario to imagine is when suppose we have water above its boiling point (so it is in vapour phase). The Gibbs potential has its minima at two volumes as shown in Fig.5 for curve at T_1. The system takes the minima which is lower (the right one).

As we decrease the temperature, at some temperature, both the minima become equal, as for T_2. This is the *critical temperature*. As temperature is reduced further, the other minima becomes the more stable one. The system was in the right minima which was till now the *stable* one. It still remains in the right one, however, it now becomes *metastable*. In a very small timescale, due to some fluctuations, a *nucleus* of condensed liquid (the stable state) forms which grows rapidly and the entire system undergoes the transition.

3.2. Grand canonical basis of phase coexistence

Having seen the physical picture, we will discuss how the liquid-gas phase transition is brought about by considering the partition function that we had found out earlier from Eq(2). However, we used the uniform density approximation for this which is not entirely correct at phase coexistence since the gas (low density) and liquid phases (high density) have weirdly different densities (however, each phase can be assumed to have a uniform density separately).

This problem can be circumvented by considering the *grand canonical ensemble* where we fix the chemical potential μ and the number of particles (and in turn, the density) is appropriately adjusted for different phases. The grand partition function Ξ is defined as,

$$\Xi(\mu, T, V) = \sum_{N=0}^{\infty} e^{\beta\mu N} \mathcal{Z}(N, T, V) \tag{9}$$

where $\mathcal{Z}$ is the canonical partition function. We can appropriately modify the canonical partition function to write is as an expontential:

$$\begin{aligned}
e^{\beta\mu N + \ln \mathcal{Z}} &= \exp\left[\beta\mu N\right] \cdot \exp\left[\frac{\beta a N^2}{V}\right] \cdot \exp\left[N \ln\left(V - \frac{N\omega}{2}\right)\right] \cdot \exp\left[-\ln N! - N \ln \lambda_{\mathrm{T}}^3\right] \\
&= \exp\left[\beta\mu N\right] \cdot \exp\left[\frac{\beta a N^2}{V}\right] \cdot \exp\left[N \ln N + N \ln\left(\frac{V}{N} - \frac{\omega}{2}\right)\right] \cdot \exp\left[-\ln N! - N \ln \lambda_{\mathrm{T}}^3\right] \\
&= \exp\left[\beta\mu N + \frac{\beta a N^2}{V} + N \ln N + N \ln\left(\frac{V}{N} - \frac{\omega}{2}\right) - \ln N! - N \ln \lambda_{\mathrm{T}}^3\right] \\
&= \exp\left[\beta\mu N + \frac{\beta a N^2}{V} + \cancel{N \ln N} + N \ln\left(\frac{V}{N} - \frac{\omega}{2}\right) - \cancel{N \ln N} + N - N \ln \lambda_{\mathrm{T}}^3\right] \\
&= \exp\left[\frac{\beta a N^2}{V} + N \ln\left(\frac{V}{N} - \frac{\omega}{2}\right) + N\Delta\right]
\end{aligned}$$

where we have used Sterling's approximation, $\ln N! \approx N \ln N - N$ and $\Delta := (1 + \beta\mu - \ln \lambda_{\mathrm{T}}^3)$. We can now use the saddle-point approximation to evaluate the sum, which gives only a significate contribution for some $N = N^*$.

$$\Xi \approx \exp\left[\frac{\beta a N^{*2}}{V} + N^* \ln\left(\frac{V}{N^*} - \frac{\omega}{2}\right) + N^*\Delta\right] \tag{10}$$

From appendix A, the grand potential is,

$$-PV = \Phi = -k_{\mathrm{B}}T \ln \Xi \implies \beta P = \frac{\ln \Xi}{V} \approx \left[\frac{\beta a N^{*2}}{V^2} + \frac{N^*}{V} \ln\left(\frac{V}{N^*} - \frac{\omega}{2}\right) + \frac{N^*}{V}\Delta\right]$$

We define $n^* = \frac{N^*}{V}$, where n^* is the solution of the equation $\frac{\partial \Psi}{\partial n} = 0$ where $\Psi(n)$ is defined as,

$$\Psi(n) = \beta a n^2 + n \ln\left(\frac{1}{n} - \frac{\omega}{2}\right) + n\Delta$$

Carrying out the differentiation $\frac{\partial \Psi}{\partial n}$, we obtain

$$2\beta a n + \ln\left(\frac{1}{n} - \frac{\omega}{2}\right) + \frac{n}{\frac{1}{n} - \frac{\omega}{2}} \times \left(-\frac{1}{n^2}\right) + \Delta = 0 \implies \boxed{\Delta = \frac{1}{1 - \frac{\omega n}{2}} - 2\beta a n - \ln\left(\frac{1}{n} - \frac{\omega}{2}\right)} \tag{11}$$

Substituting this value of Δ in $\Psi(n)$ we get,

$$\Psi(n^*) = \beta a N^{*2} + \cancel{n^* \ln\left(\frac{1}{N^*} - \frac{\omega}{2}\right)} + \frac{n^*}{1 - \frac{n^*\omega}{2}} - 2\beta a n^{*2} - \cancel{n^* \ln\left(\frac{1}{n^*} - \frac{\omega}{2}\right)} = \frac{1}{\frac{1}{n^*} - \frac{\omega}{2}} - \beta a N^{*2}$$

Comparing this with Van der Waal's equation, this gives us $P = P_{\text{can.}}$ where $P_{\text{can.}}$ is the canonical ensemble pressure. This tells us that the grand canonical and the canonical pressure are identical at particular value of the density n^*. Here we have assumed only a unique n^* which maximises the sum. However, the sum in Eq (10) can be peaked at multiple different values of densities and the appropriate uniform density is chosen for that value which maximises $\Psi(n)$.

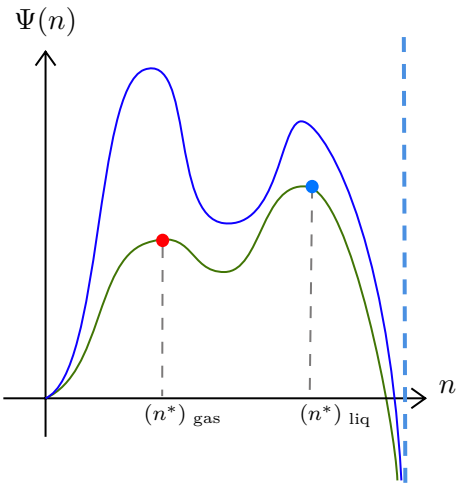


Figure 6: Plot of $\Psi(n)$ vs. n at different temperature. Green plot is for $T < T_c$ and blue is for $T > Tc$. The lower density corresponds to gas and higher density correpsonds to liquid. At $n = \frac{2}{\omega}$, $\Psi(n) \to -\infty$ which has been shown by the blue vertical dashed line.

In the above figure, the blue curve denotes $T > T_c$ and the green curve denotes $T < T_c$. For both $T < T_c$ and $T > T_c$, we have two peaks in the $\Psi(n)$ vs. n plot, however, only the right peak is chosen for $T < T_c$ (corresponding to liquid density) and the left peak is chosen for $T > T_c$ (corresponding to gas density). Considering contribution from both peaks,

$$\ln \Xi \approx \ln\left(e^{V\Psi(n^*_{\text{liq}})} + e^{V\Psi(n^*_{\text{gas}})}\right) = V\Psi(n^*_{\text{liq}}) + \ln\left(1 + e^{V(\Psi(n^*_{\text{gas}}) - \Psi(n^*_{\text{liq}}))}\right)$$

In the thermodynamic limit, if $T > T_c$, $\Psi(n^*_{\text{gas}}) > \Psi(n^*_{\text{liq}})$ then $\ln \Xi \approx V\Psi(n^*_{\text{gas}})$ and hence the gas phase dominates. For $T < T_c$, $\Psi(n^*_{\text{gas}}) < \Psi(n^*_{\text{liq}})$ and hence the liquid phase dominates. From this, we can say that only in the thermodynamic limit, there is a *singularity* in the density at $T = T_c$ (there are no phase transitions in finite systems)!

Lecture 04: Yang-Lee Theory for Phase Transition

We will now discuss about a mathematical basis of condensation based on Yang and Lee's theory of phase transition [1] which is based on the analysis of the zeroes of the grand partition function. The partition function seems to be an analytic function since it essentially consists of sums of well-behaved exponentials.

However, phase transitions are characterised by non-analyticity which leads us to think about how the analytic partition function will capture the essence of the non-analytic phase transition. As discussed before, *true* phase transitions occur only in the thermodynamic limit and in the thermodynamic limit, partition function can indeed become non-analytic (since the limit functions of a sequence of analytic function need not be analytic).

4.1. Singularities and Phase Transition

We will write Eq (9) in terms of the *fugacity* $z = e^{\beta\mu}$ and also consider a finite system with volume V (and then take ultimately take $V \to \infty$). Only a finite number of particles, say M, can be crammed into this finite volume, hence

$$\Xi(z, V) = \sum_{N=0}^{M} z^N \mathcal{Z}(N, V, T) = 1 + z\mathcal{Z}_1 + z^2\mathcal{Z}_2 + \ldots + z^M \mathcal{Z}_M \tag{12}$$

Note that the above equation is a well-behaved polynomial of degree M in z and its coefficients $\mathcal{Z}_N$ are all positive which implies that $\Xi(z, V)$ has no real positive root. From the grand potential $\Phi = -PV = -k_B T \ln \Xi$, we can write the pressure P and density ρ in the thermodynamic limit,

$$\begin{aligned} P &= \lim_{V\to\infty} \frac{k_B T}{V} \ln \Xi(z, V) \\ \langle N \rangle = z\frac{\partial \ln \Xi}{\partial z} \implies \rho &= \lim_{V\to\infty} \frac{\langle N \rangle}{V} = \lim_{V\to\infty} \frac{z}{V} \frac{\partial \ln \Xi(z, V)}{\partial z} \end{aligned} \tag{13}$$

These quantities will not have any singularity unless $\Xi(z, V) = 0$ which cannot hold true, unless we cosider a *complex* fugacity. Then for finite V, the algebraic equation $\Xi = 0$ has M roots appearing in complex-conjugate pairs. As V increases, the number of roots also increases (linearly with V) and moves around in the complex plane, excluding the real axis. In the limit $V \to \infty$, some of these roots touch the real axis and this describes a phase transition. With regard to this, we discuss two theorems as stated in the original paper.

Theorem 1:
For all positive values of z, the limit

$$L = \lim_{V\to\infty} \frac{1}{V} \ln \Xi(z, V)$$

exists and is independent of the shape of the volume holding the particles, with the assumption that the surface area does not scale faster than $V^{2/3}$.

Moreover, $L(z)$ is a continuous, monotonically increasing function of z.

Theorem 2:
Suppose in the complex z plane, there exists a region $\mathcal{R}$ containing the positive real axis, which has no roots of Ξ, then $\lim_{V\to\infty} \frac{1}{V} \frac{\partial^k \ln \Xi}{\partial z^k}$ is uniformly convergent and the limit function is analytic for all $z \in \mathcal{R}$.

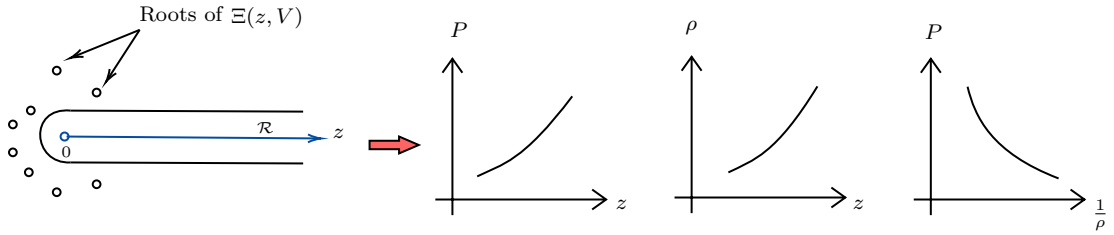
Moreover, the operations $\lim_{V\to\infty}$ and $z\frac{\partial}{\partial z}$ can be interchanged.

The above theorem implies that,

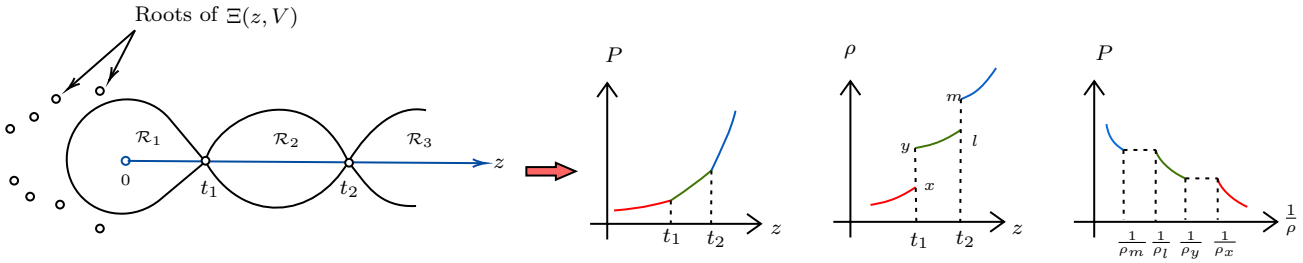
$$\rho = \lim_{V\to\infty} \frac{z}{V}\frac{\partial \ln \Xi}{\partial z} \iff z\frac{\partial}{\partial z}\left(\lim_{V\to\infty}\frac{1}{V}\ln\Xi\right) = z\frac{\partial(\beta P)}{\partial z} \tag{14}$$

If such a region $\mathcal{R}$ does not exist, then the limit does not exist which makes sense physically, since the density ρ as defined in Eq (13), does not assume a single value at the condensation point. Hence, everything depends on the existence of $\mathcal{R}$

- As $V \to \infty$, if a region $\mathcal{R}$ exists which fully encloses the positive real axis, then P exists from Thm (1) and is an analytic, increasing function of z. From Thm (2), ρ also exists and is an analytic function of z. It can be shown that ρ is also increasing with z. P and ρ are related by Eq (14). The system under consideration is in a *single phase*.



- On the other hand, if the roots of $\Xi(z, V)$ approach some specific values $z = t_1, t_2 \ldots$ on the real axis as $V \to \infty$, from the figure below, there will exist regions $\mathcal{R}_1, \mathcal{R}_2 \ldots$ within which Thm (2) will be satisfied piecewise and hence, within these regions, the system exists in a single phase as argued before. At the points $t_1, t_2 \ldots$, the pressure P will be continuous from Thm (1), but ρ might have some non-analyticity since this does not satisfy the condition for Thm (2). The system now possess *multiple phases*.



  It is to be noted that the discontinuity in the density is only possible in the thermodynamic limit. For finite system, we will get a *continuous crossover* due to *finite-size effects*.

  If $\frac{\partial P}{\partial z}$ is discontinuous, then we have a *first-order phase transition* as shown in the figure above. If $\frac{\partial P}{\partial z}$ is continuous but $\frac{\partial^2 P}{\partial z^2}$ is discontinuous, then we obtain a *second-order phase transition*.

From this discussion, we observe that the study of phase transitions can be reduced to just studying the distribution of the zeroes of the grand partition function.

Lecture 05: More on Van der Waal's Equation

In the previous section, we saw a mathematical theory of condensation based on the zeroes of the grand partition function. Let us now move back to the Van der Waal's equation and try to analyse the critical point.

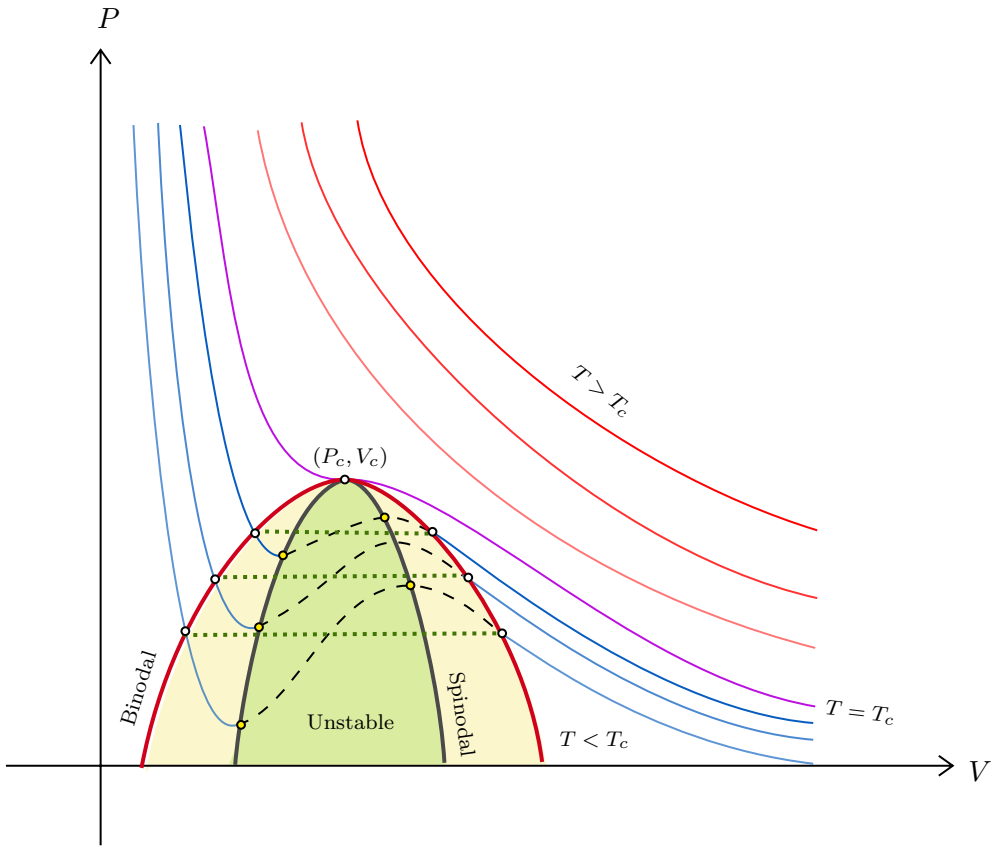


Figure 7: Van der Waal's isotherm. The figure shows Van der Waal's isotherms for $T < T_c$ ($T > T_c$) with blue (red) lines. The curve for $T = T_c$ is shown with purple line. Maxwell's construction is shown with green dotted line. The red line denotes the *binodal line* and the gray line denotes the *spinodal* line. The yellow region denote the metastable state while the green region denote the unstable states.

In Fig.??, we see the Van der Waal's isotherms at different temperature regime. There exists a temperature T_c such that at a particular point (V_c, P_c), the isotherm has zero slope and zero curvature. Thus the critical point is characterised by

$$\frac{\partial P}{\partial V} = 0 \qquad \frac{\partial^2 P}{\partial V^2} = 0$$

Defining $v = \frac{V}{N}$, from Van der Waal's equation we can write,

$$P = \frac{k_B T}{v - b} - \frac{a}{v^2} \implies \frac{\partial P}{\partial V} = -\frac{k_B T}{(v-b)^2} + \frac{2a}{v^3} \implies \frac{\partial^2 P}{\partial V^2} = \frac{2k_B T}{(v-b)^3} - \frac{6a}{v^4} \tag{15}$$

Equating the derivative to zero, we get $2a(v_c - b)^2 = k_B T v_c^3$ and equating the second derivative to zero, we get $3a(v_c - b)^3 = k_B T v_c^4$. Dividing both these equations, we get

$$\frac{3}{2}(v_c - b) = v_c \implies 3(v_c - b) = 2v_c \implies v_c = 3b$$

Substituting this in any one of the above equation we get $k_B T_c = \frac{8a}{27b}$ and substituting v_c and T_c in Van der Waal's equation, we get $P_c = \frac{a}{27b^2}$. Thus our critical parameters are,

$$\boxed{P_c = \frac{a}{27b^2} \qquad v_c = 3b \qquad k_B T_c = \frac{8a}{27b}}$$

5.1. Approaching Universality

The Van der Waal's equation depends on the microscopic details of the system, a and b. These vary for different gases and hence, the equation cannot describe universal properties. However, let us define the

reduced parameters,

$$\Pi = \frac{P}{P_c} \qquad \nu = \frac{v}{v_c} \qquad \tau = \frac{T}{T_c}$$

We now put these in the equation of state, which gives us

$$\begin{aligned}\left(\Pi P_c + \frac{a}{\nu^2 v_c^2}\right)(\nu v_c - b) = k_{\mathrm{B}}\tau T_c \implies \left(\frac{\Pi a}{27b^2} + \frac{a}{9\nu^2 b^2}\right)(3b\nu - b) = \frac{8a\tau}{27b} \\ \implies \frac{3ab}{27b^2}\left(\Pi + \frac{3}{\nu^2}\right)\left(\nu - \frac{1}{3}\right) = \frac{8a\tau}{27b} \\ \implies \boxed{\left(\Pi + \frac{3}{\nu^2}\right)\left(\nu - \frac{1}{3}\right) = \frac{8\tau}{3}}\end{aligned} \tag{16}$$

The above dimensionless Van der Waal's equation in terms of the reduced parameters, is independent of a and b and is thus *universal*, in the sense that, different gases are expected to follow the same equation. The generalisation is known as the *principle of corresponding states*, which says that all fluids when compared with respect to reduced parameters, have the same *compressibility factor*. The compressibility factor is defined as $Z = \frac{Pv}{k_{\mathrm{B}}T}$, with the critical value predicted by Van der Waal to be,

$$Z_c = \frac{P_c v_c}{k_{\mathrm{B}} T_c} = \frac{3ab}{27b^2 \times \frac{8a}{27b}} = \frac{3}{8} = 0.375$$

Experimentally, the critical value of the compressibility factor is found to be in the range $0.28 - 0.33$, thus, Van der Waal's equation does not provide an accurate quantitative estimate.

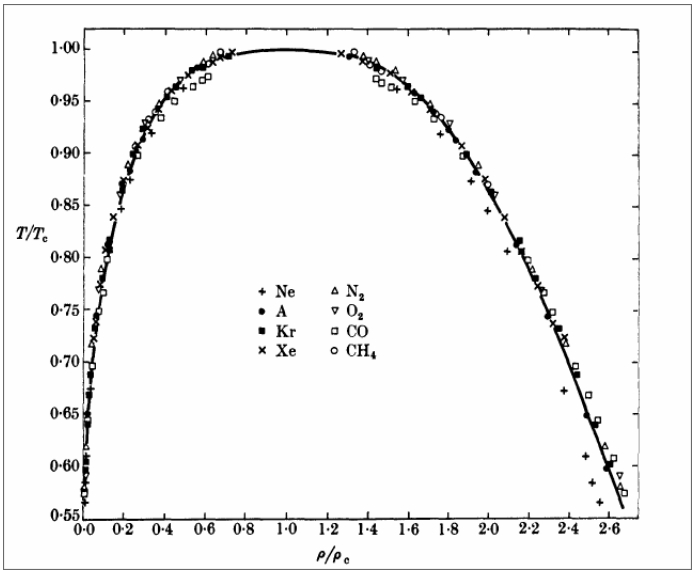


Figure 8: The Guggenheim plot for different gases with reduced parameter, showing that the trend follows a universal function (Source: Guggenheim (1945) [2]).

5.2. Critical Opalescence

Critical opalescence refers to an enhanced scattering of light by a substance in this critical region. Such enhanced scattering renders the substance milky white in reflected light.

As we know, at the critical point, $\mathcal{K}_{\mathrm{T}} = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_T \to \infty$ since the slope of the isotherm is zero at the critical point. As $\mathcal{K}_{\mathrm{T}} \propto \sigma_{\mathrm{N}}$ where σ_{N} is the number fluctuations in the system, there is a huge number fluctuation, due to which the scattering of light is intensified.

5.3. Critical Point Behaviour

We will now discuss the behaviour of gases in the vicinity of the critical point to analyse universality. For $T > T_c$, there is always a unique volume corresponding to each pressure and hence, we can apply

Taylor expansion around v_c to write the pressure as,

$$P(T,v) = P(T,v_c) + \left.\frac{\partial P}{\partial v}\right|_T (v-v_c) + \frac{1}{2}\left.\frac{\partial^2 P}{\partial v^2}\right|_T (v-v_c)^2 + \frac{1}{6}\left.\frac{\partial^3 P}{\partial v^3}\right|_T (v-v_c)^3 + \mathcal{O}\left[\left(\frac{v-v_c}{v_c}\right)^4\right]$$

Each of the coefficients are functions of temperature and hence, can be Taylor expanded about T_c.

$$\begin{aligned}
P(T,v_c) &= \underbrace{P(T_c,v_c)}_{P_c} + \alpha(T-T_c) + \mathcal{O}\left[\left(\frac{T-T_c}{T_c}\right)^2\right] \\
\left.\frac{\partial P}{\partial v}\right|_{T,v_c} &= \cancelto{0}{\left.\frac{\partial P}{\partial v}\right|_{T_c,v_c}} - a(T-T_c) + \mathcal{O}\left[\left(\frac{T-T_c}{v_c}\right)^2\right] \\
\left.\frac{\partial^2 P}{\partial v^2}\right|_{T,v_c} &= \cancelto{0}{\left.\frac{\partial^2 P}{\partial v^2}\right|_{T_c,v_c}} + b(T-T_c) + \mathcal{O}\left[\left(\frac{T-T_c}{T_c}\right)^2\right] \\
\left.\frac{\partial^3 P}{\partial v^3}\right|_{T,v_c} &= -c + \mathcal{O}\left[\left(\frac{T-T_c}{T_c}\right)\right]
\end{aligned}$$

At the critical point the slope and the curvature vanishes and hence the first terms in the second and third equation is zero. Using the stability condition in Eq. (6), $a > 0$ for $T > T_c$ and $c > 0$. b can have any arbitrary sign[1]. Let us put these expression in the original Taylor expansion.

$$P(T,v) = P_c + \alpha(T-T_c) - a(T-T_c)(v-v_c) + \frac{b}{2}(T-T_c)(v-v_c)^2 - \frac{c}{6}(v-v_c)^3 + \text{higher orders}\ldots \tag{17}$$

From this, we can predict the following things about different quantities:

- Let us consider only upto linear order in $(T-T_c)$ and $(v-v_c)$, hence we neglect the fourth, fifth and higher order terms. This gives us an approximate analytic solution for the pressure,

  $$\boxed{P(T,v) = P_c + \alpha(T-T_c) - a(T-T_c)(v-v_c)}$$

  We obtain $\frac{\partial P}{\partial v} = -a(T-T_c)$ and hence the isothermal compressibility at v_c scales as,

  $$\lim_{T\to T_c^+} \mathcal{K}(T,v_c) = -\frac{1}{v_c}\frac{\partial v}{\partial P} \sim \frac{1}{T-T_c}$$

  Experimental results identify the exponent as $\gamma \approx 1.3$ where $\mathcal{K}(T,v_c) \sim (T-T_c)^{-\gamma}$.

- At $T = T_c$, the isotherm behaves as

  $$P = P_c - \frac{c}{6}(v-v_c)^3 \implies (P-P_c) \sim (v-v_c)^3$$

  Experimental results identify the exponent as $\delta \approx 5.0$ where $(P-P_c) \sim (v-v_c)^\delta$.

The above analysis cannot be applied for $T < T_c$ since then for each pressure, we have two volumes and Taylor expansion cannot be effectively applied. Let us do the analysis in an alternate way using Eq. (16). Consider the two volumes v_{liq} and v_{gas} for which the pressure is same at say some temperature T. Then, from the equation we can write,

$$\Pi = \frac{8\tau/3}{\nu_g - 1/3} - \frac{3}{\nu_g^2} = \frac{8\tau/3}{\nu_l - 1/3} - \frac{3}{\nu_l^2}$$

[1] These a, b are not the ones appearing in the Van der Waal's equation.

From this we obtain,

$$8\tau\left[\frac{1}{\nu_g-1}-\frac{1}{\nu_l-1}\right]=3\left[\frac{1}{\nu_l^2}-\frac{1}{\nu_g^2}\right]=3\left[\frac{\nu_g^2-\nu_l^2}{\nu_l^2\nu_g^2}\right]\implies\boxed{\tau=\frac{(3\nu_l-1)(3\nu_g-1)(\nu_l+\nu_g)}{8\nu_g^2\nu_l^2}}$$

Note that the equation is symmetric in ν_g and ν_l and $\nu_g=\nu_l=1$ at the critical point, which implies that we can write

$$\nu_g=1+\frac{\varepsilon}{2}\qquad\nu_l=1-\frac{\varepsilon}{2}$$

where $\varepsilon\equiv\nu_g-\nu_l$. We substitute this in the expression for τ, leading us to

$$\tau=\frac{2\left(2-\frac{3\varepsilon}{2}\right)\left(2+\frac{3\varepsilon}{2}\right)}{8\left[\left(1+\frac{\varepsilon}{2}\right)\left(1-\frac{\varepsilon}{2}\right)\right]^2}=\frac{\left(4-\frac{9\varepsilon^2}{4}\right)}{4\left(1-\frac{\varepsilon^2}{4}\right)^2}=\left(1-\frac{9\varepsilon^2}{16}\right)\left(1-\frac{\varepsilon^2}{4}\right)^{-2}\approx\left(1-\frac{9\varepsilon^2}{16}\right)\left(1+\frac{\varepsilon^2}{2}\right)=1-\frac{\varepsilon^2}{16}+\mathcal{O}(\varepsilon^4)$$

Then substituting for the real variables, we have

$$(v_{\text{gas}}-v_{\text{liq}})\sim(T_c-T)^{1/2}$$

Experimental results predict an exponent $\beta\approx0.3$ where $(v_{\text{gas}}-v_{\text{liq}})\sim(T_c-T)^{\beta}$.

Van der Waal's equation thus does not provide a perfect quantitative description of condensation, however, qualitative descriptions are more or less accurate. The exponents $\beta,\gamma,\delta\ldots$ are called *critical exponents* and many people dedicate their lives in finding the numerical value of these exponents.

Lecture 06: Correlations and Fluctuations

In here, we discuss a bit about an important quantity, *the correlation function*, which is an important quantity to look at while studying phase transition. Recall from Eq. (1) that the density was given by a sum over delta functions. We define the *density-density correlation function* (or simply the correlation function) as,

$$\mathcal{G}(\mathbf{r},\mathbf{r}')=\Big\langle[n(\mathbf{r})-\langle n(\mathbf{r})\rangle][n(\mathbf{r}')-\langle n(\mathbf{r}')\rangle]\Big\rangle=\langle n(\mathbf{r})n(\mathbf{r}')\rangle-\langle n(\mathbf{r})\rangle\langle n(\mathbf{r}')\rangle$$

where $n(\mathbf{r})-\langle n(\mathbf{r})\rangle$ denotes the fluctuation of the density from its average value and $\langle\cdot\rangle$ represent the *thermal (ensemble) average*, using the distribution. For translationally invariant system, we have $\mathcal{G}(\mathbf{r},\mathbf{r}')\equiv\mathcal{G}(\mathbf{r}-\mathbf{r}')$ and also, $n(\mathbf{r})=n(\mathbf{r}')$. Then the above equation can also be written as,

$$\mathcal{G}(\mathbf{r}-\mathbf{r}')=\langle n(\mathbf{r})n(\mathbf{r}')\rangle-n^2$$

where $\langle n(\mathbf{r})\rangle=n$. As $|\mathbf{r}-\mathbf{r}'|\to\infty$, that is, the distance between two particles become very large, we do expect them to be independent and no longer 'correlated'. Thus, $\mathcal{G}(\mathbf{r}-\mathbf{r}')\to0$ as $|\mathbf{r}-\mathbf{r}'|\to\infty$.

The correlation function kind of quantifies the fluctuations in the density. Earlier, we saw that the isothermal compressibility also characterises the number fluctuations. Then, these two must be related on some level. To see this, we note that

$$\begin{aligned}\Big\langle(N-\langle N\rangle)^2\Big\rangle&=\Big\langle\int\mathrm{d}^3r\,\{n(\mathbf{r}-\langle n(\mathbf{r})\rangle)\}\int\mathrm{d}^3r'\,\{n(\mathbf{r}'-\langle n(\mathbf{r}')\rangle)\}\Big\rangle\\&=\int\mathrm{d}^3r\mathrm{d}^3r'\,\Big\langle\{n(\mathbf{r}-\langle n(\mathbf{r})\rangle)\}\{n(\mathbf{r}'-\langle n(\mathbf{r}')\rangle)\}\Big\rangle=\int\int\mathrm{d}^3r\mathrm{d}^3r'\,\mathcal{G}(\mathbf{r}-\mathbf{r}')\end{aligned}$$

Introducing the variables $\mathbf{r}''=\mathbf{r}-\mathbf{r}'$ and $\mathbf{R}=\mathbf{r}+\mathbf{r}'$, the integral changes accordingly.

$$\Big\langle(N-\langle N\rangle)^2\Big\rangle=\int\mathrm{d}^3R\int\mathrm{d}^3r''\mathcal{G}(r'')=V\int\mathrm{d}^3r''\mathcal{G}(r'')$$

The number fluctuation can also be written as,

$$\Big\langle(N-\langle N\rangle)^2\Big\rangle=\frac{\langle N\rangle^2\,k_{\text{B}}T}{V}\mathcal{K}_{\text{T}}=\langle N\rangle\,nk_{\text{B}}T\mathcal{K}_{\text{T}}$$

Consider an ideal gas, with $PV = Nk_{\mathrm{B}}T$ which gives us,

$$\left(\frac{\partial P}{\partial V}\right)_T = -\frac{Nk_{\mathrm{B}}T}{V^2} \implies \mathcal{K}_{\mathrm{T}}^{\circ} = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right) = \frac{V}{Nk_{\mathrm{B}}T} = \frac{1}{nk_{\mathrm{B}}T}$$

Using this, we can write the dimensionless compressiblity as,

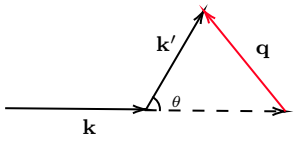
$$\left(\frac{\mathcal{K}_{\mathrm{T}}}{\mathcal{K}_{\mathrm{T}}^{\circ}}\right) = \frac{\left\langle (N - \langle N\rangle)^2\right\rangle}{\langle N\rangle} = \frac{V\int \mathrm{d}^3 r\ \mathcal{G}(r)}{\langle N\rangle} = \frac{1}{n}\int \mathrm{d}^3 r\ \mathcal{G}(r)$$

The above is a very simple example of the *fluctuation-dissipation theorem* which relates the correlation to the linear response of the system (compressibility, in our case).

Since the isothermal compressibility diverges at T_c, the integral also diverges and this implies that the correlation function also becomes long ranged. The correlation length ξ (the characteristic length scale after which $\mathcal{G}(\mathbf{r})$ decays) becomes as large as the wavelength of light and the density fluctuations scatter light strongly, resulting in critical opalescence, as mentioned in sec. 5.2.

6.1. Structure Factor

Let us now try to quantify the scattering intensity when our fluid is subjected to some radiation. Assume a *quasielastic scatetring*, that is, the incoming radiation has much larger energy than the typical excitation energy of the system. Hence, the system can only absorb or emit very small amounts of energy and very small energy transfer occurs.



From elastic scattering, $|\mathbf{k}| \approx |\mathbf{k}'|$, the momentum transfer vector $\mathbf{q} = \mathbf{k}' - \mathbf{k}$ has a magnitude,

$$|\mathbf{q}| = \sqrt{|\mathbf{k}|^2 + |\mathbf{k}'|^2 - 2|\mathbf{k}||\mathbf{k}'|\cos\theta} \approx \sqrt{2|\mathbf{k}|^2(1-\cos\theta)} = 2|\mathbf{k}|\sin\left(\frac{\theta}{2}\right)$$

Now, suppose that there are N particles in the target and the *scattering amplitude* for scattering from particle i is $a_i(\mathbf{q})$. Then the total intensity of the scattered radiation is given by,

$$\mathcal{I}(q) = \left\langle \left| \sum_{j=1}^{N} a_j(\mathbf{q}) \right|^2 \right\rangle$$

The scattering amplitude for particles at $\mathbf{r}_i$ and $\mathbf{r}_j$ are related just by a phase factor,

$$a_j(\mathbf{q}) = a_i(\mathbf{q}) e^{-i\mathbf{q}\cdot(\mathbf{r}_j - \mathbf{r}_i)}$$

Using this, we can write the internsity as,

$$\mathcal{I}(\mathbf{q}) = \left\langle \left| \sum_{j=1}^{N} a_1(\mathbf{q}) e^{-i\mathbf{q}\cdot(\mathbf{r}_j - \mathbf{r}_1)} \right|^2 \right\rangle = |a_1(\mathbf{q})|^2 \left\langle \left| \sum_{j=1}^{N} e^{-i\mathbf{q}\cdot(\mathbf{r}_j - \mathbf{r}_1)} \right|^2 \right\rangle = |a_1(\mathbf{q})|^2 \left\langle \left| \sum_{j=1}^{N} e^{-i\mathbf{q}\cdot\mathbf{r}_j} \right|^2 \right\rangle \tag{18}$$

as $\left|e^{i\mathbf{q}\cdot\mathbf{r}_1}\right| = 1$. If no correlations exist between the particles, then $\sum\limits_j e^{-i\mathbf{q}\cdot(\mathbf{r}_j - \mathbf{r}_1)} = N + \sum\limits_{j\neq 1} e^{-i\mathbf{q}\cdot(\mathbf{r}_j - \mathbf{r}_1)}$ and $\sum\limits_{j\neq 1} \left\langle e^{-i\mathbf{q}\cdot(\mathbf{r}_j - \mathbf{r}_1)} \right\rangle \approx 0$ due to randomised phases which leads to,

$$\mathcal{I}^{\circ}(\mathbf{q}) = N|a_1(\mathbf{q})|^2$$

Then we can write the dimensionless intensity as,

$$\begin{aligned}
\frac{\mathcal{I}(\mathbf{q})}{\mathcal{I}^{\circ}(\mathbf{q})} &= \frac{1}{N}\left\langle \left(\sum_{j=1}^{N} e^{i\mathbf{q}\cdot\mathbf{r}_j}\right)\left(\sum_{i=1}^{N} e^{-i\mathbf{q}\cdot\mathbf{r}_i}\right)\right\rangle = \frac{1}{N}\left\langle \left(\sum_{i,j} e^{i\mathbf{q}\cdot(\mathbf{r}_j-\mathbf{r}_i)}\right)\right\rangle \\
&= \frac{1}{N}\int \mathrm{d}^3r\mathrm{d}^3r' \left\langle \left(\sum_{i,j} \delta^{(3)}(\mathbf{r}-\mathbf{r}_i)\delta^{(3)}(\mathbf{r}'-\mathbf{r}_j)e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}\right)\right\rangle \\
&= \frac{1}{N}\int \mathrm{d}^3r\mathrm{d}^3r' \left\langle e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}\left(\sum_{i,j} \delta^{(3)}(\mathbf{r}-\mathbf{r}_i)\delta^{(3)}(\mathbf{r}'-\mathbf{r}_j)\right)\right\rangle \\
&= \frac{1}{N}\int \mathrm{d}^3r\mathrm{d}^3r' \; e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}\left\langle \left(\sum_{i} \delta^{(3)}(\mathbf{r}-\mathbf{r}_i)\right)\left(\sum_{j} \delta^{(3)}(\mathbf{r}'-\mathbf{r}_j)\right)\right\rangle \\
&= \frac{1}{N}\int \mathrm{d}^3r\mathrm{d}^3r' \; e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}\left\langle n(\mathbf{r})n(\mathbf{r}')\right\rangle \\
&= \frac{1}{N}\int \mathrm{d}^3r\mathrm{d}^3r' \; e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}(\mathcal{G}(\mathbf{r}-\mathbf{r}')+n^2)
\end{aligned}$$

Again using the same variable substitution, we obtain

$$\frac{\mathcal{I}(\mathbf{q})}{\mathcal{I}^{\circ}(\mathbf{q})} = \frac{V}{N}\int \mathrm{d}^3r \; e^{-i\mathbf{q}\cdot\mathbf{r}}\mathcal{G}(\mathbf{r}) + \frac{V^2}{N}\int \mathrm{d}^3r \; e^{-i\mathbf{q}\cdot\mathbf{r}} = \frac{V}{N}\int \mathrm{d}^3r \; e^{-i\mathbf{q}\cdot\mathbf{r}}\mathcal{G}(\mathbf{r}) + \frac{V^2n^2}{N}\delta^{(3)}(\mathbf{q})$$

The last term contributes only when $\mathbf{q} = 0$ which is for $\theta = 0$ (forward-scattering) and is omitted in most cases. Hence, we define the structure factor $\mathcal{S}(\mathbf{q})$ as

$$\mathcal{S}(\mathbf{q}) = \frac{n\mathcal{I}(\mathbf{q})}{\mathcal{I}^{\circ}(\mathbf{q})} = \int \mathrm{d}^3r \; e^{-i\mathbf{q}\cdot\mathbf{r}}\mathcal{G}(\mathbf{r})$$

$\mathcal{S}(\mathbf{q})$ is just the spatial Fourier transform of the correlation function. $\mathcal{S}(\mathbf{q})$ becomes extremely large as we approach the critical point, for small values of $|\mathbf{q}|$.

Lecture 07: Introduction to Ising Model

The Ising model is a prototypical model to study phase transitions in magnetic systems. Since its fomulation by *Lenz* in 1920 and subsequent 1D solution by *Ising* and 2D solution by *Onsager*, Ising model has penetrated deep into all fields. The Ising model is defined fairly simply, by the Hamiltonian,

$$\mathcal{H} = -J\sum_{\langle ij\rangle}\sigma_i\sigma_j - h\sum_j \sigma_j \tag{19}$$

where $\sigma_j \in \{+1, -1\}$ is a random variable which is given an interpretation of a *classical spin*. J and h respectively denote the spin-coupling constant and the external field. The notation $\langle ij\rangle$ means that the spins i and j are nearest-neighbours. The Ising model provides interesting numerical and analytical artefacts till date which makes it an important system to study. The 1D solution is fairly simple, using a *transfer-matrix* method which is provided in Appendix B.

7.1. Mean-field solution

In the mean-field solution for the Ising model, we 'throw' away the fluctuations in each spin, which makes the spins interact with an 'effective' field resulting from the average orientation of the neighboring spins. Consider the identity,

$$(\sigma_i - \langle\sigma_i\rangle)(\sigma_j - \langle\sigma_j\rangle) = \sigma_i\sigma_j - \sigma_i\langle\sigma_j\rangle - \sigma_j\langle\sigma_i\rangle + \langle\sigma_i\rangle\langle\sigma_j\rangle \tag{20}$$

The LHS is zero since we are neglecting the spin fluctuations in the mean-field and hence the Ising Hamiltonian in Eq. (19) becomes,

$$\mathcal{H} = -J\sum_{\langle ij\rangle}\sigma_i\langle\sigma_j\rangle - J\sum_{\langle ij\rangle}\sigma_j\langle\sigma_j\rangle + J\sum_{\langle ij\rangle}\langle\sigma_i\rangle\langle\sigma_j\rangle - h\sum_i\sigma_i$$

Due to translation invariance, $\langle\sigma_i\rangle = \langle\sigma_j\rangle \equiv \langle\sigma\rangle$ and hence can be taken out of the sum.

$$\begin{aligned}\mathcal{H} &= -J\langle\sigma\rangle\sum_{\langle ij\rangle}\sigma_i - J\langle\sigma\rangle\sum_{\langle ij\rangle}\sigma_j + J\langle\sigma\rangle^2\sum_{\langle ij\rangle}-h\sum_i\sigma_i \\ &= -2J\langle\sigma\rangle\sum_{\langle ij\rangle}\sigma_i + J\langle\sigma\rangle^2\sum_{\langle ij\rangle}-h\sum_i\sigma_i\end{aligned}$$

For each spin σ_i, let us suppose that we have γ neighbours. Since the sums are now independent of j, these can be reduced to a sum over spins,

$$\begin{aligned}\sum_{\langle ij\rangle}f(\sigma_i) = \frac{1}{2}\sum_i f(\sigma_i)\sum_{j\in \mathrm{NN}(i)} \equiv \frac{\gamma}{2}\sum_{i=1}^{N}f(\sigma_i) \implies \mathcal{H} &= -J\gamma\langle\sigma\rangle\sum_i\sigma_i + \frac{JN\gamma}{2}\langle\sigma\rangle^2 - h\sum_i\sigma_i \\ &= -\mathrm{h_{eff}}\sum_i\sigma_i + \frac{JN\gamma}{2}\langle\sigma\rangle^2\end{aligned} \tag{21}$$

where $\mathrm{h_{eff}} = h + J\gamma\langle\sigma\rangle$ is kind of the *mean field* which is subjected to each spin. The Hamiltonian depends on $\langle\sigma\rangle$, however, given the Hamiltonian, we can also calculate $\langle\sigma\rangle$ from the partition function. This leads to a *self-consistent* equation which we need to tackle!

Lecture 08: Mean-field solution for Ising model

We will continue our discussion of the mean-field solution of the Ising model. Previously, we had reduced the Hamiltonian to a simplified expression, with an effective field.

$$\mathcal{H}_{\mathrm{MF}} = -\mathrm{h_{eff}}\sum_i\sigma_i + \frac{JN\gamma}{2}\langle\sigma\rangle^2 \tag{22}$$

This is simple to solve, since this is N independent spins in a field. The partition function is,

$$\mathcal{Z} = \sum_{\{\sigma_i\}} e^{\beta\mathrm{h_{eff}}\sum\sigma_i}\cdot e^{-\beta\mathcal{E}_0} \tag{23}$$

where $\mathcal{E}_0 = \frac{J\gamma N}{2}\langle\sigma\rangle^2$. Since the particles are independent, the sum over spins can be simplified as,

$$\mathcal{Z} = \left[\sum_{\sigma\in\{-1,1\}} e^{\beta\mathrm{h_{eff}}\sigma}\right]^N\cdot e^{-\beta\mathcal{E}_0} = [2\cosh(\beta\mathrm{h_{eff}})]^N e^{-\beta\mathcal{E}_0}$$

From this, the free energy is obtained as,

$$F(T,h) = -k_{\mathrm{B}}T\ln\mathcal{Z} = k_{\mathrm{B}}T[\beta\mathcal{E}_0 - N\ln(2\cosh\beta\mathrm{h_{eff}})] = \mathcal{E}_0 - Nk_{\mathrm{B}}T\ln(2\cosh\beta\mathrm{h_{eff}})$$

From the free-energy, we can obtain the magnetisation,

$$\mathcal{M} = -\frac{\partial F}{\partial B} = Nk_{\mathrm{B}}T\tanh\beta\mathrm{h_{eff}}\times\beta = N\tanh\beta\mathrm{h_{eff}}$$

The magnetisation per spin is thus obtained as a *transcendental equation*,

$$\boxed{\langle\sigma\rangle = \frac{\mathcal{M}}{N} = \tanh(\beta J\gamma\langle\sigma\rangle + \beta h)} \tag{24}$$

We are interested in finding whether we have any spontaneous magnetisation in the system, that is, magnetisation without an external field. Thus, let us take the case when $h = 0$. Now, define $x := \frac{\langle\sigma\rangle}{\beta J\gamma}$, so that the equation changes to,

$$\frac{x}{\beta J\gamma} = \tanh x$$

Now, note that $\beta J\gamma$ should be dimensionless as x is dimensionless. This implies that $J\gamma$ should have dimension of $k_{\mathrm{B}}T$. Let us define $k_{\mathrm{B}}T_c := J\gamma$ which leads us to,

$$\left(\frac{T}{T_c}\right)x = \tanh(x)$$

Given a temperature T, the left-hand side is just an equation of a line, with slope $\frac{T}{T_c}$. Let us analyse the situation graphically.

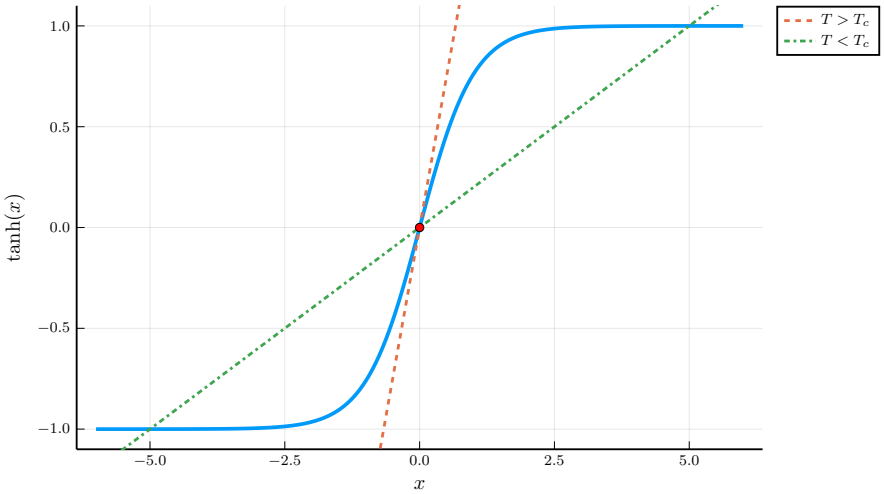


Figure 9: Graphical analysis of the transcendental equation

In Fig.9, we have plotted $\tanh(x)$ and two straight lines, with $T > Tc$ and $T < T_c$. For $T > Tc$, we see that the line does not cut $\tanh(x)$ at any point other than $x = 0$. However, for $T < T_c$, we see that two solutions exist, other than the trivial solution $x = 0$. As $\tanh(-x) = -\tanh(x)$, if one of the solution is $x = +x_0$, then the other solution is $x = -x_0$. A solution of x corresponds to a solution of $\langle\sigma\rangle$. Thus,

- $T > T_c$: $\langle\sigma\rangle = 0$ is the only solution and there is no spontaneous magnetisation.
- $T < T_c$: Apart from $\langle\sigma\rangle = 0$, we have two other solutions $\langle\sigma\rangle = \pm m_0$.

The mean-field solution, which predicts a finite critical temperature, is clearly wrong for the 1D case, where we know that no phase transition occur at any finite temperature. In 1D, the fluctuations are too strong to throw away, since there are only two nearest neighbours to interact with.

For the Ising model, two important things to note are *dimensionality* and lattice structure. However, in the mean-field Hamiltonian, γ (which is the only parameter depending on the topology of the lattice) cannot distinguish between these two factors. For example, for a cubic lattice in 3D, we have six nearest neighbours. Also, a triangular lattice in 2D has six nearest neighbours. Hence, these two lattices have the same γ, however, Ising dynamics in both the lattices are expected to be quite different.

Mean-field analysis becomes exact if we increase the dimensionality of the lattice and also if we increase the range of interaction, that is, we include higher order neighbours also. This ensures that the interaction between the spins is indeed an *effective interaction*.

Lecture 09: More on Ising Model

We have predicted a phase transition for the Ising model using mean-field approximation. However, the approximation seems to be inconsistent on many grounds, working well for higher dimensions and

long-range interactions. It predicted that in 1D too, Ising model has a spontaneous magnetisation at some finite temperature which cannot be. Even though we have solved the Ising system for dimension $d = 1$ in appendix. B (and it has been painfully solved by many stalwarts for $d = 2$ case too), let us see some arguments on why phase transitions cannot occur for 1D but it is possible in 2D Ising system.

9.1. Phase Transition in 1D Ising System

We will show that for $T > 0$ in $d = 1$ zero-field Ising Model, there exists no *long-range order*. Consider the ground state of the Ising model at $T = 0$, which is *ordered*, with all spins aligned in the same direction. Under open boundary conditions, this configuration has minimum energy $E_0 = -J(N-1)$.

$$\ldots \uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow \ldots$$

The above configuration has entropy $S = 0$, since all the spins are aligned. Hence, the free energy of the system is $F_{\text{grnd}} = E - TS = -J(N-1)$.

On increasing the temperature, the spins flips randomly due to interactions and this increases the energy of the system (since the interaction term is $-J(-1) = +J$ only if neighbouring spins are oppositely aligned). We need to check whether this destroys the long-range order. Now, consider a configuration with one *domain wall*[1] introduced at some point in the Ising chain, as shown in red below.

$$\ldots \uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow \; | \; \downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow \ldots$$

Introducing the domain wall increases the energy, due to the spins on either side of the domain wall.

$$E_{\text{dw}} = -J(N_+ - 1) - J(N_- - 1) - J(-1) = -J(N-1) + 2J$$

Thus introducing one domain wall incurs a cost of $\Delta E = 2J$. Now, since there are N spins, this domain wall can be placed at any of the $(N-1)$ positions. Then the entropy of the system with one domain wall is $S = k_{\text{B}} \ln(N-1)$ and the free energy is $F_{\text{dw}} = -J(N-1) + 2J - k_{\text{B}}T \ln(N-1)$. The change in free energy is,

$$\Delta F = F_{\text{dw}} - F_{\text{grnd}} = 2J - k_{\text{B}}T \ln(N-1)$$

In the thermodynamic limit $N \to \infty$ which implies that $\Delta F \to -\infty$. The system can always lower the free energy by creating a domain wall for any temperature $T > 0$. In fact, the free energy is further lowered by introducing arbitrary number of domain walls, untill no domains remain at all. This implies that the long-ranged order is unstable and there is no spontaneous magnetisation at any finite temperature in the zero-field $d = 1$ Ising model.

9.2. Phase Transition in 2D Ising System (Peierls' Argument)

The situation becomes a bit different for $d = 2$ Ising model. To prove the existence of phase transition at a finite temperature in $d = 2$, consider a case where all the outer layer spins in the lattice are of the same type, say $\uparrow$. Now, consider the spin in the center of the lattice, highlighted yellow in Fig. 10.

[1] In simple terms, a domain wall is an imaginary boundary which separates *domains*. Domains are regions with the same kind of spins, that is, all up or all down.

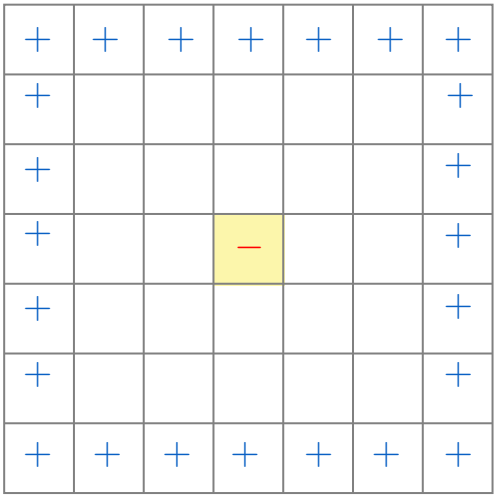
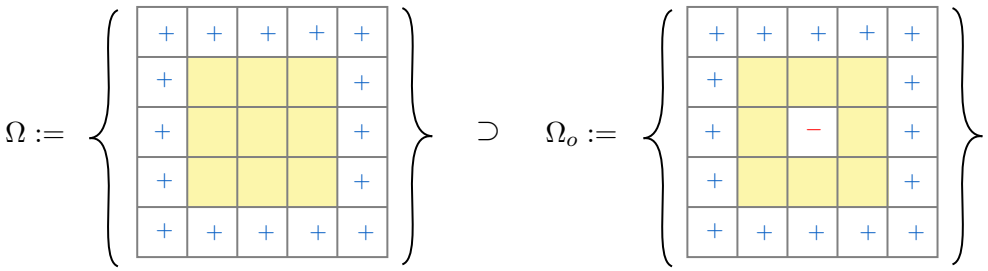


Figure 10: 2D Ising lattice; the outer layer have all same spins while the center spin is oppositely aligned with the outer spins.

If there is spontaneous magnetisation at some finite temperature, then the probability of the center spin to be oppositely aligned to the outer spins become zero (since the lattice becomes *ordered*). Also, note that the central spin is not particularly important and is just a representative of the bulk spin.



Now, consider Ω to be the set of all configurations where all the outer layers have spin $+$. Naturally, if we define Ω_0 to be the set of all configurations where the central spin is $-$ and all the outer layers have spin $+$, we have $\Omega_0 \subset \Omega$, as shown in the above figure. To have a phase transition is to show that the probability of any configuration $\{\sigma\} \in \Omega_0 \to 0$ as $N \to \infty$.

To show that, we define a *shoreline* which is an imaginary closed loop separating $+$ spins from $-$ spins. So, along the boundary of the shoreline, we have all opposite spins on either side. A given shoreline thus separates spins σ_i and σ_j such that $\sigma_i \cdot \sigma_j = -1$. Note that, in the interior of the shoreline, there can be $+$ or $-$ spins.

We define another set of configurations, Ω_s in which every configuration has the central spin to be $-$ and all the outer layers have spin $+$. In addition to it, there is a *fixed* shoreline S surrounding the central spin. Clearly, $\Omega_s \subset \Omega_0$

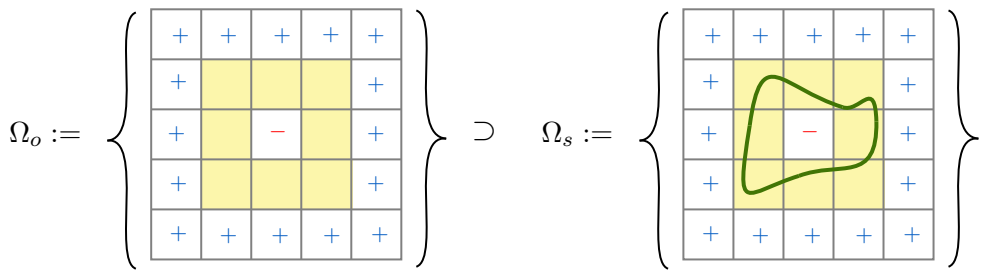


Figure 11: The set of configurations showing the shoreline with a green line.

The probability of a configuration inside Ω_s is given by,

$$\text{Prob}(\{\sigma\} \in \Omega_s) = \frac{1}{\mathcal{Z}} \sum_{\{\sigma\}\in\Omega_s} e^{-\beta\mathcal{H}(\{\sigma\})} = \frac{1}{\mathcal{Z}} \sum_{\{\sigma\}\in\Omega_s} \exp\left(\beta J \sum_{\langle ij\rangle \in S} \sigma_i\sigma_j\right) \exp\left(\beta J \sum_{\langle ij\rangle \notin S} \sigma_i\sigma_j\right) \tag{25}$$

where we have broken the nearest neighbour sum into two parts: spins which are separated by the shoreline and spins which are not. Note that if the spins are separated by the shoreline, then $\sigma_i\sigma_j = -1$ and the sum is just $-n(S)$, where $n(S)$ denotes the *length* of the shoreline. Thus, the probability becomes,

$$\text{Prob}(\{\sigma\} \in \Omega_s) = \frac{1}{\mathcal{Z}} \sum_{\{\sigma\}\in\Omega_s} e^{-\beta J n(S)} \exp\left(\beta J \sum_{\langle ij\rangle \notin S} \sigma_i\sigma_j\right) \tag{26}$$

The remaining sum, where spins are not separated by the shoreline, is hard to calculate exactly and we need to find an estimate for that.

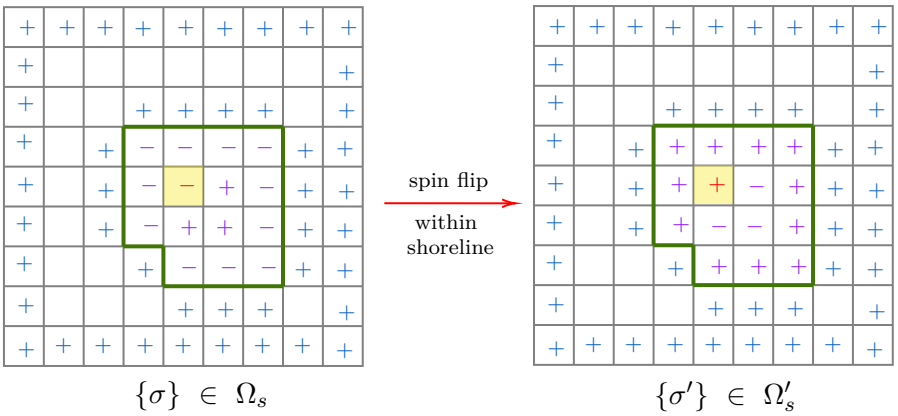


Figure 12: Flipping of all the spins inside the shoreline, taking $\sigma \to \sigma'$

We consider a specific configuration $\{\sigma\} \in \Omega_s$ and then flip all the spins in the inner side of the shoreline as shown in Fig. 12. We call this configuration $\{\sigma'\}$. If a spin in this configuration is outside the shoreline, then $\sigma_i = \sigma'_i$ since the spins outside the shoreline remains unchanged. If the spins belong inside the shoreline, then both spins have flipped and we have $\sigma'_i\sigma'_j = (-\sigma_i)(-\sigma_j) = \sigma_i\sigma_j$. If the spins are separated by shoreline, only one of the spins (which is in the inner side of the shoreline) changes and $\sigma'_i\sigma'_j = -\sigma_i\sigma_j = -(-1) = +1$. Thus we have,

$$\sum_{\langle ij\rangle} \sigma'_i\sigma'_j = \sum_{\langle ij\rangle \in S} \sigma'_i\sigma'_j + \sum_{\langle ij\rangle \notin S} \sigma'_i\sigma'_j = n(S) + \sum_{\langle ij\rangle \notin S} \sigma_i\sigma_j$$

Note that $n(S) > 0$ always which give us the inequality,

$$\sum_{\langle ij\rangle \notin S} \sigma_i\sigma_j = \sum_{\langle ij\rangle} \sigma'_i\sigma'_j - n(S) < \sum_{\langle ij\rangle} \sigma'_i\sigma'_j$$

Also note that $\sigma_i \to \sigma'_i$ is a one-to-one map and hence the sum of spins over Ω_s is equal to the sum of spins over Ω'_s. Using this and the estimate of the sum, Eq. (26) becomes,

$$\begin{aligned} \text{Prob}(\{\sigma\} \in \Omega_s) &< \frac{1}{\mathcal{Z}} \sum_{\{\sigma'\}\in\Omega'_s} e^{-\beta J n(S)} \exp\left[\beta J \sum_{\langle ij\rangle} \sigma'_i\sigma'_j\right] \\ &= \frac{e^{-\beta J n(S)}}{\mathcal{Z}} \sum_{\{\sigma'\}\in\Omega'_s} \exp\left[\beta J \sum_{\langle ij\rangle} \sigma'_i\sigma'_j\right] \end{aligned} \tag{27}$$

Now, the RHS is the sum over all configurations in Ω'_s. Since $e^x > 0$ for all x, this term is less than the sum over all the configurations $\{\sigma\} \in \Omega$. Thus,

$$\text{Prob}(\{\sigma\} \in \Omega_s) < e^{-\beta J n(S)} \frac{1}{\mathcal{Z}} \sum_{\{\sigma\}\in\Omega} \exp\left[\beta J \sum_{\langle ij\rangle} \sigma_i\sigma_j\right] = e^{-\beta J n(S)}$$

since the red term is just the definition of the partition function. Thus the probability of any configuration in Ω_s is less than $e^{-\beta J n(S)}$. However, we were interested in the situation where the configuration belonged to Ω_0 which can be obtained by summing over all such possible shorelines S.

$$\text{Prob}(\{\sigma\} \in \Omega_0) = \sum_{\{S\}} \text{Prob}(\Omega_S) < \sum_{\{S\}} e^{-\beta J n(S)}$$

Note that the length n of a shoreline can be $n = 4, 5, 6 \ldots$. The minimum value is 4, for the shoreline which contains only the central spin and this length increases. Then the sum over shorelines can be written as,

$$\text{Prob}(\{\sigma\} \in \Omega_0) < \sum_{n=4}^{\infty} s(n) e^{-\beta J n}$$

where $s(n)$ denote the number of shorelines with length n. The final thing to do is to have an estimate for $s(n)$. For this, note that shorelines are closed curves. To form a shoreline, start from any point P. We can move in only three directions (not in four) since shorelines are self-avoiding, so we cannot move in the direction in which we had already formed a line.

The number of ways to form a shoreline of length n is thus $\sim 3^n$. Note that in this case, the choice of P was arbitrary and we can essentially start from any of the n points. Thus, the number of shorelines of length n is $s(n) \sim 3^n n$. Substituting this in the above expression,

$$\text{Prob}(\{\sigma\} \in \Omega_0) < \sum_{n=4}^{\infty} 3^n n e^{-\beta J n} \equiv \sum_{n=4}^{\infty} n r^n < \sum_{n=1}^{\infty} n r^n \qquad \text{where, } r = 3e^{-\beta J}$$

From the ratio test, we have

$$\lim_{k\to\infty} \left|\frac{a_{k+1}}{a_k}\right| = \lim_{k\to\infty} \left|\frac{(k+1)r^{k+1}}{kr^k}\right| = \lim_{k\to\infty} \left(1 + \frac{1}{k}\right)|r| = |r|$$

and hence the sum converges if $|r| < 1 \implies e^{\beta J} > 3$. The value of the sum in the RHS is $\frac{r}{(r-1)^2}$ and hence,

$$\text{Prob}(\{\sigma\} \in \Omega_0) < \frac{r}{(r-1)^2} = \frac{3e^{-\beta J}}{(3e^{-\beta J} - 1)^2}$$

As $\beta \to \infty$ (corresponding to $T \to 0$), $\text{Prob}(\{\sigma\} \in \Omega_0) \to 0$ and hence for sufficiently low temperatures all spins in the systems tend to align even without an external magnetic field, proving the existence of a phase transition.

9.3. Symmetries of the Ising Model

The zero-field Ising Hamiltonian has an obvious symmetry of $\sigma_i \mapsto -\sigma_i$, which is broken if $h \neq 0$. In non-zero field, from Eq. (19), we can see that if $h \to -h$ and $\{\sigma\} \to \{-\sigma\}$, then the Ising Hamiltonian remains invariant.

$$\mathcal{H}(J, h, \{\sigma\}) = \mathcal{H}(J, -h, \{-\sigma\})$$

This is called the *time-reversal* symmetry or $\mathbb{Z}_2$ symmetry. Let us see what happens to the partition function under $h \to -h$.

$$\begin{aligned}
\mathcal{Z}(-h, J, T) &= \sum_{\{\sigma\}} \exp\left[-\beta \mathcal{H}(-h, J, \{\sigma\})\right] \\
&= \sum_{\{\sigma\}} \exp\left[-\beta \mathcal{H}(-h, J, \{-\sigma\})\right] \\
&= \sum_{\{\sigma\}} \exp\left[-\beta \mathcal{H}(h, J, \{\sigma\})\right] = \mathcal{Z}(h, J, T)
\end{aligned}$$

where in the second sum we used the fact that changing $\sigma \to -\sigma$ will not matter since we are summing over both -1 and $+1$ spins. The free energy is just the logarithm of the partition function, hence it also enjoys the symmetry,

$$F(-h, J, T) = F(h, J, T)$$

From the free energy, we obtain the magnetisation

$$\mathcal{M}(h) = -\frac{\partial F(h, J, T)}{\partial h} = -\frac{\partial F(-h, J, T)}{\partial h} = \frac{\partial F(-h, J, T)}{\partial(-h)} = -\mathcal{M}(-h) \tag{28}$$

From the above expression, if $h = 0$ then we have $\mathcal{M}(0) = 0$ for all temperatures, which apparently says that *phase transition is impossible in zero-field!*

This situation arises since we assumed the derivative of the free energy is well-behaved which is indeed true for finite systems, however, in the thermodynamic limit, F develops a kink for $T < T_c$ and hence $\left(\frac{\partial F}{\partial h}\right)$ develops a discontinuity as shown in Fig. 13 (a)

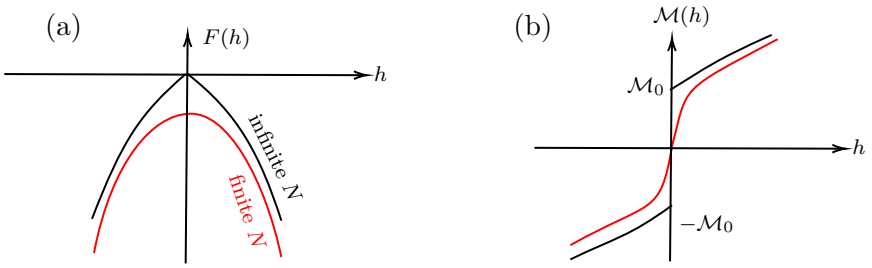


Figure 13: (a) Free energy and (b) Magnetisation behaviour in finite N and thermodynamic limit for $T < T_c$.

In the thermodynamic limit, near $h = 0$ the free energy behaves as,

$$F(h) = F(0) - \mathcal{M}_0|h| + \mathcal{O}(h^{q>1})$$

From this, if $h < 0$ then $\mathcal{M}(0^-) = -\mathcal{M}_0$ and if $h > 0$ then $\mathcal{M}(0^+) = +\mathcal{M}_0$ which is clearly discontinuous as shown in Fig. 13 (b). It is clear that if we take the thermodynamic limit first and then take $h \to 0$ and if we first take $h \to 0$ for a finite N and then take $N \to \infty$, we get two different behaviours. Thus, the limits do not commute.

$$\lim_{N\to\infty}\lim_{h\to 0}\left(\frac{1}{N}\frac{\partial F(h)}{\partial h}\right) \neq \lim_{h\to 0}\lim_{N\to\infty}\left(\frac{1}{N}\frac{\partial F(h)}{\partial h}\right)$$

9.3.1. Spontaneous Symmetry Breaking

When the Hamiltonian of the system has a particular symmetry but the statistical behavior of the system breaks that symmetry, we say that the symmetry is broken spontaneously. As seen before, the zero-field Ising Hamiltonian enjoys a $\mathbb{Z}_2$ symmetry, under the exchange $\{\sigma_i\} \to \{-\sigma_i\}$. For $T < T_c$ in the thermodynamic limit, we saw that

$$m = \lim_{N\to\infty}\frac{1}{N}\sum_i \langle\sigma_i\rangle \neq 0$$

Hence, at all temperature $\mathcal{H}$ has a symmetry under the exchange of spins but $\langle\sigma_i\rangle$ does not. Thus we say that the symmetry is spontaneously broken for $T < T_c$.

This is different from the uninteresting explicit symmetry breaking in the $h \neq 0$ case, where the Hamiltonian itself does not have the $\mathbb{Z}_2$ symmetry from beginning.

Spontaneous symmetry breaking seems a bit counterintuitive if we naively see a probabilistic viewpoint of the situation. Since the Hamiltonian has $\mathbb{Z}_2$ symmetry, the Boltzmann factor $P(\{\sigma\}) =$

$\frac{1}{\mathcal{Z}} \exp\left(-\beta \mathcal{H}(\{\sigma\})\right)$ is also invariant under this symmetry. Then the expectation,

$$\langle \sigma_i \rangle = \sum_{\{\sigma\}} \sigma_i P(\{\sigma\}) = 0$$

The sum is zero because for a configuration $\{\sigma_i\}$, the opposite configuration $\{-\sigma_i\}$ will have the same Boltzmann factor, however, the σ_i factor in the sum will become $-\sigma_i$, which will cancel with the configuration. Thus, in the thermodynamic limit, we have to be careful with the calculation!

Consider the Ising model when $h \neq 0$. In this case, consider two configurations A and B which differ by the fact that all spins in configuration B are the flipped spins of configuration A. Due to the field term $-h \sum \sigma_i = -hNm$, the probability of these two contributions will be

$$\frac{P_{\mathrm{A}}}{P_{\mathrm{B}}} = \frac{\exp[\beta h N m]}{\exp[-\beta h N m]} \implies \frac{P_{\mathrm{B}}}{P_{\mathrm{A}}} = \exp[-2\beta h N m]$$

In the thermodynamic limit, for $h > 0$, $\frac{P_{\mathrm{B}}}{P_{\mathrm{A}}} \to 0$ and hence the system must be in configuration A, with magnetisation $+m$ for any $h > 0$ (in particular, true for $h \to 0^+$). For $h < 0$, $\frac{P_{\mathrm{B}}}{P_{\mathrm{A}}} \to \infty$ and hence the system must be in configuration B, with magnetisation $-m$ for any $h < 0$ (in particular, true for $h \to 0^-$).

Thus, in an infinitesimal field close to zero and in the thermodynamic limit, there is a large weight assigned to states with particular magnetisation $+m$ or $-m$, for $h > 0$ and $h < 0$ respectively. This is equivalent to setting $h = 0$ but taking a *restricted ensemble*, where we exclude the configurations with the 'unpreferred' magnetisation and thus, their Boltzmann weight is identically zero. Two such probability distribution can be defined P_+ and P_- based on the magnetisation values. I haven't gone through the rigorous mathematical arguments for this, however, Goldenfeld advised to refer to [3], where this has apparently been dealt with rigor.

Lecture 10: Some more on Ising Model

In the previous section, we noted some properties based on the symmetry of the Ising model. Let us now continue our discussion on the mean field solution, focussing on critical exponents, that we previously saw in the phase transition in fluids.

10.1. Critical Exponents

Critical exponents are defined as the limiting *power-law* behaviour of some thermodynamic quantities near the critical point.

$$f(t) \sim t^{\lambda} \qquad \implies \qquad \lambda = \lim_{t \to 0} \frac{\ln f(t)}{\ln t}$$

The variable t is often taken to be the reduced temperature $t := \pm \frac{(T - T_c)}{T_c}$ depending on whether we want to approach from below or above T_c. The reduced temperature kinda is a measure of the distance from critical point. It is taken to be dimensionless so that different models can be compared.

The critical exponents for T_c^+ and T_c^- are found to be always equal, if they exist (like for magnetisation, $m = 0$ for $T > T_c$ so no exponent can be obtained in that case and hence, magnetisation is approached only from below T_c).

From Eq. (24), the mean field magnetisation was written as $\langle \sigma \rangle = \tanh(\beta h + \beta J \gamma \langle s \rangle)$. Let us denote $m = \langle \sigma \rangle$ and $\tau = \frac{T_c}{T} = \beta J \gamma$. In terms of the reduced temperature $t = \frac{T_c - T}{T_c}$, we have $\tau = \frac{1}{1-t}$. Using $\tanh(x) \simeq x - \frac{x^3}{3}$ for $x \ll 1$, we get

$$m = \tanh(\tau m) = \tanh\left(\frac{m}{1-t}\right) = \frac{m}{(1-t)} - \frac{m^3}{3(1-t)^3} + \dots$$

Solving this, we get $m = 0$ or $m^2 = (3t)(1-t)^2$. Note that for $T > T_c$, $t < 0$ while $(1-t)^2 > 0\ \forall t$. Hence, m^2 comes out to be negative, which is not possible. Thus for $T > T_c$ we only have one solution $m = 0$. The non-zero magnetisation is thus interesting for us and let us check what is the scaling of this,

$$m^2 = (3t)(1-t)^2 = 3t + \mathcal{O}(t^2) \implies m \sim \pm(3t)^{1/2}$$

Thus we obtain the first critical exponent from the mean-field analysis,

$$m \sim \left(\frac{T_c - T}{T_c}\right)^{\beta} \qquad \text{where, } \beta = \frac{1}{2}$$

Now, let us check what happens when $h \neq 0$, along the critical isotherm $T = T_c \implies \tau = 1$. For small m and $({}^{h}/_{k_{\mathrm{B}}T_c}) \ll m$, the magnetisation equation becomes,

$$\begin{aligned} m = \tanh(\beta h + m) &\simeq (\beta h + m) - \frac{1}{3}(\beta h + m)^3 + \dots \\ &= (\beta h + m) - \frac{m^3}{3}\left(\frac{3\beta h}{m} + 1\right) + \dots \end{aligned}$$

From this we obtain a scaling between the field and magnetisation,

$$\beta h[1 - m^2] = \frac{m^3}{3} \implies h = \frac{m^3}{3\beta(1-m^2)} = \frac{m^3}{3\beta} + \dots \implies h \sim m^3$$

We obtained the second critical exponent from the mean-field analysis,

$$m \sim h^{1/\delta} \qquad \text{where, } \delta = 3$$

We will now deal with the third exponent, but we have to be more careful here, since this will have scaling both above and below T_c. For this, again consider the transcendental equation $m = \tanh(\beta h + \tau m)$ which, after expansion around small m and $h \ll m k_{\mathrm{B}} T$, can be written as,

$$h = \frac{m(1-\tau) + \frac{\tau^3 m^3}{3}}{\beta(1 - \tau^2 m^2)}$$

Differentiating and retaining terms only upto $\mathcal{O}(m^2)$,

$$\left(\frac{\partial h}{\partial m}\right)_T = \frac{m^2\tau^2 + (1-\tau)}{\beta\left(m^2\tau^2 - 1\right)^2}$$

The denominator cannot provide any more m^2 term and hence upto $\mathcal{O}(m^2)$, the derivative is given by,

$$\left(\frac{\partial h}{\partial m}\right)_T = \frac{1}{\beta}\left[\frac{m^2}{(1-t)^2} - \frac{t}{(1-t)}\right]$$

For $T > T_c$, $m = 0$ and for $T < T_c$, $m^2 = 3t(1-t)^2$ as found before. Substituting this above, we get

$$\begin{aligned} \chi_+ = \left(\frac{\partial m}{\partial h}\right)_{T_c^+} &= \frac{\beta(t-1)}{t} = \frac{1}{k_{\mathrm{B}}T}\left[1 - \frac{T_c}{T_c - T}\right] = \frac{1}{k_{\mathrm{B}}(T - T_c)} \\ \chi_- = \left(\frac{\partial m}{\partial h}\right)_{T_c^-} &= \frac{\beta(1-t)}{t(2-3t)} \simeq \frac{\beta(1-t)}{2t} = \frac{1}{2k_{\mathrm{B}}T}\left[\frac{T_c}{T_c - T} - 1\right] = \frac{1}{2k_{\mathrm{B}}(T_c - T)} \end{aligned}$$

We obtained the scaling of the susceptibility,

$$\begin{aligned} \chi_+ &\sim (T - T_c)^{-\gamma'} \quad \text{where, } \gamma' = 1 \\ \chi_- &\sim (T_c - T)^{-\gamma} \quad \text{where, } \gamma\ = 1 \end{aligned}$$

For $T \gg T_c$ then $\chi_+ \sim \frac{1}{T}$, in accordance with Curie's law. We see that $\gamma = \gamma'$ and hence, approach from both side of the critical point is the same. Also, $\frac{\chi_+}{\chi_-} = 2$ which is called the *amplitude ratio.*

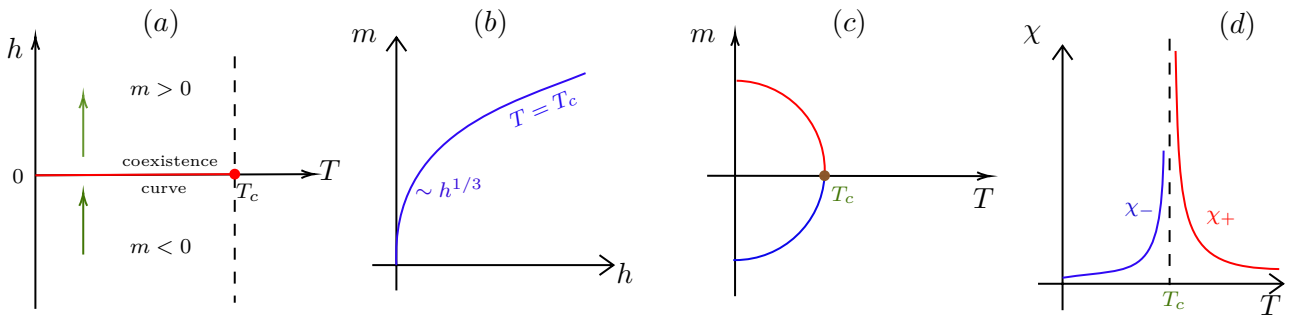


Figure 14: Scaling of various quantities in Ising model

Fig. 14 (a) shows the Ising model phase diagram. For low temperatures $T < T_c$, the system undergoes a discontinuous phase transition in which m changes abruptly as it crosses from $h < 0$ to $h > 0$, denoting a first-order transition. Shown in red is the *coexistence curve*, which ends at T_c. Beyond T_c, m changes continuously across the $h < 0$ to $h > 0$ transition.

As we vary T for a fixed h, the magnetisation varies smoothly as shown in Fig. 14 (c) until T_c, after which it becomes zero. The Ising model shows a first-order transition as a function of h but a second-order transition as a function of T.

10.2. Bragg-Williams Approximation

This is kind of an alternate mean-field description of the Ising model. Consider the Ising lattice containing N spins, with say, N_+ up spins and N_- down spins. Then the average magnetisation is given by,

$$m = \frac{N_+ - N_-}{N_+ + N_-} = \frac{2N_+ - N}{N} \implies \frac{N_+}{N} = \frac{1}{2}(m+1)$$

The entropy of the system is defined as the number of ways by which a configuration with magnetisation m can be produced. Hence, out of N spins, we choose N_+ spins and the rest are set to N_-, which gives us,

$$\Omega(N_+, N_-) = \frac{N!}{N_+!N_-!} = \frac{N!}{\left(\frac{N(1+m)}{2}\right)!\left(\frac{N(1-m)}{2}\right)!} \qquad S = k_\mathrm{B} \ln \Omega(N_+, N_-)$$

Using Sterling's approximation, $\ln N! \approx N \ln N - N$ we obtain,

$$\begin{aligned}
\ln \Omega &\approx (N \ln N - N) - \frac{N(1+m)}{2} \ln\left(\frac{N(1+m)}{2}\right) - \frac{N(1-m)}{2} \ln\left(\frac{N(1-m)}{2}\right) + N \\
&= N\left[\ln N - \frac{(1+m)}{2} \ln\left(\frac{N(1+m)}{2}\right) - \frac{(1-m)}{2} \ln\left(\frac{N(1-m)}{2}\right)\right] \\
&= N\left[\ln N - \frac{(1+m)}{2} \ln(1+m) - \frac{(1-m)}{2} \ln(1-m) - \ln N - \ln 2\right] \\
&= N\left[\ln 2 - \frac{1+m}{2} \ln(1+m) - \frac{1-m}{2} \ln(1-m)\right]
\end{aligned}$$

The mean-field energy of the Ising model is given by,

$$U = -\frac{J\gamma N m^2}{2} - Nhm$$

We can now calculate the free energy and minimise it to find the equation of state.

$$F(T, m, N) = U - TS = -\frac{J\gamma N m^2}{2} - Nhm - Nk_\mathrm{B}T\left[\ln 2 - \frac{1+m}{2} \ln(1+m) - \frac{1-m}{2} \ln(1-m)\right]$$

which implies that,

$$\frac{\partial F}{\partial m} = -JN\gamma m - Nh + \frac{Nk_{\mathrm{B}}T}{2}[1+\ln(1+m) - 1 - \ln(1-m)] = -JN\gamma m - Nh + \frac{Nk_{\mathrm{B}}T}{2}\ln\frac{1+m}{1-m} = 0$$
$$\implies \frac{1+m}{1-m} = e^{2\beta(J\gamma m+h)} \implies m = \frac{e^{2\beta(J\gamma m+h)}-1}{e^{2\beta(J\gamma m+h)}+1} = \frac{e^{\beta(J\gamma m+h)}-e^{-\beta(J\gamma m+h)}}{e^{\beta(J\gamma m+h)}+e^{-\beta(J\gamma m+h)}} = \tanh(\beta(J\gamma m+h))$$

Thus we obtained the same previous self-consistent equation $m = \tanh(\beta J\gamma m + \beta h)$ from this method.

10.3. Towards the Landau free energy

Instead of writing the Ising partition function $\mathcal{Z}(T,h,N)$ as a sum over all spin configurations, we can write it as a sum over all possible magnetisations m. We can write,

$$\mathcal{Z}(T,h,N) = \sum_m \sum_{\{\sigma\}|m} e^{-\beta\mathcal{H}(\{\sigma\},N,h)} \approx \sum_m \Omega(m,N)e^{-\beta\mathcal{H}_{\mathrm{MF}}(m,N,h)}$$

where $\Omega(m,N)$ is just the *degeneracy factor*, which tells us how many states are there with magnetisation m and $\mathcal{H}_{\mathrm{MF}}$ is the mean-field Hamiltonian from Eq. (22). The above sum can be approximated by an integral from -1 to 1, taking magnetisation to be continuous:

$$\begin{aligned}
\mathcal{Z}(T,h,N) &= \int_{-1}^{1} \mathrm{d}m\ \Omega(m,N)e^{-\beta\mathcal{H}_{\mathrm{MF}}(m,N,h)} \\
&= \int_{-1}^{1} \mathrm{d}m\ e^{\ln\Omega(m,N)}e^{-\beta\mathcal{H}_{\mathrm{MF}}(m,N,h)} \\
&= \int_{-1}^{1} \mathrm{d}m\ e^{\ln\Omega(m,N)-\beta\mathcal{H}_{\mathrm{MF}}(m,N,h)} \\
&= \int_{-1}^{1} \mathrm{d}m\ e^{-\beta N\left(\frac{-J\gamma m^2}{2} - mh - \frac{k_{\mathrm{B}}T}{N}\ln\Omega(m,N)\right)}
\end{aligned} \tag{29}$$

The blue term feels like some kind of thermodynamic potential but it depends both on m and h. Hence this is some kind of pseudo-free energy called the *Landau free energy* denoted by $\mathcal{L}(m,h)$,

$$\mathcal{L}(m,h) = -\frac{\gamma J m^2}{2} - mh - k_{\mathrm{B}}T\ln 2 + \frac{k_{\mathrm{B}}T}{2}[(1+m)\ln(1+m) + (1-m)\ln(1-m)]$$

From saddle-point approximation, the integral will take the value at $m = m^*$, such that $N\mathcal{L}(m^*,h)$ is minimum. Thus,

$$\left.\frac{\partial\mathcal{L}}{\partial m}\right|_{m^*} = -\gamma J m^* - h + \frac{k_{\mathrm{B}}T}{2}[1+\ln(1+m^*) - 1 - \ln(1-m^*)] = 0$$

From this we obtain the same transcendental equation $\tanh(\beta h + \beta J\gamma m) = m$ as before. Let us see some insights from the plot of the Landau free energy.

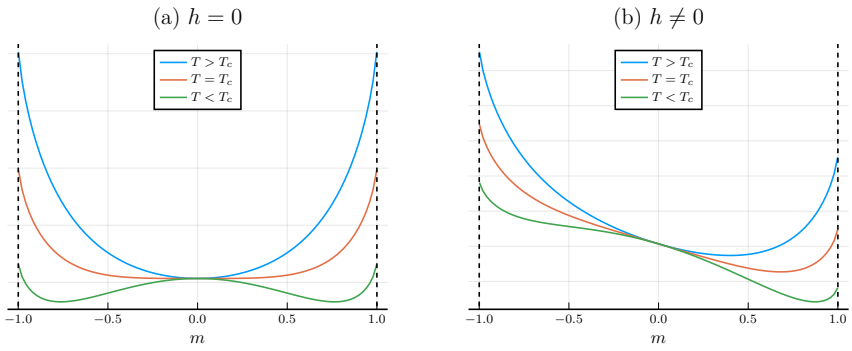


Figure 15: $\mathcal{L}$ vs. m at different temperature regimes. The curves have been appropriately shifted so that $\mathcal{L}(m = 0) = 0$

Fig. 15 (a) shows the variation of $\mathcal{L}(m)$ as m is varied between -1 and $+1$. For the zero-field case, $\mathcal{L}$ is symmetric about $m = 0$. For $T > T_c$ we have only one minima at $m = 0$ and for $T < T_c$ we have two mimima at $\pm m_0$ while $m = 0$ is a local maxima. The second derivative of the Landau free energy at $m = 0$

$$\left.\frac{\partial^2 \mathcal{L}}{\partial m^2}\right|_{m=0} = -\gamma J + \frac{k_B T}{2}\left[\frac{1}{1+m} + \frac{1}{1-m}\right]\Bigg|_{m=0} = -J\gamma + k_B T \implies \left.\frac{\partial^2 \mathcal{L}}{\partial m^2}\right|_{m=0, T=T_c} = 0$$

from our definition of $k_B T_c = J\gamma$. Thus, for all values of h, $m = 0$ is an *inflection point* for $T = T_c$ where the curvature disappears, as is evident in Fig. 15.

For $T < T_c$, $\mathcal{L}$ has two degenerate minima for $h = 0$. However, when we take $h \neq 0$ then these minima becomes non-degenerate, one becomes the stable minima and one becomes the metastable one (depending on the sign of h). On increasing h, the magnetisation metastable minima keeps getting shallower and at some $h = h^*$ (called the *spinodal field*), it disappears completely as shown in Fig. 16. The condition for this is that $\frac{\partial \mathcal{L}}{\partial m} = 0$ and $\frac{\partial^2 \mathcal{L}}{\partial m^2} = 0$, which gives us

$$m - \tanh\left(\beta h + \beta J\gamma m\right) = 0 \qquad 1 - \beta J\gamma \operatorname{sech}^2\left(\beta h + \beta J\gamma m\right) = 0$$

Using $\operatorname{sech}^2(\beta h + \beta J\gamma m) = 1 - \tanh^2(\beta h + \beta J\gamma m)$ we obtain $m^* = \pm\sqrt{1 - \frac{1}{\beta J\gamma}}$. What happens is that, for $h > 0$ the metastable minima is at $m < 0$ and this is given by $m^* = -\sqrt{1 - \frac{1}{\beta J\gamma}}$ while for $h < 0$, $m^* = +\sqrt{1 - \frac{1}{\beta J\gamma}}$ is the metastable magnetisation. From these *spinodal magnetisation*, we obtain the spinodal fields by substituting this in the expression of $\beta h = \tanh^{-1}(m) - \beta J\gamma m$ according to whether $h < 0$ or $h > 0$.

$$\beta h^* = \frac{1}{2}\ln\left[\frac{1+m^*}{1-m^*}\right] - \beta J\gamma m^*$$

Hence to summarise, we have the following cases:

- $h = 0 \longrightarrow$ degenerate, equally likely minima at $\pm m_0$ for $T < T_c$.
- $h \neq 0, h < h^* \longrightarrow$ one stable and one metastable minima.
- $h \neq 0, h > h^* \longrightarrow$ only one stable minima.

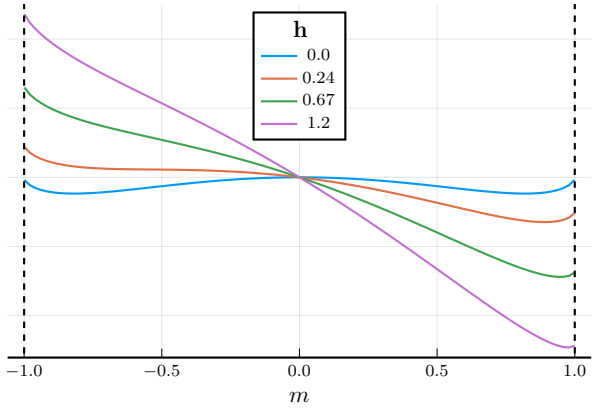


Figure 16: $\mathcal{L}$ vs. m for different values of h at $T < T_c$. On increasing h, the metastable minima at $m < 0$ disappears.

The metastable state exists only between $(-h^*, +h^*)$. At $T = T_c$ we have $\beta J\gamma = 1$ which implies $m^* = 0$ and hence $\pm h^*$ coalesce to the same point. The phase diagram for h vs. T is shown below:

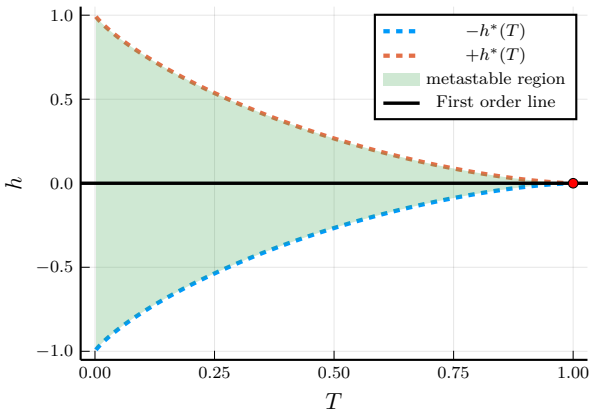


Figure 17: Phase diagram for h and T. The blue shaded region denotes the states (h, T) where the metastable regions exist. The black line denotes the first order phase coexistence curve, ending at T_c. Here T_c is taken to be 1 for the simulation.

10.4. Hysterisis

On varying the magnetic field at some fixed temperature $T < T_c$, we obtain a hysterisis in the Ising model. Suppose we start with a high negative value of $h \gg -|h^*|$. In this case, only one *global minima* is present (see Fig. 18 (a)). As we decrease the field magnitude (take the field towards zero), then at $h = -|h^*|$, the metastable minima will appear, but the system will be sitting in the global minima. At $h = 0$, the global and the metastable minima will become degenerate. On increasing h further in the positive side, the previous global minima now become the metastable minima.

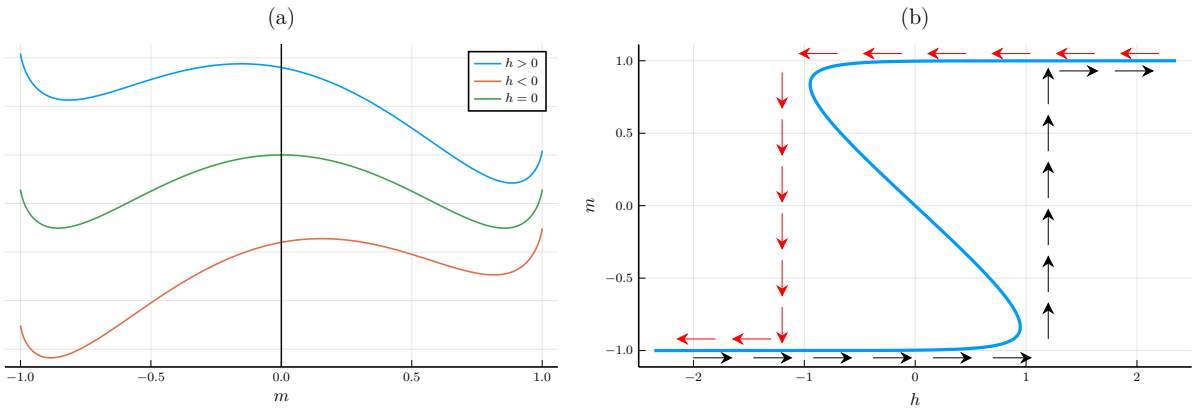


Figure 18: Hysterisis curve from mean-field theory. (a) $\mathcal{L}(m)$ vs. m in different field regimes. The global minima shifts on moving h from negative to positive. (b) Magnetisation vs. h curve, showing the hysterisis loop.

The system should technically be sitting in the global minima, however, since it was previously occupying the other minima (which has now become metastable), due to some kind of *inertia*, it still stays in the metastable state, which happens until h hits $+|h^*|$. After that, the metastable minima disappears and the system is forced to relocate to the global minima.

As shown in Fig. 18 (b), the black arrows traverse the path when we start from $h < 0$ while the red arrows show the same when starting from $h > 0$. We can see that the paths are not the same and the resulting $m(h)$ curve is not reversible in time. This is the characteristic case of *hysterisis*!

Lecture 11: Landau Theory for Phase Transition: I

We move on to a formal description of the process encountered in the previous lecture. Here, will be be doing away with the microscopic details. Although, time and again, we will be taking the Ising model as our basis to build intuition and stuff, the method can be possibly generalised to other systems. We will define the system in terms of an *order parameter* which we will take to be a scalar. However, order parameters can literally be *anything* as long as it can distinguish between two phases.

11.1. Order Parameter

Order parameters can be scalars, or in general tensors or an element from a group, it can be real or complex; there is a lot of diversity. The basic necessity is that, it should distinguish between phases. It is usually zero in the unordered phase and non-zero in the ordered phase. For example, in the *Heisenberg model* with the Hamiltonian,

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j - \mathbf{h} \cdot \sum_i \boldsymbol{\sigma}_i \tag{30}$$

where the spins on the lattice are *vectors*, the magnetisation $\mathbf{M}$ is a vector, such that $\mathbf{M} = 0$ for $T > T_c$ and $\mathbf{M} = M\hat{\mathbf{n}}$, pointing in some arbitrary direction $\hat{\mathbf{n}}$ for $T < T_c$.

For the superfluid transition in ^{3}He, the order parameter is something called a *pairing amplitude* which is kinda a complex matrix and has to do with formation of Cooper pairs. In superconductors, the energy gap Δ is often taken to be the order parameter. In fluid systems, as seen before, we took the density difference between the phases to be the order parameter. In each of these, the number of components in the order parameter are different.

11.2. Expanding the energy

The Landau theory has to do with expanding a function $\mathcal{L}$ in powers of the *order parameter*. The function $\mathcal{L}$ must obey the symmetry of the system. With all our might we write the phenomenological expansion,

$$\mathcal{L} = \sum_{i=0}^{\infty} a_i(\{K\}, T)m^i \tag{31}$$

where $\{K\}$ denote the set of couplings in the model (for example, in the Ising model, J was our coupling constant and also h, kinda). The expansion in itself is not that helpful, unless we do something stupid with it. We expect that m should be small in and around T_c and hence we truncate the expansion upto m^4, leaving us with the quartic free energy,

$$\mathcal{L} = a_0 + a_1 m + a_2 m^2 + a_3 m^3 + a_4 m^4$$

For the time being, let us consider the $\mathbb{Z}_2$ symmetry case as in zero-field Ising model. Thus, $\mathcal{L}(m) = \mathcal{L}(-m)$ which forces the odd terms to be zero viz. $a_1 = a_3 = 0$. Moreover, we want $\mathcal{L}$ to be bounded below, since we hope to extract physical insights from minimising the free energy. If $\mathcal{L}$ has no finite minima, then we can arbitrarily make that small by taking $\eta \to \infty$ which is unphysical. Thus, $a_4 > 0$ is taken to make $\mathcal{L}$ bounded below.

All the coefficients here are dependent on temperature and the coupling. In the unordered phase, $m = 0$ and hence a_0 denotes the value of $\mathcal{L}$ in the disordered phase. Since this coefficient is independent of the order parameter, we can think of this as a *smooth background field*, containing the irrelevant degrees of freedom, upon which the phase transition stuff is superimposed. We set $a_0 = 0$, that's it! We expand the remaining coefficients with respect to the reduced temperature, $t = \frac{T - T_c}{T_c}$:

$$\begin{aligned} a_2 &= a_2^{(0)} + a_2^{(1)} t + \mathcal{O}(t^2) \\ a_4 &= a_4^{(0)} + a_4^{(1)} t + \mathcal{O}(t^2) \end{aligned} \tag{32}$$

We don't need a_4 upto the linear term also, since a_4 comes with m^4, which is itself assumed to be tiny. So, we just take a_4 to be some positive constant. We now minimise $\mathcal{L}$, hoping to get some insights.

$$\frac{\partial \mathcal{L}}{\partial m} = 2a_2 m + 4a_4 m^3 = 0 \implies m = 0 \quad \text{or} \quad m = \sqrt{-\frac{a_2}{2a_4}} \tag{33}$$

We assume m to be continuous across the transition, and hence $a_2(T_c) \to 0$, which implies that $a_2^{(0)} = 0$. To summarise, with all our assumptions, we get the expression for the Landau free energy upto m^4 to be,

$$\mathcal{L} = a_2(T - T_c)m^2 + a_4 m^4 \tag{34}$$

where we have redefined the constants a_2 and a_4 by absorbing some constants. Let us now add the magnetic field term h, which breaks the $\mathbb{Z}_2$ symmetry. The simplest way to incorporate this is through a linear term. The free energy can then be written as,

$$\mathcal{L} = \frac{a_2}{2}(T - T_c)m^2 + \frac{a_4}{4}m^4 - mh \tag{35}$$

Minimising this gives us,

$$\frac{\partial \mathcal{L}}{\partial m} = a_2(T - T_c)m + a_4 m^3 - h = 0 \implies \boxed{a_2(T - T_c)m + a_4 m^3 = h}$$

which is the equation of state. It is a cubic equation with potentially three roots.

11.3. Finding Critical Exponents

Suppose $h = 0$. Then, from minimising $\mathcal{L}$ we get,

$$m = 0 \qquad m = \left(-\frac{a_2}{a_4}(T - T_c)\right)^{1/2} \sim (T - T_c)^{1/2} \tag{36}$$

We can easily see from here that the critical exponent $\boxed{\beta = \frac{1}{2}}$. Now, suppose $h \neq 0$. Then at $T = T_c$ we have $a_4 m^3 = h \implies m \sim h^{1/3}$ which gives us the critical exponent $\boxed{\delta = \frac{1}{3}}$. From the equation of state, we find that

$$\frac{\partial h}{\partial m} = a_2(T - T_c) + 3a_4 m^2 \implies \frac{\partial m}{\partial h} = \frac{1}{a_2(T - T_c) + 3a_4 m^2}$$

For $T > T_c$, we have $m^* = 0$ and for $T < T_c$ we have $m^* = \sqrt{-\frac{a_2}{a_4}(T - Tc)}$, using which we can obtain the zero-field susceptibility,

$$\chi_{T_c^+} = \frac{1}{a_2(T - T_c)} \implies \boxed{\gamma' = 1}$$

$$\chi_{T_c^-} = \frac{1}{a_2(T - T_c) - 3a_4 \cdot \frac{a_2}{a_4}(T - Tc)} = \frac{1}{2a_2(T_c - T)} \implies \boxed{\gamma = 1}$$

The last exponent comes from the susceptibility which can be obtained from the specific heat $C_v = -T\frac{\partial^2 \mathcal{L}}{\partial T^2}$ for $h = 0$. For $T > T_c$, $\mathcal{L} = 0$ as $m^* = 0$. For $T < T_c$ we have,

$$\mathcal{L} = -\frac{a_2^2}{2a_4}(T - T_c)^2 + \frac{a_2^2}{4a_4}(T - T_c)^2 = -\frac{a_2^2}{4a_4}(T - T_c)^2 \implies C_v = \frac{a_2^2}{2a_4}T$$

Thus, between T_c^+ and T_c^-, we have $\Delta C = \frac{a_2^2}{2a_4}T_c > 0$ and thus there is a discontinuity in the specific heat. It is clear from here that $\boxed{\alpha = 0}$ which is the remaining critical exponent.

Lecture 12: Landau Theory for Phase Transition: II

We now add a cubic term to the free energy, which will lead to a first order transition.

12.1. First Order Transition

$$\mathcal{L} = \frac{1}{2}a_2(T - T_c)m^2 - \frac{1}{3}a_3 m^3 + \frac{1}{4}a_4 m^4 \qquad a_4, a_2 > 0 \tag{37}$$

We can assume the $a_3 > 0$, if not, define $m' = -m$. The free energy no longer enjoys the $\mathbb{Z}_2$ symmetry. Minimising the free energy gives us,

$$\frac{\partial \mathcal{L}}{\partial m} = a_2(T - T_c)m - a_3 m^2 + a_4 m^3 = 0 \implies m = 0 \quad \text{or} \quad a_4 m^2 - a_3 m + a_2(T - T_c) = 0$$

The quadratic part gives us two solutions, namely,

$$m_\pm = \frac{a_3}{2a_4} \pm \sqrt{\left(\frac{a_3}{2a_4}\right)^2 - \frac{a_2}{a_4}(T - T_c)}$$

From this, we see that if $a_3^2 < 4a_2a_4(T - T_c)$ then the above two solutions become complex and we are left with only $m = 0$ as the real solution. If $a_3^2 > 4a_2a_4(T - T_c) \implies T < T_c + \frac{a_3^2}{4a_2a_4}$, then we have three real solutions. Let us denote $T^* = T_c + \frac{a_3^2}{4a_2a_4} > T_c$, which implies that even above T_c, for T satisfying $T_c < T < T^*$, three solutions do appear.

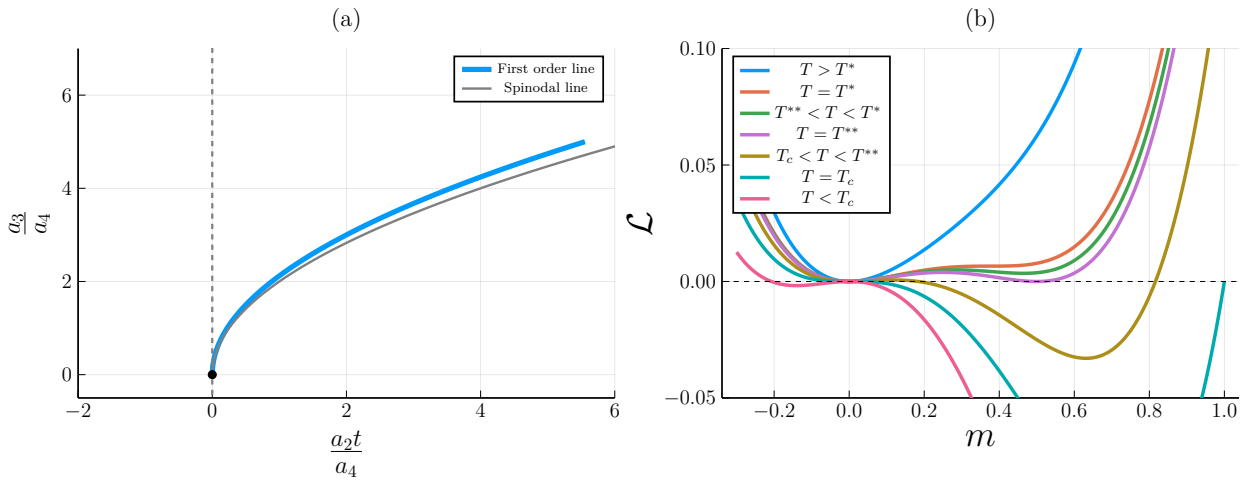


Figure 19: Landau free energy $\mathcal{L}$ with the cubic term. (a) Phase diagram in the a_3 vs. t plane. The blue line denotes the first order line $a_3^2 = (9/2)a_2a_4t$ while the dashed grey line denotes the spinodal line $a_3^2 = 4a_2a_4t$ (b) Behavious of $\mathcal{L}$ in different temperature regime.

Okay, now let us see the position of these three extremas. Note that $m_+ > m_-$ and $m_+ > 0$ from the form of the expression, so only the position with respect to zero needs to be ascertained for m_-. If we want $m_- > 0$, then

$$\left(\frac{a_3}{2a_4}\right)^2 > \left(\frac{a_3}{2a_4}\right)^2 - \frac{a_2}{a_4}(T - T_c) \implies T > T_c$$

Thus, for $T > T_c$ we have $m_+ > m_- > 0$ and for $T < T_c$ we have $m_- < 0 < m_+$. The position of the extremas are fixed. Now, let's look at the curvature.

$$\frac{\partial^2 \mathcal{L}}{\partial m^2} = a_2(T - T_c) - 2a_3 m + 3a_4 m^2$$

At $m = 0$, $\frac{\partial^2 \mathcal{L}}{\partial m^2} = a_2(T - T_c)$ which implies that for $T < T_c$ we have a maxima at $m = 0$ and for $T > T_c$, there's a minima at $m = 0$. From these facts, we have:

- For $T < T_c$, $m_\pm$ are the minima and $m = 0$ is the maxima.
- For $T > T_c$, m_+ and $m = 0$ are the minima and m_- is the maxima.

Let us now see how the free energy behaves for different values of $T > T_c$, to ascertain which extremas are global. At $m = 0$, we always have an minima and hence, to find the global things, we neet to compare the other extremas with $\mathcal{L}(m = 0)$, so we look at the case when $\mathcal{L}(0) = \mathcal{L}(m_+)$ (since m_- is the maxima, we do not care about it). This is equivalent to simultaneously satisfying the two equations for $m \neq 0$,

$$\mathcal{L}(m) = 0 \qquad \frac{\partial \mathcal{L}}{\partial m} = 0$$

Eliminating m^2 from these equations and defininining $\epsilon = T - T_c$, leaves us with,

$$4\left(\frac{1}{3}a_3 m - \frac{1}{2}a_2\epsilon\right) - a_3 m + a_2\epsilon = 0$$

from which we get, $m = \frac{3a_2\epsilon}{a_3}$. Now, this m must be equal to m_+, since this is the minima.

$$\begin{aligned}
&\implies \left(\frac{3a_2}{a_3}\epsilon - \frac{a_3}{2a_4}\right)^2 = \left(\frac{a_3}{2a_4}\right)^2 - \frac{a_2}{a_4}\epsilon \\
&\implies \left(\frac{3a_2}{a_3}\right)^2\epsilon^2 - \frac{3a_2}{a_4}\epsilon = -\frac{a_2}{a_4}\epsilon \\
&\implies \frac{9a_2}{a_3^2\epsilon} = \frac{2}{a_4} \\
&\implies \boxed{a_3^2 = \frac{9}{2}a_2a_4\epsilon}
\end{aligned}$$

Define $T^{**} = T_c + \frac{2a_3^2}{9a_2a_4} < T^*$. We summarise all the cases below:

- For $T > T^*$ we have only one minima $m = 0$.
- For $T^{**} < T < T^*$ we have three extrema, the global minima is at $m = 0$ and at m_+ we have a local minima. m_- is a maxima.
- For $T_c < T < T^{**}$ we have three extrema, the global minima is at m_+ and at $m = 0$ we have a local minima. m_- is still a maxima.
- For $T < T_c$, we have three extremas and $m = 0$ is a local maxima, while the global minima is at m_+. m_- is a local minima.

But where does the first order transition take place? Note that, for $T > T^{**}$ the minima is at $m = 0$ and then, at $T = T^{**}$, we have two minima at $m = 0$ and a finite $m = m_+ > 0$. Just below T^{**} we have the global minima as m_+ which is not zero. Thus, there is a abrupt jump between the minima, which is the telltale sign of a first order transition.

12.2. Tricritical Point

We now consider a free energy with $\mathbb{Z}_2$ symmetry, but with a higher order term, m^6.

$$\mathcal{L} = \frac{1}{2}a_2(T - T_c)m^2 + \frac{1}{4}a_4m^4 + \frac{1}{6}a_6m^6 \qquad a_6, a_2 > 0 \tag{38}$$

From the same old routine, we minimise the Landau free energy

$$\frac{\partial\mathcal{L}}{\partial m} = m(a_2(T - T_c) + a_4m^2 + a_6m^4) = 0 \tag{39}$$

Denoting $t = T - T_c$, the trivial solution is $m = 0$ while the four other solutions are given by,

$$m^2 = -\frac{a_4}{2a_6} \pm \sqrt{\left(\frac{a_4}{2a_6}\right)^2 - \frac{a_2}{a_6}t} \implies \boxed{m = \pm\sqrt{-\frac{a_4}{2a_6} \pm \sqrt{\left(\frac{a_4}{2a_6}\right)^2 - \frac{a_2}{a_6}t}}}$$

Suppose that, $T > T_c$ and $a_4 > 0$, which implies that $a_2t + a_4m^2 + a_6m^4 > 0$ and cannot produce any root, for all m and hence, $\frac{\partial\mathcal{L}}{\partial m}$ has a unique root at $m = 0$. For $T < T_c$, consider $a_2t + a_4x + a_6x^2 = 0$ where we defined $x = m^2$.

The discriminant of this equation is $a_4^2 - 4a_6a_2t$. As $T < T_c$, we have $t < 0$ and hence the discriminant is positive. This implies the existence of two roots to the equation. However, note that the product of the roots is $\frac{a_2t}{a_6} < 0$ which implies that one of the root is negative and the other is positive. We discard the negative root, as $x = m^2 > 0$ by definition. Then, apart from $m = 0$, only two root survive from this, corresponding to $x_+ \longrightarrow m = \pm\sqrt{x_+}$, which are:

$$m = \pm\sqrt{-\frac{a_4}{2a_6} + \sqrt{\left(\frac{a_4}{2a_6}\right)^2 - \frac{a_2}{a_6}t}}$$

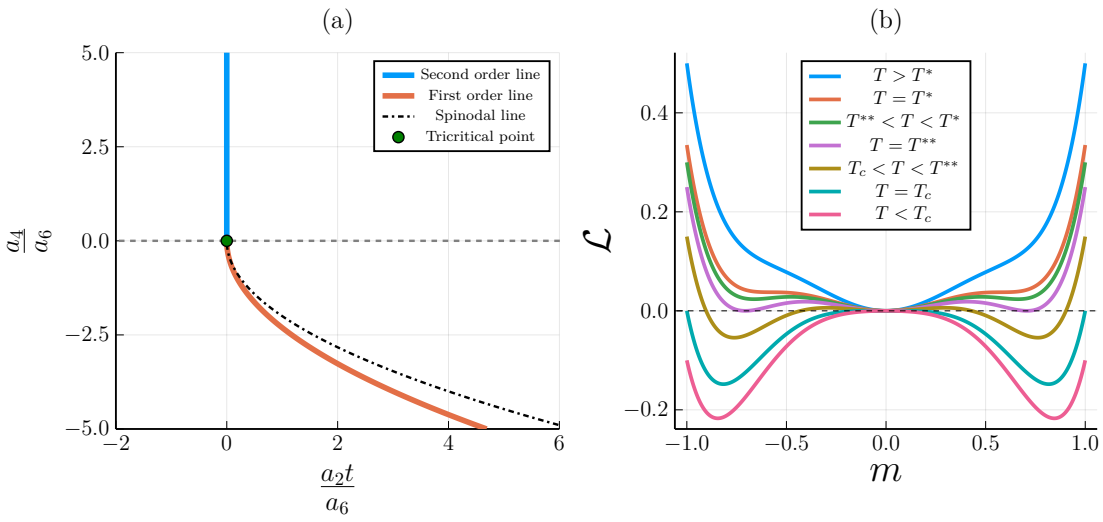


Figure 20: Landau free energy $\mathcal{L}$ with the sixth order term. (a) Phase diagram in the a_4 vs. t plane. The blue line denotes the second order line ($a_2 = 0$) while the dashed grey line denotes the spinodal line $a_4^2 = 4a_2a_6t$ (b) Behavious of $\mathcal{L}$ in different temperature regime.

as the '$-$' root inside the square root gives imaginary solution. To see this, note that $\frac{a_2}{a_6}t < 0$ and hence,

$$\sqrt{\left(\frac{a_4}{2a_6}\right)^2 - \frac{a_2}{a_6}t} = \sqrt{\left(\frac{a_4}{2a_6}\right)^2 + \left|\frac{a_2}{a_6}t\right|} > \left|\frac{a_4}{2a_6}\right|$$

Let us now look at the case when $T > T_c$ but $a_4 < 0$, which has all five real roots, provided $a_4^2 > 4a_2a_6t \implies a_4 < -2\sqrt{a_2a_6t}$. If $a_4 > -2\sqrt{a_2a_6t}$, then the quantity under the root becomes imaginary and all the four roots become complex, so only real root is $m = 0$.

As $\mathcal{L} \to \infty$ as $m \to \pm\infty$, we must have three minima, separated by two maximas. From $\mathbb{Z}_2$ symmetry or otherwise, we can say that for $T > T_c$, $m = 0$ is always going to be a minima (and for $T < T_c$, it is a maxima). We now need to check whether the other two minima are lower in energy than $m = 0$ or not; so we check as before, $\mathcal{L}(m) = \mathcal{L}(0) = 0$ along with $\frac{\partial \mathcal{L}}{\partial m} = 0$ which gives us two simultaneous equations,

$$\begin{aligned} 6a_2t + 3a_4m^2 + 2a_6m^4 &= 0 \\ a_2t + a_4m^2 + a_6m^4 &= 0 \end{aligned} \tag{40}$$

Multiplying the second equation by 2 and subtracting, we obtain:

$$4a_2t + a_4m^2 = 0 \implies m^2 = -\frac{4a_2}{a_4}t$$

Substituting this again the one of the equations gives us,

$$a_4 = -\frac{4}{\sqrt{3}}\sqrt{a_2a_6t} < 0$$

Now, we summarise the cases for $T > T_c$:

- If $a_4 > -2\sqrt{a_2a_6t}$ then only minima is $m = 0$.
- If $-\frac{4}{\sqrt{3}}\sqrt{a_2a_6t} < a_4 < -2\sqrt{a_2a_6t}$, then five real roots appear, but the global minima is still $m = 0$.
- If $a_4 < -\frac{4}{\sqrt{3}}\sqrt{a_2a_6t}$, then five real roots appear and zero minima is the local minima, while the other two (degenerate) minimas are global.

For $T < T_c$, three extremas are three; $m = 0$ is a maxima while two other global minimas are present. As before, there are two temperature scales involved, first is the spinodal temperature $T^* = T_c + \frac{a_4^2}{4a_2a_6}$ where the minima first start to appear and $T^{**} = T_c + \frac{3a_4^2}{16a_2a_6}$ where the first order transition take place (minima is the same as the minima at $m = 0$), as shown in Fig. 20. The point $(t = 0, a_4 = 0)$ in the phase diagram, where the first and the second order line meet is called the *tricritical point*.

Lecture 13: Landau Theory for Phase Transition: III

In this lecture, we focus on how the order parameter changes and the emergence of interesting phenomenon like hysterisis, for the m^3 and m^6 Landau theory.

13.1. Order Parameter Flow for m^3

Consider the previous case of $\mathcal{L}$ with m^3 term. We can change this to a one-parameter problem, following a transformation. We want to keep the one parameter r associated with a_2, since this is where the temperature dependence is there. The other parameters need to be scaled somehow. If we say, $a_3 = ca_4$, then we obtain

$$\mathcal{L} = a_4\left(\frac{a_2}{2a_4}(T - T_c)m^2 - \frac{1}{3}cm^3 + \frac{1}{4}m^4\right)$$

If we now define the scaling $m = cu$ then we obtain,

$$\mathcal{L} = a_4\left(\frac{a_2}{2a_4}(T - T_c)c^2u^2 - \frac{1}{3}c^4u^3 + \frac{1}{4}c^4u^4\right)$$

The last two terms contain c^4. If the first term also somehow had c^4 we can take it common. So let us try the definition

$$\frac{a_2(T - T_c)}{a_4} = rc^2 \implies a_2(T - T_c) = \frac{a_3^2}{a_4}r$$

where r is our new parameter and the Landau free energy becomes,

$$\mathcal{L} = a_4c^4\left(\frac{1}{2}ru^2 - \frac{1}{3}u^3 + \frac{1}{4}u^4\right)$$

Rescaling $\mathcal{L}$ by a_4c^4, we obtain the following transformed function,

$$\varphi(u) = \frac{1}{2}ru^2 - \frac{1}{3}u^3 + \frac{1}{4}u^4 \tag{41}$$

which depends only on the parameter r (note that r contains the temperature dependence). The fixed point for $\varphi(u)$ are found from solving $\varphi'(u) = 0$,

$$ru - u^2 + u^3 = 0 \implies u = 0 \qquad u_\pm = \frac{1}{2} \pm \sqrt{\frac{1}{4} - r}$$

From the second derivative, we have $\varphi''(u) = r - 2u + 3u^2$. For $r > \frac{1}{4}$ we only have one fixed point, $u = 0$ and $\varphi''(u) = r > 0$, hence $u = 0$ is a *stable fixed point*. Now, for $0 < r < \frac{1}{4}$ we have three extremas for $\varphi(u)$.

For this case, $0 < u_- < u_+$ and hence, 0 and u_+ are the minimas while u_- is the maxima (from the form of the potential). We need to check which of the minima is lower, for which we check $\varphi(u) = \varphi(0) = 0$.

Multiplying this by 12 and ignoring the $u = 0$ roots, we have $6r - 4u + 3u^2 = 0$. From minimisation condition, we further have $r - u + u^2 = 0$. Solving this simultaneously yields $u = 3r$ and substituting this in any one of the equation gives us $r = \frac{2}{9}$ and $u = \frac{2}{3}$. Hence, for $r > \frac{2}{9}$, $u = 0$ is the global minima while $u = u_+$ is the local minima and this becomes opposite for $0 < r < \frac{2}{9}$.

For $r < 0$, $u_- < 0 < u_+$ and hence $u = 0$ becomes the *unstable* maxima and the minimas are that $u = u_\pm$.

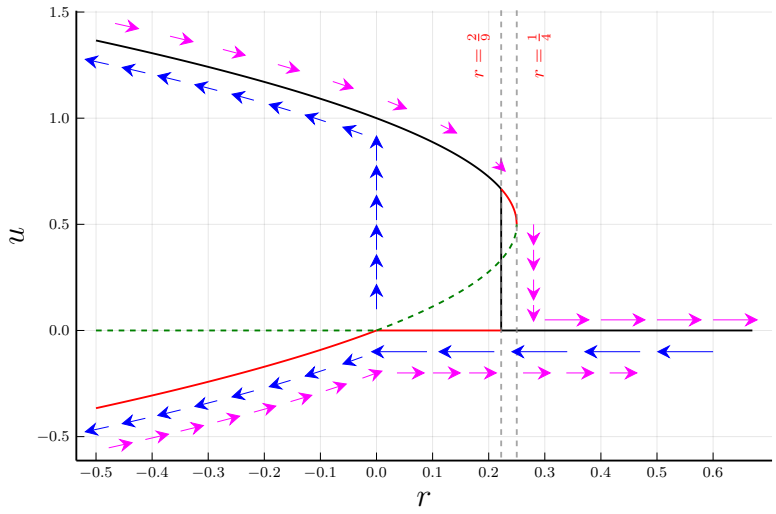


Figure 21: Hysterisis plot for $\varphi(u)$ with the cubic term. The black line denotes the stable fixed points while the red line represents the metastable fixed points. The dashed green line denote the unstable points.

So, say if we start from a negative value of u and r, then the system quickly moves to the red line (which is locally stable). As we increase r, we move along the red line to reach past $r = 0$ (shown by the magenta arrows in the lower region of Fig. 21), still following the same line, since the line is locally stable. In this case, there is no hysterisis.

Instead, if we start from some positive value of u initially, the system moves to follow the upper black line; it continues to move like this till $r = \frac{1}{4}$, at which point the line ceases to exist and it quickly drops down to $u = 0^+$.

When coming back (starting with a high positive value of r), the system remains in $u = 0$ line, until $u = 0$ becomes unstable at $r = 0$. At this point, the system jumps to the globally stable upper black line and continues to move there (shown by the blue lines in the upper part of Fig. 21)).

Clearly, these paths, while going and returning, are not the same, and this demonstrates the hysterisis in the theory.

13.2. Order Parameter Flow for m^6

Let us move on to the sextic potential that we saw earlier,

$$\mathcal{L} = \frac{1}{2}a_2(T - T_c)m^2 + \frac{1}{4}a_4 m^4 + \frac{1}{6}a_6 m^6$$

We can perform the same kind of transformation here also. Taking a_6 common we have,

$$\mathcal{L} = a_6\left(\frac{a_2}{2a_6}(T - T_c)m^2 + \frac{a_4}{4a_6}m^4 + \frac{1}{6}m^6\right)$$

Taking the scaling $a_4 = \pm c^2 a_6$ [1] and $m = cu$ we obtain,

$$\mathcal{L} = a_6\left(\frac{a_2}{2a_6}(T - T_c)c^2u^2 \pm \frac{c^6}{4}u^4 + \frac{1}{6}c^6u^6\right)$$

Defining the new scaling,

$$\frac{a_2(T - T_c)}{a_6} = rc^4 \implies a_2(T - T_c) = \frac{a_4^2}{a_6}r$$

[1] If a_4 is positive, then we take the $+$ sign, else take the $-$ sign.

Taking c^6 common and rescaling $\mathcal{L}$ by $c^6 a_6$, we get the transformed function,

$$\varphi(u) = \frac{1}{2}ru^2 \pm \frac{1}{4}u^4 + \frac{1}{6}u^6 \tag{42}$$

We do not focus on the case with the + sign. We will deal mainly with the negative coefficient of u^4. Minimising $\varphi(u)$ we obtain,

$$ru - u^3 + u^5 = 0 \implies r - u^2 + u^4 = 0$$

which gives us the roots,

$$u = \pm\sqrt{\frac{1}{2} \pm \sqrt{\frac{1}{4} - r}} \qquad u = 0$$

If $r > \frac{1}{4}$, then the only root is $u = 0$ (other roots become imaginary). If $0 < r < \frac{1}{4}$ then we have all the roots. If $r < 0$ then $\sqrt{\frac{1}{4} - r} > \frac{1}{2}$, then there are only three roots, $u = 0, \pm\sqrt{\frac{1}{2} + \sqrt{\frac{1}{4} - r}}$.

Note that $\varphi''(0) = r$ which implies that for $r > 0$, $u = 0$ is a minima and it is a maxima otherwise. For $r > 0$, to check which is the global minima, we check $\varphi(u) = \varphi(0) = 0$ and $\varphi'(u) = 0$, which leads to the simultaneous equations,

$$\begin{aligned} 6r - 3u^2 + 2u^4 &= 0 \\ r - u^2 + u^4 &= 0 \end{aligned}$$

solving which, we obtain $u^2 = 4r$ and $r = 0$ or $r = \frac{3}{16}$. Then, for $r > \frac{3}{16}$, $u = 0$ is the global minima. For $r < \frac{3}{16}$, u_{++} and u_{-+} are the global stable minimas. Between $\frac{3}{16} < r < \frac{1}{4}$, u_{++} and u_{-+} are the metastable minimas. From this, we obtain the following u vs. r plot.

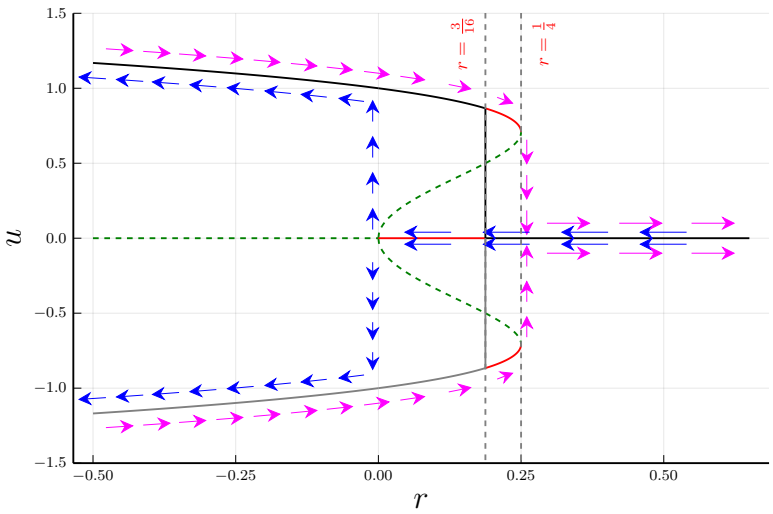


Figure 22: Hysterisis plot for $\varphi(u)$ with m^6. The solid black and grey line denote the stable fixed points while the red line represents the metastable fixed points. The dashed green line denote the unstable points.

There is an obvious $u \to -u$ symmetry in Fig. 22. When r is positive, the flow is towards the fixed point $u = 0$, which persists even when $r < \frac{1}{4}$. When it reaches $r = 0$, $u = 0$ becomes unstable and the flow shifts to either of the global fixed points u_{++} or u_{-+}.

If we instead start from a higher positive value of u when $r < 0$, the system shifts to the upper black branch and follows that line till $r = \frac{1}{4}$ where the stable point is annihilated and the system abruptly shifts to $u = 0+$, where it remains on increasing r further. We thus see that between $0 < r < \frac{1}{4}$, the dynamics is irreversible and there is *hysterisis*.

Lecture 14: Spontaneous Symmetry Breaking

Let us re-visit the spontaneous symmetry breaking seen earlier, through the perspective of Landau theory. SSB, as stated before, refers to the fact that in some regime, the ground state does not respect the symmetry of the Hamiltonian. For a finite system, we observe no SSB since everything is analytic. In the thermodynamic limit, we had seen,

$$m = -\lim_{h\to 0}\frac{\partial}{\partial h}\left[\lim_{N\to\infty}\frac{F}{N}\right] \neq -\lim_{N\to\infty}\left[\lim_{h\to 0}\left(\frac{1}{N}\frac{\partial F}{\partial h}\right)\right]$$

With the definition of the partition function using $\mathcal{L}$, we can write the free energy from Eq. (29) as,

$$F = -k_{\mathrm{B}}T\ln\left[\int_{-\infty}^{\infty}\mathrm{d}m e^{-\beta N\mathcal{L}}\right] \tag{43}$$

where we have extended the integral limits to $\pm\infty$. Taking derivative with respect to the field, we obtain,

$$\frac{\partial F}{\partial h} = -k_{\mathrm{B}}T\cdot -\beta N\frac{\int \mathrm{d}m\ e^{-\beta N\mathcal{L}}(-m)}{\int \mathrm{d}m\ e^{-\beta N\mathcal{L}}} = -N\frac{\int \mathrm{d}m\ me^{-\beta N\mathcal{L}}}{\int \mathrm{d}m\ e^{-\beta N\mathcal{L}}} \tag{44}$$

where we assumed that $\mathcal{L}$ has the coupling term $-mh$ with the field. Let us focus on the numerator only, since the denominator is just the partition function and is always positive.

$$\lim_{h\to 0}\frac{\partial F}{\partial h} \propto \lim_{h\to 0}\int \mathrm{d}m\ me^{-\beta N\mathcal{L}} = \lim_{h\to 0}\left[\int_{-\infty}^{0}\mathrm{d}m\ me^{-\beta N\mathcal{L}} + \int_{0}^{\infty}\mathrm{d}m\ me^{-\beta N\mathcal{L}}\right] \tag{45}$$

Now, in the zero field limit, $\mathcal{L}(m) = \mathcal{L}(-m)$ (presence of $\mathbb{Z}_2$ symmetry). Let we change the integral variable $m \to -m$, using which we get

$$\lim_{h\to 0}\frac{\partial F}{\partial h} \propto \lim_{h\to 0}\left[-\int_{0}^{\infty}\mathrm{d}m\ me^{-\beta N\mathcal{L}} + \int_{0}^{\infty}\mathrm{d}m\ me^{-\beta N\mathcal{L}}\right] = 0 \tag{46}$$

Thus, on taking the zero-field limit first, we get an overall zero magnetisation, even if we take the thermodynamic limit after this. Let us now try to take the thermodynamic limit first and then take the zero-field limit.

$$\begin{aligned}\lim_{N\to\infty} -\frac{k_{\mathrm{B}}T}{N}\ln\left[\int_{-\infty}^{\infty}\mathrm{d}m\ e^{-\beta N(\widetilde{\mathcal{L}}-hm)}\right] &= \lim_{N\to\infty} -\frac{k_{\mathrm{B}}T}{N}\ln\left[\int_{-\infty}^{0}\mathrm{d}m\ e^{-\beta N(\widetilde{\mathcal{L}}-hm)} + \int_{0}^{\infty}\mathrm{d}m\ e^{-\beta N(\widetilde{\mathcal{L}}-hm)}\right] \\ &= \lim_{N\to\infty} -\frac{k_{\mathrm{B}}T}{N}\ln\left[\int_{0}^{\infty}\mathrm{d}m\ \left(e^{-\beta N(\widetilde{\mathcal{L}}-hm)} + e^{-\beta N(\widetilde{\mathcal{L}}+hm)}\right)\right]\end{aligned} \tag{47}$$

where $\widetilde{\mathcal{L}}$ denotes the Landau free energy without the field coupling. In the last step, we had used the substitution $m \to -m$ as before. Let us suppose $h > 0$, then the integral can be written as,

$$\lim_{N\to\infty} -\frac{k_{\mathrm{B}}T}{N}\ln\left[\int_{0}^{\infty}\mathrm{d}m\ e^{-\beta N(\widetilde{\mathcal{L}}-hm)}\left[1 + e^{-2\beta Nhm}\right]\right] \tag{48}$$

For a finite positive h, if $N \to \infty$, then the blue term is really really small and hence can be neglected. The remaining integral (evaluated by the saddle point approximation) takes the value where it peaks at m^*. Taking the thermodynamic limit and $h \to 0^+$, we have:

$$-\lim_{h\to 0^+}\lim_{N\to\infty}\frac{\partial}{\partial h}\left[-\frac{k_{\mathrm{B}}T}{N}\ln e^{-\beta N(\widetilde{\mathcal{L}}(m^*)-hm^*)}\right] = -\lim_{h\to 0^+}\lim_{N\to\infty}\frac{\partial}{\partial h}\left[\widetilde{\mathcal{L}}(m^*) - hm^*\right] = m^* \tag{49}$$

which gives a finite magnetisation. Suppose we had taken $h < 0$ initially,

$$\lim_{N\to\infty} -\frac{k_B T}{N} \ln \left[\int_0^\infty \mathrm{d}m \; e^{-\beta N(\widetilde{\mathcal{L}}+hm)} \left[1 + e^{+2\beta N h m}\right] \right] \tag{50}$$

Since $h < 0$ then the red term goes to zero and exactly similarly, we obtain a finite magnetisation $-m^*$ when taking the zero field limit after the thermodynamic limit. This gives us the correct prescription of analysing the spontaneous magnetisation, depicting SSB.

Lecture 15: Landau-Ginzburg Theory

In the Landau theory, we had assumed an average value m of the magnetisation for the entire system and used this as the order parameter. However, this method is too rough as it misses any spatial dependence of the order parameter. m was spatially homogenous which perhaps is not what we want. We now generalise $m \to m(\mathbf{x})$ where $m(\mathbf{x})$ is now a field.

We focus on magnetic systems only, however, this can be applied to more general systems. To see this clearly, divide the system into N' different cells $\{I_1, I_2 \dots I_{N'}\}$, each with a characteristic length $\sim l$ as shown below. Here l is a mesoscopic length scale, $a \ll l \ll L$ where a is the lattice spacing and L is the typical linear dimension of the lattice.

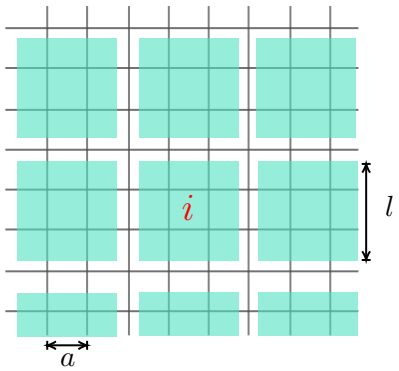


Figure 23: Coarse graining the lattice

Let the centre of cell I be $\mathbf{x}$ and define the local order parameter,

$$m_{\mathrm{I}}(\mathbf{x}) = \frac{1}{N_{\mathrm{I}}} \sum_{i\in I} \sigma_i \tag{51}$$

where N_{I} is the number of spins in cell I. This process is called *coarse graining*, since we are defining an order parameter, averaged over N_{I} spins in each cell. Let us now define $\mathcal{L}$ in this case. At first glance, it seems that

$$\mathcal{L}(\{m_{\mathrm{I}}\}) = \sum_i^{N'} \left[\frac{1}{2} a_2 (T - T_c) m_i^2 + \frac{1}{4} a_4 m_i^4 - h_i m_i \right]$$

We have suppressed the $\mathbf{x}$ parameter, since $\mathbf{x}$ is dependent on i itself. Note that the above free energy does not take into account the cost of maintaining the local magnetisation in adjacent cells. Every m_i is independent and this can lead to large difference in the order parameter in adjacent cells. We assume that the spatial variation of the local order parameter is 'slow' and for this, we introduce a symmetric coupling term,

$$\mathcal{L}(\{m_{\mathrm{I}}\}) = \sum_i^{N'} \left[\frac{1}{2} a_2 (T - T_c) m_i^2 + \frac{1}{4} a_4 m_i^4 - h_i m_i \right] + \frac{1}{2} \sum_{ij} \mathcal{C}_{ij} (m_i - m_j)^2 \tag{52}$$

where $\mathcal{C}_{ij}$ is the short-range coupling and based on a characteristic cutoff length R, is defined as,

$$\mathcal{C}_{ij} = \begin{cases} c_0 & |i-j|l < R \\ 0 & |i-j|l > R \end{cases}$$

There are some subtleties here though. Note that $\mathbf{x}$ can take only discrete values, based on the position of the cell. Hence we assume that $\frac{N'}{N}$ is small enough that $\mathbf{x}$ can be taken to be continuous. Moreover, within each cell, $m_{\rm I}(\mathbf{x})$ is quantised in terms of $\frac{1}{N_{\rm I}}$. We choose $N_{\rm I}$ large enough, so that $m_{\rm I}(\mathbf{x})$ can take any value between -1 and $+1$. This allows us to replace $m_{\rm I}(\mathbf{x})$ by just a continuous function $m(\mathbf{x})$. Let us now manipulate the coupling term now. Assume a 1D system for ease.

$$\begin{aligned} \frac{1}{2}\sum_{ij}\mathcal{C}_{ij}(m_i - m_j)^2 &= \sum_i \sum_{j=1}^{R/l} c_0 (m_{i+j} - m_i)^2 \\ &= \sum_i \sum_{j=1}^{R/l} c_0 \left[\frac{(m_{i+j}-m_i)^2}{(jl)^2}\right](jl)^2 \end{aligned} \tag{53}$$

The thing in the bracket looks like the discrete version of a derivative. In the continuum limit, this leads to $(\partial_x m(x))^2$, which becomes the gradient term $(\boldsymbol{\nabla} m(\mathbf{x}))\cdot(\boldsymbol{\nabla} m(\mathbf{x}))$ in general d dimensions. The sum over i can be converted to a d-dimensional integral,

$$\sum_i \equiv \frac{1}{l^d}\int \mathrm{d}^d x$$

where l^d is the elemental volume in each cell with centre $\mathbf{x}$. The sum over j is just a constant and depends on the interaction range R. Thus, absorbing every constants into a single parameter γ, the coupling term becomes,

$$\frac{1}{2}\sum_{ij}\mathcal{C}_{ij}(m_i - m_j)^2 \simeq \frac{\gamma}{2}\int \mathrm{d}^d x\ (\boldsymbol{\nabla} m(\mathbf{x}))^2$$

The final expression for the Landau free energy is,

$$\mathcal{L}[m(\mathbf{x})] = \int \mathrm{d}^d x\ \left[\frac{1}{2}a_2(T-T_c)(m(\mathbf{x}))^2 + \frac{1}{4}a_4(m(\mathbf{x}))^4 - h(\mathbf{x})m(\mathbf{x}) + \frac{\gamma}{2}(\boldsymbol{\nabla} m(\mathbf{x}))^2\right] \tag{54}$$

Note that, $\mathcal{L}$ has now become a *functional*, that is, it takes a function $m(\mathbf{x})$ and spits out a scalar. The partition function calculation becomes a bit involved, since it contains the term $\exp(-\beta\mathcal{L}[m(\mathbf{x})])$ and we have to perform an integral. However, this is not an ordinary integral, since the integration variable is now a function $m(\mathbf{x})$.

What happens is that there are infinite realisations of the function $m(\mathbf{x})$ and we need to 'integrate' over all these realisations. The process through which it is done is called *functional integral* or a more cool sounding, *path integral*. The formal notation of the functional integral is,

$$\mathcal{Z} = \int \mathcal{D}m(\mathbf{x})\ e^{-\beta\int \mathrm{d}^d x\ \left[\frac{1}{2}a_2(T-T_c)(m(\mathbf{x}))^2 + \frac{1}{4}a_4(m(\mathbf{x}))^4 - h(\mathbf{x})m(\mathbf{x}) + \frac{\gamma}{2}(\boldsymbol{\nabla} m(\mathbf{x}))^2\right]} \tag{55}$$

Out of the infinite realisations of $m(\mathbf{x})$, the one which gives the equation of state is the one which minimises the free energy functional. For minimisation purpose, we have to invoke the concept of function derivative since $m(\mathbf{x})$ is a function. Thus, we have the equation of state as,

$$m^*(\mathbf{x})\ :\quad \frac{\delta\mathcal{L}}{\delta m} = 0$$

Before formally going down this rabbit hole, let us find the minima by simply calculating the variation $\delta\mathcal{L}$ when the function $m(vbx)$ is varied from the minimising function as $m(\mathbf{x}) = m^*(\mathbf{x}) + \delta m(\mathbf{x})$, such that at the boundaries, $\delta m = 0$.

$$\delta\mathcal{L} = \int \mathrm{d}^d x\ \left[a_2(T-T_c)m\delta m + a_4 m^3\delta m - h\delta m + \frac{\gamma}{2}\times 2(\delta(\boldsymbol{\nabla} m)\cdot(\boldsymbol{\nabla} m))\right]$$

Let us calculate the variation of the gradient term.

$$\begin{aligned}\int \mathrm{d}^d x\ (\boldsymbol{\nabla} m)\cdot\delta(\boldsymbol{\nabla} m) &= \int \mathrm{d}^d x\ (\boldsymbol{\nabla} m)\cdot\boldsymbol{\nabla}(\delta m)\\ &\overset{\text{IBP}}{=} -\int \mathrm{d}^d x\ (\boldsymbol{\nabla}^2 m)\delta m + \text{Boundary terms}\\ &= -\int \mathrm{d}^d x\ (\boldsymbol{\nabla}^2 m)\delta m\end{aligned}$$

The boundary term is zero, since δm is zero at the boundaries. From the variation of the functional, we obtained

$$\delta\mathcal{L} = \int \mathrm{d}^d x\ \left[a_2(T-T_c)m(\mathbf{x}) + a_4(m(\mathbf{x}))^3 - h(\mathbf{x}) - \gamma\boldsymbol{\nabla}^2 m(\mathbf{x})\right]\delta m = 0$$

Since δm is arbitrary, we have the equation of state satisfied by,

$$\boxed{a_2(T-T_c)m^*(\mathbf{x}) + a_4(m^*(\mathbf{x}))^3 - h(\mathbf{x}) - \gamma\boldsymbol{\nabla}^2 m^*(\mathbf{x}) = 0}$$

Lecture 16: Kink Solutions

In the previous lecture, we introduced a spatial variation of the order parameter, $m(\mathbf{x})$. Consider the 1D Ising chain as an example. Suppose in the extreme left end of the chain, we have a $\uparrow$ spin while in the extreme right, we have a $\downarrow$ spin.

If we keep this constraint fixed, then it is evident that somewhere in the middle, there should be a spin flip (that is, we cannot *continuously deform* the left side to bring it to the right side). This inability to continuously deform a configuration aptly indicates that this is a *topological artifact*.

This spin flip is nothing but a *domain wall* if we think about it. The domain wall is also exotically called a *kink* or *soliton* depending on the context and the type of system used. Note that if there are two kinks, then there are two spin flips and hence these cancel each other (that is, the boundaries have the same spins). Thus, this configuration can be continuously deformed to the ground state which is uniform.

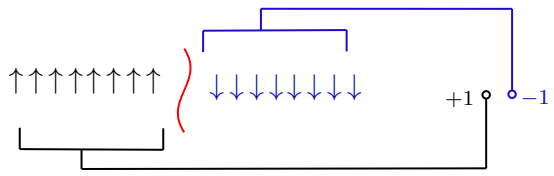


Figure 24: Mapping of spins to the order parameter space.

The spins left and right of the kink can be mapped from the real space (of the lattice) to the order-parameter space, where there are two points $+1$ and -1, as shown in Fig. 24. Thus a state $(+,+)$ or $(-,-)$ will have all up spins and down spins respectively and hence are the ground states. The state $(+,-)$ (state $(-,+)$) will have up spins on the left (right) and down spins on the right (left) of the kink. These are the four topologically distinct sectors for the 1D Ising model. The state $(-,+)$ is called the kink state where we have up spins on the right of the chain while $(+,-)$ is called the anti-kink state.

We want to see the variation of the order parameter across the domain wall. For this, consider the following Landau functional,

$$\mathcal{L}[m(\mathbf{x})] = \int \mathrm{d}^d x\ \left[\frac{1}{2}a_2(T-T_c)(m(\mathbf{x}))^2 + \frac{1}{4}a_4(m(\mathbf{x}))^4 - h(\mathbf{x})m(\mathbf{x}) + \frac{\gamma}{2}(\boldsymbol{\nabla} m(\mathbf{x}))^2\right]$$

Now, suppose spatial variations persist only in one direction, while all the other $(d-1)$ dimensions are spatially uniform. Hence $m(\mathbf{x}) \equiv m(x)$ and let A be the integral over the rest of the spatially uniform

$(d-1)$ dimensions (hence $A \sim l^{d-1}$).

$$\frac{\mathcal{L}}{A} = \int \mathrm{d}x \left[\frac{1}{2}a_2(T-T_c)(m(x))^2 + \frac{1}{4}a_4(m(x))^4 - h(x)m(x) + \frac{\gamma}{2}\left(\frac{\partial m(x)}{\partial x}\right)^2\right] \tag{56}$$

Considering $h(x) = 0$, we get the equation of motion:

$$\gamma\frac{\mathrm{d}^2m}{\mathrm{d}x^2} = a_2(T-T_c)m + a_4m^3 \tag{57}$$

Multiplying both sides by $\frac{\mathrm{d}m}{\mathrm{d}x}$ we get,

$$\begin{aligned}
\gamma\left(\frac{\mathrm{d}m}{\mathrm{d}x}\right)\frac{\mathrm{d}^2m}{\mathrm{d}x^2} = \left[a_2(T-T_c)m + a_4m^3\right]\left(\frac{\mathrm{d}m}{\mathrm{d}x}\right) &\implies \frac{\gamma}{2}\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\mathrm{d}m}{\mathrm{d}x}\right)^2 = \frac{\partial}{\partial x}\left[\frac{1}{2}a_2(T-T_c)m^2 + \frac{1}{4}a_4m^4\right] \\
&\implies \frac{\mathrm{d}}{\mathrm{d}x}\left[\frac{\gamma}{2}\left(\frac{\mathrm{d}m}{\mathrm{d}x}\right)^2 - \frac{1}{2}a_2(T-T_c)m^2 - \frac{1}{4}a_4m^4\right] = 0 \\
&\implies -\frac{\gamma}{2}\left(\frac{\mathrm{d}m}{\mathrm{d}x}\right)^2 + \frac{1}{2}a_2(T-T_c)m^2 + \frac{1}{4}a_4m^4 = C
\end{aligned}$$

where C is a constant determined by the boundary conditions. So let's set $m(x \to +\infty) = m_\infty = \sqrt{-\frac{a_2}{a_4}(T-T_c)} > 0$ and $\left.\frac{\mathrm{d}m}{\mathrm{d}x}\right|_\infty = 0$. Using this, we obtain the value of C

$$C = \frac{1}{2}a_2(T-T_c) \times \left(-\frac{a_2(T-T_c)}{a_4}\right) + \frac{1}{4}a_4 \times \frac{(a_2(T-T_c))^2}{a_4^2} = -\frac{[a_2(T-T_c)]^2}{4a_4}$$

Substituting this value above, we get the equation as,

$$\begin{aligned}
0 &= -\frac{\gamma}{2}\left(\frac{\mathrm{d}m}{\mathrm{d}x}\right)^2 + \frac{1}{2}a_2(T-T_c)m^2 + \frac{1}{4}a_4m^4 + \frac{[a_2(T-T_c)]^2}{4a_4} \\
&= -\frac{\gamma}{2}\left(\frac{\mathrm{d}m}{\mathrm{d}x}\right)^2 + \frac{a_4}{4}\left[\frac{2a_2}{a_4}(T-T_c)m^2 + m^4 + m_\infty^4\right] \\
&= -\frac{\gamma}{2}\left(\frac{\mathrm{d}m}{\mathrm{d}x}\right)^2 + \frac{a_4}{4}\left[-2m^2m_\infty^2 + m^4 + m_\infty^4\right] \\
&= -\frac{\gamma}{2}\left(\frac{\mathrm{d}m}{\mathrm{d}x}\right)^2 + \frac{a_4}{4}(m^2 - m_\infty^2)^2
\end{aligned} \tag{58}$$

from which get two solutions,

$$\sqrt{\frac{2\gamma}{a_4}}\frac{\mathrm{d}m}{\mathrm{d}x} = \pm(m^2 - m_\infty^2)$$

We take the $-$ve solution and then we integrate to get,

$$\sqrt{\frac{2\gamma}{a_4}}\int_{m(x_0)}^{m}\frac{\mathrm{d}m}{m_\infty^2 - m^2} = \int_{x_0}^{x}\mathrm{d}x = (x - x_0)$$

where x_0 is the centre of the domain wall and we assume $m(x_0) = 0$. On solving the integral, we obtain the solution,

$$\begin{aligned}
\sqrt{\frac{2\gamma}{a_4}}\frac{1}{m_\infty}\tanh^{-1}\left(\frac{m}{m_\infty}\right) = (x - x_0) \implies m(x) &= m_\infty\tanh\left[\frac{m_\infty(x-x_0)}{\sqrt{2}(\gamma/a_4)^{1/2}}\right] \\
&= m_\infty\tanh\left[\frac{(x-x_0)}{\sqrt{2}(\gamma/a_4)^{1/2}(a_2(T_c-T)/a_4)^{-1/2}}\right]
\end{aligned}$$

Now, the red quantity has the dimension of length and we denote is by ξ. Physically, ξ denotes the length scale over which significant change occurs across the domain wall. This is appropriately called

the *correlation length* since this is the scale across which correlations between the spins persist. The correlation length is temperature dependent as seen above. It scales as, $\xi \sim (T_c - T)^{-1/2}$, hence shows a power-law divergence at $T = T_c$.

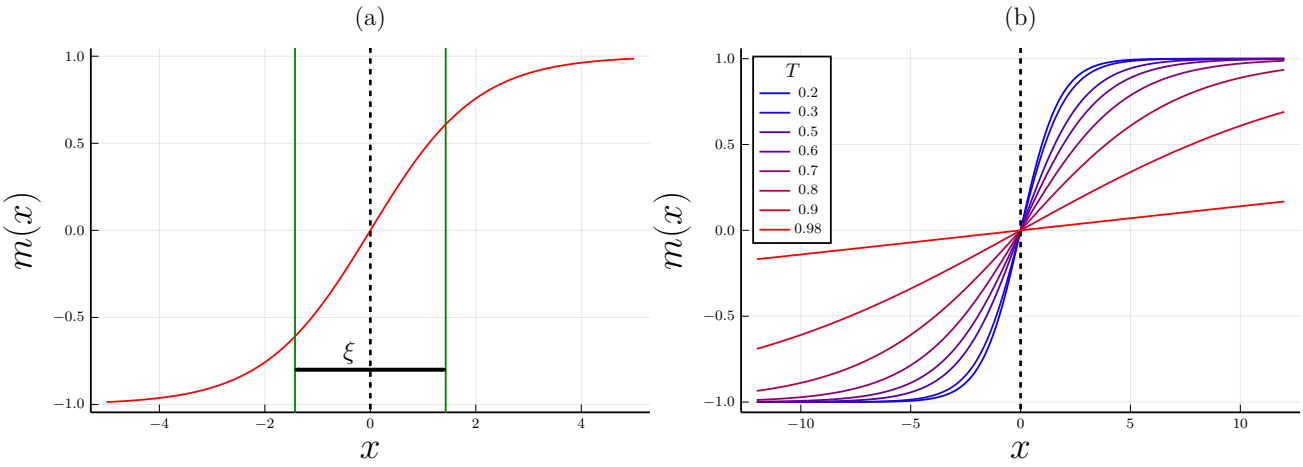


Figure 25: Spatial variation of order parameter. (a) $m(x)$ at $T < T_c$. The black vertical dashed line denotes the centre of the domain wall, while the green lines denote the extent of ξ. Within this region, most changes occur across the domain wall. (b) $m(x)$ for various temperatures. We see that the correlation length gradually increases on increasing T.

The domain wall incurs some energy cost in the system. This is reflected in terms of the surface tension σ defined as,

$$\sigma \equiv \int_{-\infty}^{\infty} \left[\frac{1}{2}a_2(T-T_c)m^2(x) + \frac{1}{4}a_4 m^4(x) + \frac{\gamma}{2}\left(\frac{\mathrm{d}m}{\mathrm{d}x}\right)^2\right] - \left[\frac{1}{2}a_2(T-T_c)m_\infty^2 + \frac{1}{4}a_4 m_\infty^4\right] \tag{59}$$

The above is just the increase in energy from the uniform ground state. This gives us,

$$\begin{aligned}
\sigma &= \int_{-\infty}^{\infty} \left[\frac{1}{2}a_2(T-T_c)\left(m^2(x) - m_\infty^2\right) + \frac{1}{4}a_4\left(m^4(x) - m_\infty^4\right) + \frac{\gamma}{2}\left(\frac{\mathrm{d}m}{\mathrm{d}x}\right)^2\right] \mathrm{d}x \\
&= \int_{-\infty}^{\infty} \left[\frac{1}{2}a_2(T-T_c)\left(m^2 - m_\infty^2\right) + \frac{1}{4}a_4\left(m^4 - m_\infty^4\right) + \frac{a_4}{4}(m^2 - m_\infty^2)^2\right] \mathrm{d}x \\
&= \int_{-\infty}^{\infty} \left(m^2 - m_\infty^2\right)\left[\frac{1}{2}a_2(T-T_c) + \frac{1}{4}a_4\left(m^2 + \cancel{m_\infty^2}\right) + \frac{a_4}{4}(m^2 - \cancel{m_\infty^2})\right] \mathrm{d}x \\
&= \int_{-\infty}^{\infty} \frac{a_4}{2}\left(m^2 - m_\infty^2\right)^2 \mathrm{d}x = \int_{-\infty}^{\infty} \frac{a_4}{2} \times \frac{2\gamma}{a_4}\left(\frac{\mathrm{d}m}{\mathrm{d}x}\right)^2 \mathrm{d}x = \gamma \int_{-\infty}^{\infty} \left[\frac{\mathrm{d}}{\mathrm{d}x}\left(m_\infty \tanh\left(\frac{x-x_0}{\sqrt{2}\xi}\right)\right)\right]^2 \mathrm{d}x
\end{aligned} \tag{60}$$

Carrying out the integral yields us,

$$\sigma = \frac{\gamma m_\infty^2}{2\xi^2} \int_{-\infty}^{\infty} \mathrm{sech}^4\left(\frac{x-x_0}{\sqrt{2}\xi}\right) \mathrm{d}x = \frac{\gamma m_\infty^2}{2\xi^2} \times \sqrt{2}\xi \int_{-\infty}^{\infty} \mathrm{sech}^4(t)\, \mathrm{d}t = \frac{4\gamma m_\infty^2}{3\sqrt{2}\xi}$$

Using the definition of ξ from before, we get

$$\sigma = \frac{4}{3\sqrt{2}} \frac{\sqrt{\gamma a_2^3 |T_c - T|^3}}{a_4} \implies \sigma \sim |T_c - T|^{3/2} \tag{61}$$

The surface tension goes to 0 at T_c and so domain walls are easy to form at the critical point.

16.1. Physical Interpretation

At the extreme left end, $m(x) \to -m_\infty$ and $m(x) \to +m_\infty$ at the extreme right end. Note that

$$\pm m_\infty$$

are the minima of the free energy density. Hence, the domain wall allows us to go from one minima to another. There is anothe physical interpretation of Eq. (57). This equation looks exactly like Newton's law $\frac{\partial^2 y}{\partial t^2} = -\frac{\partial V}{\partial y}$, with $m \leftrightarrow y$ and $x \leftrightarrow t$. Then this situation is like an inertial particle moving back and forth between two hills, situated at $\pm m_\infty$.

16.2. Topological Charge

Let us define the following quantity,

$$\mathfrak{q}_\mathrm{T} := \frac{1}{2m_0}\int_{-\infty}^{\infty} \mathrm{d}x \left(\frac{\mathrm{d}m}{\mathrm{d}x}\right) = \left[\frac{m(+\infty) - m(-\infty)}{2m_0}\right] \tag{62}$$

$\mathfrak{q}_\mathrm{T}$ is just dependent on the boundary conditions and hence, invariant under some local change of the order parameter. For the ground states, $(+,+)$ or $(-,-)$, the topological charge is zero. For the kink state $(-,+)$ we have $\mathfrak{q}_\mathrm{T} = +1$ and for the anti-kink state $(+,-)$ we have $\mathfrak{q}_\mathrm{T} = -1$. Two kinks (one kink and other anti-kink or vice versa) is topologically equivalent to one of the ground states.

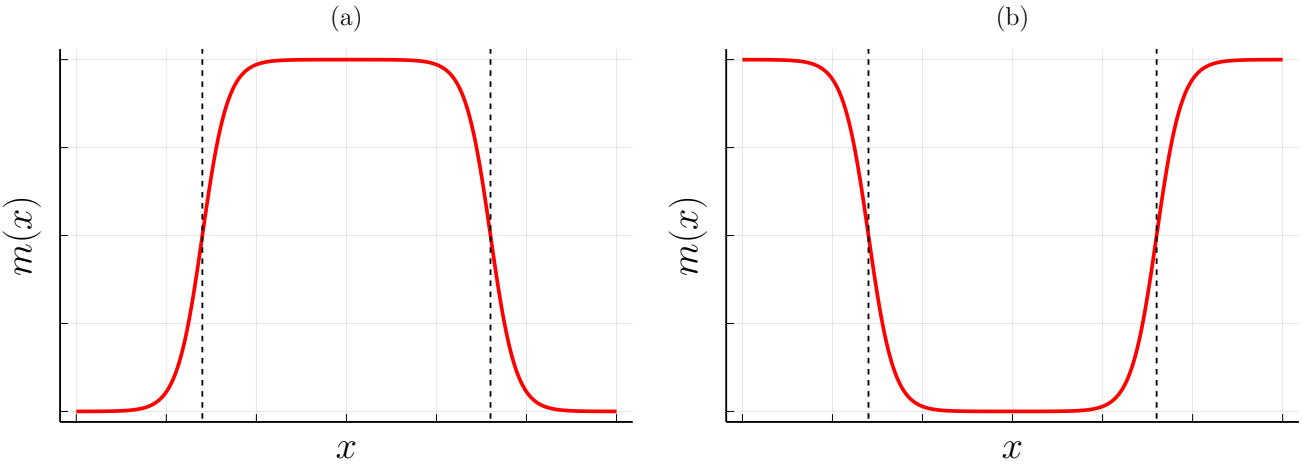


Figure 26: (a) Kink-antikink pair (b)Antikink-kink pair

Such kink and anti-kink pairs are deformable and annihilate each other as seen previously.

Lecture 17: Fluctuation-Response Relations

Given a partition function we can obtain the free energy as $F = -k_\mathrm{B}T \ln \mathcal{Z}$ and from there we can find the expectation value of the order parameter,

$$\langle m(\mathbf{r})\rangle = -\frac{\delta F}{\delta h(\mathbf{r})} = \frac{\int \mathcal{D}m\; e^{-\beta\mathcal{L}} m(\mathbf{r})}{\int \mathcal{D}m\; e^{-\beta\mathcal{L}}} \tag{63}$$

The second expression is just the definition of the expectation value. In a similar way, the generalised susceptibility (with spatial dependence) can be found out as,

$$\chi(\mathbf{r}-\mathbf{r}') = \frac{\delta\langle m(\mathbf{r})\rangle}{\delta h(\mathbf{r}')} = -\frac{\delta^2 F}{\delta h(\mathbf{r}) h(\mathbf{r}')} \tag{64}$$

Using the definition of functional derivatives we can then write the variations,

$$\delta F = -\int \mathrm{d}^d r' \ \langle m(\mathbf{r}')\rangle \, \delta h(\mathbf{r}') \qquad \delta \langle m(\mathbf{r})\rangle = \int \mathrm{d}^d r' \ \chi(\mathbf{r}-\mathbf{r}')\delta h(\mathbf{r}')$$

We assume that $\mathcal{L}$ has a term $-h(\mathbf{r})m(\mathbf{r})$. Differentiating the expectation value with respect to the field, we have

$$\begin{aligned}\chi(\mathbf{r}-\mathbf{r}') = \frac{\delta \langle m(\mathbf{r})\rangle}{\delta h(\mathbf{r}')} &= \frac{\int \mathcal{D}m \ e^{-\beta\mathcal{L}[m]}\beta m(\mathbf{r})m(\mathbf{r}')}{\int \mathcal{D}m \ e^{-\beta\mathcal{L}}} - \frac{\left[\int \mathcal{D}m \ e^{-\beta\mathcal{L}} m(\mathbf{r})\right]\left[\int \mathcal{D}m \ m(\mathbf{r}')\beta e^{-\beta\mathcal{L}}\right]}{\left[\int \mathcal{D}m \ e^{-\beta\mathcal{L}}\right]^2} \\ &= \frac{1}{k_{\mathrm{B}}T}\left[\langle m(\mathbf{r})m(\mathbf{r}')\rangle - \langle m(\mathbf{r})\rangle \langle m(\mathbf{r}')\rangle\right] = \beta\mathcal{G}(\mathbf{r}-\mathbf{r}')\end{aligned} \tag{65}$$

where $\mathcal{G}(\mathbf{r}-\mathbf{r}')$ is the correlation function defined in Lec. 6. Hence we get a simple relation,

$$\chi(\mathbf{r}-\mathbf{r}') = \beta\mathcal{G}(\mathbf{r}-\mathbf{r}')$$

Note that we have assumed translational invariance from the beginning, that's why we were writing the functions as a different of the two vectors $\mathbf{r}-\mathbf{r}'$. We can easily use the Fourier transform for translationally invariant systems.

$$\chi(\mathbf{r}-\mathbf{r}') = \int \frac{\mathrm{d}^d k}{(2\pi)^d} \ \widetilde{\chi}(\mathbf{k}) e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}$$

Using this in the above relation above, we get $\widetilde{\chi}(k) = \beta\widetilde{\mathcal{G}}(k)$, which is an aspect of *linear response theory*. The susceptibility is a response, which is linearly proportional to the correlation function, related to the fluctuations in the system. Now, if the frequency of the external perturbation (like the Fourier modes of the magnetic field) tends to zero, χ must reduce to the static isothermal susceptibility,

$$\chi_{\mathrm{T}} = \lim_{k\to 0} \widetilde{\chi}(k) = \beta\widetilde{\mathcal{G}}(0) = \beta \int \mathrm{d}^d r \ \mathcal{G}(\mathbf{r}) \tag{66}$$

17.1. Calculating the correlation function (Ornstein-Zernike relation)

Here, we outline a method to calculate the correlation function. For that, let us take the derivative of the equation of state with respect to the field.

$$\frac{\delta}{\delta h(\mathbf{r}')}\left[a_2(T-T_c)m(\mathbf{r}) + a_4 m^3(\mathbf{r}) - h(\mathbf{r}) - \gamma\boldsymbol{\nabla}^2 m\right] = 0$$

From the definition of susceptibility, we have

$$\left[-\gamma\boldsymbol{\nabla}^2 + a_2(T-T_c) + 3a_4 m^2\right]\chi(\mathbf{r}-\mathbf{r}') = \delta^{(d)}(\mathbf{r}-\mathbf{r}')$$

Using the linear response result, we have

$$\left[-\gamma\boldsymbol{\nabla}^2 + a_2(T-T_c) + 3a_4 m^2\right]\mathcal{G}(\mathbf{r}-\mathbf{r}') = k_{\mathrm{B}}T\delta^{(d)}(\mathbf{r}-\mathbf{r}')$$

It is evident that the correlation function is the *Green's function* for this differential equation. Let us focus on the spatially homogenous case, $m(\mathbf{r}) \equiv m = \sqrt{\frac{a_2(T_c-T)}{a_4}}$ for $T < T_c$ and $m = 0$ for $T > T_c$. Then,

$$\left(-\boldsymbol{\nabla}^2 + \xi_>^{-2}\right)\mathcal{G}(\mathbf{r}-\mathbf{r}') = \frac{k_{\mathrm{B}}T}{\gamma}\delta^{(d)}(\mathbf{r}-\mathbf{r}') \qquad \xi_> = \left[\frac{a_2(T-T_c)}{\gamma}\right]^{-1/2}$$

and for $T < T_c$ we have

$$\left(-\gamma\boldsymbol{\nabla}^2 + a_2(T-T_c) + 3a_4 \times \frac{a_2(T_c-T)}{a_4}\right) = (-\gamma\boldsymbol{\nabla}^2 - 2a_2(T-T_c)) \implies \left(-\boldsymbol{\nabla}^2 + \xi_<^{-2}\right)\mathcal{G}(\mathbf{r}-\mathbf{r}') = \frac{k_{\mathrm{B}}T}{\gamma}\delta^{(d)}(\mathbf{r}-\mathbf{r}')$$

where $\xi_< = \left[\frac{2a_2(T_c-T)}{\gamma}\right]^{-1/2}$. These are the *correlation length* defined above and below T_c. We see the scaling of ξ with $|T_c - T|$ and conclude that, $\xi \sim (T_c - T)^{-\nu}$ for $T < T_c$ and $\xi \sim (T - T_c)^{\nu'}$ for $T > T_c$ with $\nu = \nu' = \frac{1}{2}$ from the mean-field theory. In summary, the two-point correlation function satisfies the differential equation,

$$(-\boldsymbol{\nabla}^2 + \xi^{-2})\mathcal{G}(\mathbf{r} - \mathbf{r}') = \frac{k_\mathrm{B}T}{\gamma}\delta^{(d)}(\mathbf{r} - \mathbf{r}')$$

Fourier transform of the equation yields,

$$\widetilde{\mathcal{G}}(k) = \frac{k_\mathrm{B}T}{\gamma}\frac{1}{k^2 + \xi^{-2}} \tag{67}$$

This is kinda the Fourier transform of the Yukawa potential. Note that, at $T = T_c$, $\xi \to \infty$ and hence $\widetilde{\mathcal{G}}(k) \sim k^{-2}$. We can revert back to the real space correlation function using the polar coordinates which we do now. For that, let us choose $\mathbf{r}' = 0$ and write the Laplacian in polar coordinates in d dimensions which gives us,

$$\left[-\frac{1}{r^{d-1}}\frac{\partial}{\partial r}\left(r^{d-1}\frac{\partial}{\partial r}\right) + \xi^{-2}\right]\mathcal{G}(\mathbf{r}) = \frac{k_\mathrm{B}T}{\gamma}\delta^{(d)}(\mathbf{r}) \tag{68}$$

Let us define $\rho := r/\xi$ and $G(\rho) = \mathcal{G}(r/\xi)$. Moreover, the d-dimensional delta function gives $\delta^{(d)}(\rho\xi) = \frac{1}{\xi^d}\delta^{(d)}(\rho)$. Using these variables, the differential equation becomes,

$$\left[-\frac{1}{\rho^{d-1}}\frac{\partial}{\partial \rho}\left(\rho^{d-1}\frac{\partial}{\partial \rho}\right) + 1\right]G(\rho) = g\delta^{(d)}(\rho)$$

where we have defined $g := \frac{k_\mathrm{B}T}{\gamma}\xi^{2-d}$. g is a strength of the fluctuations since this contains the correlation length. Now, if $\rho \neq 0$, then

$$\frac{\partial}{\partial \rho}\left(\rho^{d-1}\frac{\partial G}{\partial \rho}\right) = \rho^{d-1}G(\rho) \implies G'' + \frac{(d-1)}{\rho}G' - G = 0$$

Define $G(\rho) = \rho^{-\nu}F(\rho)$ and carrying out the derivatives,

$$\begin{aligned}
G' &= -\nu\rho^{-(1+\nu)}F + \rho^{-\nu}F' = \rho^{-\nu}\left(F' - \frac{\nu F}{\rho}\right) \\
G'' &= -\nu\left[\rho^{-(1+\nu)}F' - (1+\nu)\rho^{-(\nu+2)}F\right] - \nu\rho^{-(1+\nu)}F' + \rho^{-\nu}F'' \\
&= \rho^{-\nu}F'' - 2\nu F'\rho^{-(\nu+1)} + \nu(1+\nu)\rho^{-(2+\nu)}F \\
&= \rho^{-\nu}\left[F'' - \frac{2\nu}{\rho}F' + \frac{\nu(\nu+1)}{\rho^2}F\right]
\end{aligned} \tag{69}$$

Let us substitute these in the above differential equation,

$$\begin{aligned}
G'' + \frac{(d-1)}{\rho}G' - G &= \rho^{-\nu}\left[\left(F'' - \frac{2\nu}{\rho}F' + \frac{\nu(\nu+1)}{\rho^2}F\right) + \frac{(d-1)}{\rho}F' - \frac{\nu(d-1)}{\rho^2}F - F\right] \\
&= \rho^{-\nu}\left[F'' + \frac{d-1-2\nu}{\rho}F' + \frac{\nu(\nu+1) - \nu(d-1) - \rho^2}{\rho^2}F\right] = 0
\end{aligned} \tag{70}$$

Let us choose $d-1-2\nu = 1 \implies \nu = \frac{d}{2} - 1$. Then $\nu(\nu+1) - \nu(d-1) = \nu(\nu+1-d+1) = \nu(\nu+2-d) = -\nu^2$. Finally, we get the simplified differential equation,

$$\rho^2 F'' + \rho F' - (\nu^2 + \rho^2)F = 0$$

This is the *modified Bessel equation* and its solutions are given by the modified Bessel functions,

$$G(\rho) = \rho^{-\nu}(c_1 I_\nu(\rho) + c_2 K_\nu(\rho))$$

Note that $I_\nu \sim e^\rho$ and hence it exponentially grows up, which we do not want. Thus, we keep only $K_\nu(\rho)$ in the solution and hence, $G(\rho) \sim \rho^{-\nu} K_\nu$. The constant can be fixed by another complicated process (which I skip) and finally we get,

$$\frac{G(\rho)}{g} = \begin{cases} e^{-\rho} & d = 1 \\ \frac{1}{(2\pi)^{d/2}} \frac{1}{\rho^{(d-2)/2}} K_{\frac{d-2}{2}}(\rho) & d \geq 2 \end{cases} \tag{71}$$

For $\rho \gg 1 \implies r \gg \xi$, $K_\nu(\rho) \sim \left(\frac{\pi}{2\rho}\right)^{1/2} e^{-\rho}$ and hence for $d \geq 2$,

$$\begin{aligned} \mathcal{G}(r) = \frac{g}{(2\pi)^{d/2}} \frac{1}{\rho^{(d-2)/2}} K_{\frac{d-2}{2}}(\rho) &\longrightarrow \frac{g}{(2\pi)^{d/2}} \frac{\xi^{(d-2)/2}}{r^{(d-2)/2}} \left(\frac{\pi\xi}{2r}\right)^{1/2} e^{-r/\xi} \\ &= \xi^{2-d} \frac{k_\mathrm{B}T}{\gamma} \frac{1}{2^{d/2}\pi^{d/2}} \frac{\xi^{d/2-1}}{r^{d/2-1}} \frac{\pi^{1/2}\xi^{1/2}}{2^{1/2}r^{1/2}} e^{-r/\xi} \\ &= \frac{k_\mathrm{B}T}{\gamma} \cdot \frac{\pi^{(1-d)/2}}{2^{(1+d)/2}} \cdot \frac{e^{-r/\xi}}{r^{(d-1)/2}} \cdot \frac{1}{\xi^{(d-3)/2}} \end{aligned} \tag{72}$$

For $r \ll \xi$ (near T_c where correlation length diverges), $K_\nu \sim \frac{1}{2}\Gamma(\nu)\left(\frac{\rho}{2}\right)^{-\nu}$ and we get the expression:

$$\begin{aligned} \mathcal{G}(r) = \frac{g}{(2\pi)^{d/2}} \frac{1}{\rho^{(d-2)/2}} K_{\frac{d-2}{2}}(\rho) &\longrightarrow \frac{g}{(2\pi)^{d/2}} \frac{\xi^{(d-2)/2}}{r^{(d-2)/2}} \cdot \frac{1}{2}\Gamma\left(\frac{d-2}{2}\right)\left(\frac{2\xi}{r}\right)^{(d-2)/2} \\ &= \frac{k_\mathrm{B}T}{\gamma} \cdot \xi^{2-d} \cdot \frac{1}{2^{d/2}\pi^{d/2}} \frac{\xi^{d-2}}{r^{(d-2)/2}} \Gamma\left(\frac{d-2}{2}\right) 2^{d/2-2} \\ &= \frac{k_\mathrm{B}T}{\gamma} \cdot \frac{1}{4\pi^{d/2}} \cdot \frac{1}{r^{d-2}} \cdot \Gamma\left(\frac{d-2}{2}\right) \implies \mathcal{G}(r) \sim r^{-(d-2)} \end{aligned} \tag{73}$$

Thus, near $T = T_c$, $\mathcal{G}(r)$ becomes a power-law and it is self-similar. There is no inherent length scale. It has been experimentally seen that the exponent is not exactly $(d-2)$, hence we add a correction η, which is a new critical exponent. Thus,

$$\mathcal{G}(r) \sim \frac{1}{r^{d-2+\eta}} \tag{74}$$

From mean-field, η is obtained to be zero. The critical exponents heavily depend on the dimensionality of space. As d increases, the exponents becomes closer to that of the mean-field theory. In general, the exponents are not simple rational fractions, however, in $d = 2$ due to *conformal symmetry* (about which I do not have any idea), the exponents become rational numbers.

Lecture 18: Some More Fluctuations

By now, we have realised that the mean-field theory is very unstable and in many cases, it breaks down. Let us analyse when it is effective and when it is not. In MFT, we threw away the fluctuations and hence, if the fluctuations become more than the order parameter scale, then it breaks down.

In general, we see that the exponents do match for $d \geq 4$ using numerical results. What is so special about $d = 4$?

18.1. Ginzburg-Levanyuk Criterion

Suppose we consider only regions of extent upto order ξ in each dimensions (so correlations persist). We then define the correlation volume $V_\xi \sim \xi^d \alpha_d$ where $\alpha_d = \frac{\pi^{d/2}}{\Gamma(\frac{d}{2}+1)}$ is the volume of a unit d-sphere. Now, within this volume, if the fluctuations are way smaller than the average value of the order parameter, then we can say that MFT is kinda valid. Since the correlation is given by $\mathcal{G}(\mathbf{r})$ then, mathematically, we can define the condition for validity of Landau theory,

$$\frac{\int_{V_\xi} \mathrm{d}^d r \; \mathcal{G}(\mathbf{r})}{V_\xi} \ll \langle m \rangle^2 \tag{75}$$

This criteria is called the *Ginzburg-Levanyuk* criteria. We further analyse this,

$$\int_{V_\xi} \mathrm{d}^d r \; \mathcal{G}(\mathbf{r}) \ll \langle m \rangle^2 \, \xi^d \alpha_d$$

Now, from Eq. (66) the LHS just becomes the isothermal susceptibility[1],

$$\chi_{\mathrm{T}} k_{\mathrm{B}} T \ll \langle m \rangle^2 \, \xi^d \alpha_d \implies (-t)^{-\gamma} \ll (-t)^{2\beta} t^{-d\nu}$$

where we used the reduced temperature $t = \frac{T - T_c}{T_c}$ and the various scaling laws, $m \sim (-t)^\beta, \chi \sim (-t)^{-\gamma}$ and $\xi \sim (-t)^{-\nu}$. From this, we finally obtain:

$$(-t)^{\gamma + 2\beta - \nu d} \gg 1 \tag{76}$$

As $t \to 0$ (near T_c), this condition is only satisfied if $\gamma + 2\beta - \nu d < 0$, since then the LHS becomes less than 1 and blows up when the denominator becomes arbitrarily small. The criteria gives us,

$$\frac{\gamma + 2\beta}{\nu} < d \tag{77}$$

Defining $d_c = \frac{\gamma + 2\beta}{\nu}$ as the *upper critical dimension*, we see that for the Ising universality class (that is, those systems where the mean-field exponents are equal to that of the Ising model), $d_c = 4$ as $\gamma = 1, \beta = \nu = 1/2$ which tells us why $d = 4$ is important.

From our previous discussion, we saw that for $T < T_c$,

$$\xi = \left[\frac{\gamma}{2a_2(T_c - T)}\right]^{-1/2} \implies \xi = \left[\frac{\gamma}{2a_2 T_c(-t)}\right]^{-1/2} \implies \xi^d = \xi_1^d (-t)^{-d/2}$$

where ξ_1 is the rest of the constants, having no temperature depedence. For $T < T_c$ the susceptibility is equal to,

$$\chi = \frac{1}{2a_2(T_c - T)} = \frac{1}{2a_2 T_c(-t)}$$

Then, for $T < T_c^-$ the Ginzburg criteria gives us,

$$k_{\mathrm{B}} T_c \cdot \frac{1}{2a_2 T_c(-t)} \ll \alpha_d \xi_1^d (-t)^{-d/2} \cdot \frac{a_2(-t) T_c}{a_4} \implies \frac{k_{\mathrm{B}} a_4}{2a_2^2 T_c \xi_1^d \alpha_d} \ll (-t)^{2 - \frac{d}{2}}$$

Note that, from sec 11.3, the discontinuity in the specific heat was found out to be $\Delta C = \frac{a_2^2}{2a_4} T_c$ which exactly appears hear also. Define the GL reduced temperature as,

$$(-t_{\mathrm{GL}}) := \left[\frac{k_{\mathrm{B}}}{4\Delta C \xi_1^d \alpha_d}\right]^{2/(4-d)} \tag{78}$$

which tells us that MFT is valid only if $(-t)^{(4-d)/2} \gg (-t_{\mathrm{GL}})^{(4-d)/2}$. This relation is also dependent on the dimension.

- For $\mathbf{d > 4}$: As $t \to 0$, since $(4 - d) < 0$ the LHS can become arbitrarily large and hence the relation is always satisfied, since the RHS is just a finite constant.
- For $\mathbf{d < 4}$: As $t \to 0$, the Ginzburg criteria is not satisfied. There exists a temperature T_{GL} obtained from t_{GL} such that between $T_c - T_{\mathrm{GL}}$ and $T_c + T_{\mathrm{GL}}$, the Landau theory is not applicable. This region is called the *fluctuation dominating window*. The fluctuation dominating window is not universal and depends on the system. It is very, very narrow for conventional superconductors, so narrow that it cannot be probed by experimental means and hence experimentally it always matches with the MFT results.

[1] In Eq. (66), the integral is over the whole space, but it is well approximated by the integral over the correlation volume, since $\mathcal{G}$ is a rapidly decaying function.

- For $\mathbf{d = 4}$: Landau Theory is strictly not valid, however the Ginzburg criteria is marginally satisfied. There are some logarithmic corrections due to fluctuations.

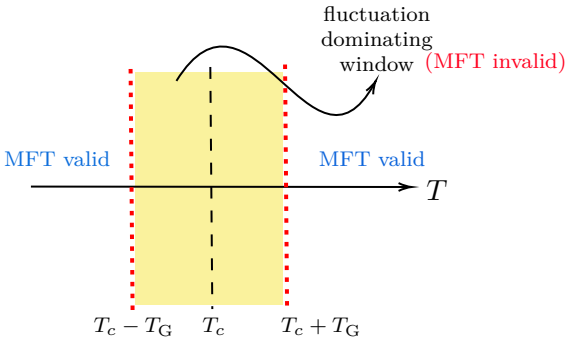


Figure 27: Fluctuation dominating window

This explains the significance of $d_c = 4$ as the upper critical dimension. Although we considered the Ising universality class, this procedure is also valid for other classes, however, $d_c \neq 4$ for those systems. Similar to the upper critical dimension, we do have a lower critical dimension d_l. Below d_l, fluctuations are so strong that they kill all the ordering and hence the mean-field theory is not even qualitatively correct (For Ising class, $d_l = 1$). Between d_l and d_c, we can qualitatively explain things using MFT but it will not provide quantitative accuracy.

Note: MFT is valid at $T = 0$, since at this temperature, no fluctuations exist. Also, when $d \to \infty$ and for infinite-range interactions, MFT is valid.

Lecture 19: Gaussian Approximation

We will try to incorporate some simple correction to MFT, to take care of the fluctuations. We try to approximate the functional integral in some way. For that, assume some deviation from the uniform magnetisation,

$$m(\mathbf{r}) = m_0 + \phi(\mathbf{r})$$

For $T > T_c$, we have $m_0 = 0$ and hence the Landau free energy becomes,

$$\mathcal{L}[\phi(\mathbf{x})] = \int \mathrm{d}^d x \left[\frac{1}{2}a_2(T - T_c)(\phi(\mathbf{x}))^2 + \frac{1}{4}a_4(\phi(\mathbf{x}))^4 - h(\mathbf{x})\phi(\mathbf{x}) + \frac{\gamma}{2}(\boldsymbol{\nabla}\phi(\mathbf{x}))^2\right]$$

We neglect terms greater than the quadratic order and also take the zero field case, which gives us,

$$\mathcal{L}[\phi(\mathbf{x})] = \int \mathrm{d}^d x \left[\frac{1}{2}a_2(T - T_c)(\phi(\mathbf{x}))^2 + \frac{\gamma}{2}(\boldsymbol{\nabla}\phi(\mathbf{x}))^2\right] \equiv \int \mathrm{d}^d x \; f(\phi(\mathbf{x})) \tag{79}$$

Let us consider a finite volume $V = L^d$, which will lead to the discretisation of the functional integral. If we decompose the field in terms of its Fourier modes, then the momenta will take discrete values in the d-dimensional space,

$$\mathbf{k} = \frac{2\pi}{L}\mathbf{n} \qquad \mathbf{n} \in \mathbb{Z}^d$$

We define the Fourier transform as,

$$\phi(\mathbf{x}) = \frac{1}{V}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}}\widetilde{\phi}_{\mathbf{k}} \xrightarrow{V\to\infty} \int \frac{\mathrm{d}^d k}{(2\pi)^d}\; e^{i\mathbf{k}\cdot\mathbf{x}}\widetilde{\phi}_{\mathbf{k}}$$

We will work with the discrete case (finite volume) for now. Let us substitute this definition carefully in the Landau functional.

$$f(\mathbf{x}) = \frac{1}{V^2}\sum_{\mathbf{k},\mathbf{k}'}\frac{\gamma}{2}\left[\boldsymbol{\nabla}_x\cdot\left(\widetilde{\phi}_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{x}}\right)\right]\left[\boldsymbol{\nabla}_x\cdot\left(\widetilde{\phi}_{\mathbf{k}'}e^{i\mathbf{k}'\cdot\mathbf{x}}\right)\right] + \frac{a_2}{2}(T-T_c)\widetilde{\phi}_{\mathbf{k}}\widetilde{\phi}_{\mathbf{k}'}e^{i(\mathbf{k}+\mathbf{k}')\cdot\mathbf{x}}$$
$$= \frac{1}{2V^2}\sum_{\mathbf{k},\mathbf{k}'}\left[-\gamma\mathbf{k}\cdot\mathbf{k}' + a_2(T-T_c)\right]\widetilde{\phi}_{\mathbf{k}}\widetilde{\phi}_{\mathbf{k}'}e^{i(\mathbf{k}+\mathbf{k}')\cdot\mathbf{x}}$$

There is only $\mathbf{x}$ dependence on the last exponential term. Integrating this over all the spatial dimensions of our system [1], we will get a Kronecker delta,

$$\int \mathrm{d}^d x\ f(\mathbf{x}) = \frac{1}{2V^2}\sum_{\mathbf{k},\mathbf{k}'}\left[-\gamma\mathbf{k}\cdot\mathbf{k}' + a_2(T-T_c)\right]\widetilde{\phi}_{\mathbf{k}}\widetilde{\phi}_{\mathbf{k}'}(V\delta_{\mathbf{k}+\mathbf{k}',0}) = \frac{1}{2V}\sum_{\mathbf{k}}\left[\gamma k^2 + a_2(T-T_c)\right]\widetilde{\phi}_{\mathbf{k}}\widetilde{\phi}_{-\mathbf{k}}$$

Since the field $\phi(\mathbf{x}) \in \mathbb{R}$, we have $\widetilde{\phi}_{-\mathbf{k}} = \widetilde{\phi}^*_{\mathbf{k}}$ which means that,

$$\int \mathrm{d}^d x\ f(\mathbf{x}) = \frac{1}{2V}\sum_{\mathbf{k},\mathbf{k}'}\left[-\gamma\mathbf{k}\cdot\mathbf{k}' + a_2(T-T_c)\right]\widetilde{\phi}_{\mathbf{k}}\widetilde{\phi}_{\mathbf{k}'}\delta_{\mathbf{k}+\mathbf{k}',0} = \frac{1}{2V}\sum_{\mathbf{k}}\left[\gamma k^2 + a_2(T-T_c)\right]\left|\widetilde{\phi}_{\mathbf{k}}\right|^2$$

Observe that $\phi(\mathbf{x}) = \widetilde{\phi}_0 + \sum_{\mathbf{k}\neq 0} e^{i\mathbf{k}\cdot\mathbf{x}}\widetilde{\phi}_{\mathbf{k}}$ which implies that, $\mathbf{k} = 0$ is the uniform mean field solution while $\mathbf{k} \neq 0$ denotes the fluctuations. Previously we had performed a coarse-graining to define the Landau-Ginzburg theory, which imposed a mesoscopic length scale l. Thus, $|\mathbf{r}| \gg l \implies |\mathbf{k}| \ll \frac{1}{l}$. Hence, there is a cutoff for the momenta, let us call it Λ. Thus the sum is restricted to only those momenta $\mathbf{k}$ which satisfies $|\mathbf{k}| < \Lambda$.

$$\mathcal{L}[\{\widetilde{\phi}_{\mathbf{k}}\}] = \frac{1}{2V}\sum_{\substack{\mathbf{k}\\|\mathbf{k}|<\Lambda}}\left[\gamma k^2 + a_2(T-T_c)\right]\left|\widetilde{\phi}_{\mathbf{k}}\right|^2 \tag{80}$$

Now, divide the k-space into two halves, Ω and Ω' such that if $\mathbf{k} \in \Omega$ then $-\mathbf{k} \in \Omega'$[2]. We need to focus only on one half, since if $\mathbf{k} \in \Omega$ then $-\mathbf{k} \in \Omega'$ and these are not indepedent. Then the Landau functional becomes,

$$\boxed{\mathcal{L}[\{\widetilde{\phi}_{\mathbf{k}}\}] = \frac{1}{V}\sum_{\substack{\mathbf{k}\in\Omega\\|\mathbf{k}|<\Lambda}}\left[\gamma k^2 + a_2(T-T_c)\right]\left|\widetilde{\phi}_{\mathbf{k}}\right|^2} \tag{81}$$

Now, let us find the partition function, where we need to perform the functional integral. Since the functional now depends on the Fourier modes, the functional integral measure will also change, which we write as,

$$\mathcal{Z} = \int \mathcal{D}\phi(\mathbf{x})\ e^{-\beta\mathcal{L}[\phi(\mathbf{x})]} \equiv \int \prod \widetilde{\phi}_{\mathbf{k}}\widetilde{\phi}^*_{\mathbf{k}}\ e^{-\beta\mathcal{L}[\{\widetilde{\phi}_{\mathbf{k}}\}]}$$

Let us elaborate this a little bit explicitly, getting rid of some subtleties.

- Firstly, note that $\widetilde{\phi}_{\mathbf{k}}$ and $\widetilde{\phi}^*_{\mathbf{k}}$ are in the same footing as the real and imaginary parts of $\widetilde{\phi}_{\mathbf{k}}$, so henceforth we will use the real and imaginary parts in the integral measure which we denote as, $\mathrm{Re}\,\widetilde{\phi}_{\mathbf{k}} \equiv \widetilde{\phi}^R_{\mathbf{k}}$ and $\mathrm{Im}\,\widetilde{\phi}^*_{\mathbf{k}} \equiv \widetilde{\phi}^I_{\mathbf{k}}$.
- Secondly, the limits of the product needs to be ascertained. Firstly, due to the same constraint that the field is real, the positive and negative modes are not independent. Moreover, we also need to take care of the cutoff. As a result, the product has the same limits as of the sum.
- While changing the measure to the Fourier modes, some constants surely crept in, which we would simply write as $\mathcal{N}$, since these would not be much of use.

[1] Note that the space is still continuous, even though the volume is finite

[2] One way to construct these regions can be to choose any arbitrary vector $\mathbf{a}$ and define $\Omega := \{\mathbf{k}|\mathbf{k}\cdot\mathbf{a} > 0\}$ and $\Omega' := \{\mathbf{k}|\mathbf{k}\cdot\mathbf{a} < 0\}$

Then the partition function becomes,

$$\boxed{\mathcal{Z} = \mathcal{N} \int \prod_{\substack{\mathbf{k}\in\Omega \\ |\mathbf{k}|<\Lambda}} \mathrm{d}\widetilde{\phi}^R_{\mathbf{k}} \mathrm{d}\widetilde{\phi}^I_{\mathbf{k}} \; \exp\left[-\frac{\beta}{V}\left[\gamma k^2 + a_2(T-T_c)\right]\left[(\widetilde{\phi}^R_{\mathbf{k}})^2 + (\widetilde{\phi}^I_{\mathbf{k}})^2\right]\right]} \tag{82}$$

where we have converted the exponential of the sum as a product of exponentials. Each integral has independent $\widetilde{\phi}^{R/I}_{\mathbf{k}}$ going from $-\infty$ to $+\infty$ and the integrand is a Gaussian. Thus, for each $\mathbf{k}$, the integral gives two Gaussian results, one for the imaginary and other for the real part. So the partition function becomes,

$$\mathcal{Z} = \mathcal{N} \prod_{\substack{\mathbf{k}\in\Omega \\ |\mathbf{k}|<\Lambda}} \frac{\pi k_{\mathrm{B}} T V}{\gamma k^2 + a_2(T-T_c)} \tag{83}$$

The free energy is then found by taking the logarithm,

$$F = -k_{\mathrm{B}}T\left[\ln \mathcal{Z}_0 + \sum_{\substack{\mathbf{k}\in\Omega \\ |\mathbf{k}|<\Lambda}} \ln\left(\frac{\pi k_{\mathrm{B}} T V}{\gamma k^2 + a_2(T-T_c)}\right)\right] = F_0 - \frac{k_{\mathrm{B}}T}{2} \sum_{|\mathbf{k}|<\Lambda} \ln\left(\frac{\pi k_{\mathrm{B}} T V}{\gamma k^2 + a_2(T-T_c)}\right)$$

In the last part, we included the sum over all k-space, which introduced the factor of ½ there. Next, we will calculate the heat capacity using this free energy and see whether any changes from MFT is seen by the introduction of fluctuations.

Lecture 20: Heat Capacity from Fluctuations

From MFT we know that the critical exponent $\alpha = 0$ and there is just a finite discontinuity across the transition point. However, in experiments, we have seen that the heat capacity actually diverges at the critical point. Let us see whether we can explain this behaviour using the fluctuations. The heat capacity at constant volume is given by,

$$C_v = -T\frac{\partial(S/V)}{\partial T} = -T\frac{\partial^2(F/V)}{\partial T^2}$$

We had calculated the free energy with incorporated fluctuations, in the previous lecture. The fluctuations are incorporated in the second term of the free energy, where the sum over $\mathbf{k}$ is there. Let us focus on that part only.

$$\begin{aligned}
\frac{C_v}{T} &= \frac{\partial^2}{\partial T^2}\left[\frac{1}{2}\frac{k_{\mathrm{B}}T}{V} \sum_{|\mathbf{k}|<\Lambda} \ln\left(\pi k_{\mathrm{B}} V T\right) - \ln\left(\gamma k^2 + a_2(T-T_c)\right)\right] \\
&= \frac{k_{\mathrm{B}}}{2V}\frac{\partial}{\partial T}\left[\sum_{|\mathbf{k}|<\Lambda} \ln\left(\pi k_{\mathrm{B}} V T\right) - \ln\left(\gamma k^2 + a_2(T-T_c)\right) + \left\{1 - \frac{a_2 T}{\gamma k^2 + a_2(T-T_c)}\right\}\right] \\
&= \frac{k_{\mathrm{B}}}{2V} \sum_{|\mathbf{k}|<\Lambda} \left[\frac{1}{T} - \frac{2a_2}{\gamma k^2 + a_2(T-T_c)} - \frac{a_2^2 T}{(\gamma k^2 + a_2(T-T_c))^2}\right] \\
&= \frac{k_{\mathrm{B}}}{2} \int_{|\mathbf{k}|<\Lambda} \frac{\mathrm{d}^d k}{(2\pi)^d} \left[\frac{1}{T} - \frac{2a_2}{\gamma k^2 + a_2(T-T_c)} - \frac{a_2^2 T}{(\gamma k^2 + a_2(T-T_c))^2}\right]
\end{aligned}$$

where we have converted the summation to an integral, taking $V \to \infty$. Now, we shall change the integral to polar coordinates. The angular part will be integrated out as the integrand has no angular dependence, giving us the solid angle S_d. We are then left with,

$$\frac{k_{\mathrm{B}}}{2}\frac{1}{(2\pi)^d} \int_0^{\Lambda} k^{d-1} \mathrm{d}k \left[\frac{1}{T} - \frac{2a_2}{\gamma k^2 + a_2(T-T_c)} - \frac{a_2^2 T}{(\gamma k^2 + a_2(T-T_c))^2}\right]$$

Let us focus on these integrals one by one:

- The first integral is,

$$\int_0^{\Lambda} k^{d-1}\mathrm{d}k\ \frac{1}{T} = \frac{1}{T}\frac{\Lambda^d}{d} \longrightarrow \text{ just a finite constant}$$

- The second integral is,

$$\frac{1}{\gamma}\int_0^{\Lambda} k^{d-1}\mathrm{d}k\ \frac{2a_2}{k^2+\frac{a_2}{\gamma}(T-T_c)} = \frac{1}{\gamma}\int_0^{\Lambda} k^{d-1}\mathrm{d}k\ \frac{2a_2}{k^2+\xi^{-2}}$$

Let us define $\mathbf{q} = \xi\mathbf{k} \implies \mathrm{d}q = \xi\mathrm{d}k$. Substituting this in the integral,

$$\frac{2a_2}{\gamma}\cdot\xi^{2-d}\int_0^{\Lambda\xi}\mathrm{d}q\ \frac{q^{d-1}}{1+q^2}$$

Since we are interested at points near T_c, where $\xi\to\infty$. Let us break the integral into two parts. The second part is for large q ($q \gg 1$) while the first part is for $q \ll 1$ or $q \sim 1$.

$$\int_0^{c}\mathrm{d}q\ q^{d-1} + \int_c^{\Lambda\xi}\mathrm{d}q\ q^{d-3} = \left[\frac{q^d}{d}\right]_0^c + \left[\frac{q^{d-2}}{d-2}\right]_c^{\Lambda\xi} \sim (w+\xi^{d-2})$$

where w is some constant, obtained from the first part. The integral overall becomes,

$$\frac{2a_2}{\gamma}\cdot(w+\xi^{d-2})\xi^{2-d} \sim \xi^{2-d} \sim t^{-(1-\frac{d}{2})}$$

ξ blows up at $T = T_c$ and hence the contribution would be finite if $2-d<0 \implies d>2$.

- Let us now focus on the third integral

$$\frac{k_\mathrm{B}}{2}\frac{1}{(2\pi)^d}\int_0^{\Lambda} k^{d-1}\mathrm{d}k\ \frac{a_2^2T}{(\gamma k^2+a_2(T-T_c))^2}$$

We do a similar kind of substitution $\mathbf{q} = \xi\mathbf{k}$ which gives us,

$$\frac{a_2^2k_\mathrm{B}T}{2\gamma^2}\frac{1}{(2\pi)^d}\cdot\xi^{4-d}\int_0^{\Lambda\xi}\mathrm{d}q\ \frac{q^{d-1}}{(1+q^2)^2}$$

Again, separating the integral into two parts gives us,

$$\int_0^{\Lambda\xi}\mathrm{d}q\ \frac{q^{d-1}}{(1+q^2)^2} = \int_0^{c}\mathrm{d}q\ q^{d-1} + \int_c^{\Lambda\xi}\mathrm{d}q\ q^{d-5} \sim (w'+\xi^{d-4})$$

Then the contribution from the third integral becomes,

$$\frac{a_2^2k_\mathrm{B}T}{2\gamma^2}\frac{1}{(2\pi)^d}\cdot\xi^{4-d}(w'+\xi^{d-4}) \sim \xi^{4-d} \sim t^{-(2-\frac{d}{2})}$$

The contribution would be finite if $4-d<0 \implies d>4$

For $d<2$, both the integrals diverge while for $d>4$, both converge. For $2<d<4$, the first converges while the second diverges. The scaling of the specific heat with the reduced temperature then becomes,

$$C_v \sim t^{-(1-\frac{d}{2})} + t^{-(2-\frac{d}{2})} \longrightarrow t^{-(2-\frac{d}{2})} \implies \boxed{C_v \sim t^{-(2-\frac{d}{2})}}$$

Hence, we see that the fluctuations have shifted the exponent α from the mean field value of zero to $\alpha = \left(2-\frac{d}{2}\right)$ and we do get a diverging behaviour at $T = T_c$, in agreement with reality. However, this is just a qualitative thing, since this exponent does not numerically agree with the experiments. Next, we will see a bit about correlation functions with fluctuations.

Lecture 21: Correlation due to Fluctuations

With respect to fluctuations, let us see how the correlation function changes. To begin our calculations, let us start with the following,

$$\left\langle \left|\widetilde{\phi}_{\mathbf{q}}\right|^2 \right\rangle = \frac{\prod\limits_{\substack{\mathbf{k}\in\Omega \\ |\mathbf{k}|<\Lambda}} \int \mathrm{d}\widetilde{\phi}^R_{\mathbf{k}}\mathrm{d}\widetilde{\phi}^I_{\mathbf{k}} \left|\widetilde{\phi}_{\mathbf{q}}\right|^2 e^{-\beta\mathcal{L}}}{\prod\limits_{\substack{\mathbf{k}\in\Omega \\ |\mathbf{k}|<\Lambda}} \int \mathrm{d}\widetilde{\phi}^R_{\mathbf{k}}\mathrm{d}\widetilde{\phi}^I_{\mathbf{k}}\ e^{-\beta\mathcal{L}}} = \frac{\prod\limits_{\substack{\mathbf{k}\in\Omega \\ |\mathbf{k}|<\Lambda}} \int \mathrm{d}\widetilde{\phi}^R_{\mathbf{k}}\mathrm{d}\widetilde{\phi}^I_{\mathbf{k}} \left[\left(\widetilde{\phi}^R_{\mathbf{q}}\right)^2 + \left(\widetilde{\phi}^I_{\mathbf{q}}\right)^2\right] e^{-\beta\mathcal{L}}}{\prod\limits_{\substack{\mathbf{k}\in\Omega \\ |\mathbf{k}|<\Lambda}} \int \mathrm{d}\widetilde{\phi}^R_{\mathbf{k}}\mathrm{d}\widetilde{\phi}^I_{\mathbf{k}}\ e^{-\beta\mathcal{L}}}$$

where $\mathcal{L}$ is the same as in Eq. (81). From this structure, we can see that if $\mathbf{k} \neq \mathbf{q}$, then the numerator and denominator gets cancelled. Thus all we are left with is just the integral over $\mathbf{q}$:

$$\begin{aligned}
&\frac{\int \mathrm{d}\widetilde{\phi}^R_{\mathbf{q}}\mathrm{d}\widetilde{\phi}^I_{\mathbf{q}} \left[\left(\widetilde{\phi}^R_{\mathbf{q}}\right)^2 + \left(\widetilde{\phi}^I_{\mathbf{q}}\right)^2\right] \exp\left(-\frac{\beta}{V}\left[\gamma q^2 + a_2(T-T_c)\right]\left[\left(\widetilde{\phi}^R_{\mathbf{q}}\right)^2 + \left(\widetilde{\phi}^I_{\mathbf{q}}\right)^2\right]\right)}{\int \mathrm{d}\widetilde{\phi}^R_{\mathbf{q}}\mathrm{d}\widetilde{\phi}^I_{\mathbf{q}}\ \exp\left(-\frac{\beta}{V}[\gamma q^2 + a_2(T-T_c)]\left[\left(\widetilde{\phi}^R_{\mathbf{q}}\right)^2 + \left(\widetilde{\phi}^I_{\mathbf{q}}\right)^2\right]\right)} \\
&= \frac{\int \mathrm{d}\widetilde{\phi}^R_{\mathbf{q}}\ \left(\widetilde{\phi}^R_{\mathbf{q}}\right)^2 \exp\left(-\frac{\beta}{V}\left[\gamma q^2 + a_2(T-T_c)\right]\left(\widetilde{\phi}^R_{\mathbf{q}}\right)^2\right)}{\int \mathrm{d}\widetilde{\phi}^R_{\mathbf{q}}\ \exp\left(-\frac{\beta}{V}[\gamma q^2 + a_2(T-T_c)](\widetilde{\phi}^R_{\mathbf{q}})^2\right)} + \frac{\int \mathrm{d}\widetilde{\phi}^I_{\mathbf{q}}\ \left(\widetilde{\phi}^I_{\mathbf{q}}\right)^2 \exp\left(-\frac{\beta}{V}\left[\gamma q^2 + a_2(T-T_c)\right]\left(\widetilde{\phi}^I_{\mathbf{q}}\right)^2\right)}{\int \mathrm{d}\widetilde{\phi}^I_{\mathbf{q}}\ \exp\left(-\frac{\beta}{V}[\gamma q^2 + a_2(T-T_c)](\widetilde{\phi}^I_{\mathbf{q}})^2\right)}
\end{aligned}$$

These two integrals are same and are typical Gaussian integrals, whose values can be found using Appendix C:

$$2 \times \frac{\int \mathrm{d}x\ x^2 e^{-c_q x^2}}{\int \mathrm{d}x\ e^{-c_q x^2}} = \frac{k_{\mathrm{B}}TV}{\gamma k^2 + a_2(T-T_c)}$$

Thus, the average correlation is obtained as,

$$\left\langle \left|\widetilde{\phi}_{\mathbf{q}}\right|^2 \right\rangle = \frac{k_{\mathrm{B}}TV}{\gamma q^2 + a_2(T-T_c)} \tag{84}$$

We can also use a heuristic equipartition method to get to this in an effortless way. From equiparition we know that each degree of freedom gets a contribution of $k_{\mathrm{B}}T/2$. Then, in Eq. (80) for each $\mathbf{k} = \mathbf{q}$, we have:

$$\frac{1}{2V}\left[\gamma q^2 + a_2(T-T_c)\right]\left\langle \left|\widetilde{\phi}_{\mathbf{q}}\right|^2 \right\rangle = \frac{1}{2}k_{\mathrm{B}}T \implies \left\langle \left|\widetilde{\phi}_{\mathbf{q}}\right|^2 \right\rangle = \frac{Vk_{\mathrm{B}}T}{\gamma q^2 + a_2(T-T_c)}$$

We thus obtain that in the Fourier space, $V\widetilde{\mathcal{G}}(\mathbf{k}) = \frac{k_{\mathrm{B}}TV}{\gamma k^2 + a_2(T-T_c)}$. Putting $\mathbf{k} = 0$ here gives us,

$$V\widetilde{\mathcal{G}}(\mathbf{k}=0) = \frac{k_{\mathrm{B}}TV}{a_2(T-T_c)} = k_{\mathrm{B}}TV\chi_{\mathrm{T}}$$

where $\chi_{\mathrm{T}} = \frac{1}{a_2(T-T_c)}$ is the isothermal susceptibility. Hence, in this case the static susceptibility rule still applies.

21.1. Hartree Approximation

We will now attempt to incorporate the quartic term in the calculations, which we neglected previously. In doing so, we will be doing some extremely stupid stuffs, without any justifications and some answers will emerge. This approximation is called the *Hartfree/self-consistent field/random phase* approximation.

What we do is, we consider a ϕ^4 theory but replace two of the ϕ with their average value, that is, $\phi^4 \longrightarrow \phi^2\left\langle\phi^2\right\rangle$.

There are six ($= {}^4C_2$) ways to choose which two out of the four ϕ's to take in the average. So the Landau functional becomes,

$$\mathcal{L}[\phi] = \int \mathrm{d}^d x\ \left[\frac{\gamma}{2}(\boldsymbol{\nabla}\phi)^2 + \frac{a_2}{2}(T-T_c)\phi^2 + \frac{6a_4}{4}\phi^2\left\langle\phi^2\right\rangle\right] \tag{85}$$

The effect of this is that the theory becomes ϕ^2 but the coefficient of ϕ^2 gets modified.

$$\frac{a_2}{2}(T-T_c) \longrightarrow \frac{a_2'}{2}(T-T_c) = \frac{a_2}{2}(T-T_c) + \frac{3a_4}{2}\left\langle\phi^2\right\rangle$$

Then the correlation found out before becomes,

$$\left\langle\left|\widetilde{\phi}_{\mathbf{q}}\right|^2\right\rangle = \frac{k_{\mathrm{B}}TV}{\gamma k^2 + a_2'(T-T_c)} = \frac{k_{\mathrm{B}}TV}{\gamma k^2 + a_2(T-T_c) + 3a_4\left\langle\phi^2\right\rangle}$$

Now, note the following,

$$\left\langle\phi^2\right\rangle \equiv \langle\phi(\mathbf{x})\phi(\mathbf{x})\rangle = \mathcal{G}(\mathbf{x},\mathbf{x}) = \int \frac{\mathrm{d}^d k}{(2\pi)^d}\widetilde{\mathcal{G}}(\mathbf{k}) = \int \frac{\mathrm{d}^d k}{(2\pi)^d}\frac{k_{\mathrm{B}}T}{\gamma k^2 + a_2(T-T_c) + 3a_4\left\langle\phi^2\right\rangle}$$

This is already a self-consistent equation for $\left\langle\phi^2\right\rangle$. From the expression of the isothermal susceptibility, $\chi_{\mathrm{T}}^{-1} = a_2'(T-T_c)$, we get:

$$\frac{\chi_{\mathrm{T}}^{-1} - a_2(T-T_c)}{3a_4} = \int \frac{\mathrm{d}^d k}{(2\pi)^d}\,\frac{k_{\mathrm{B}}T}{\gamma k^2 + \chi_{\mathrm{T}}^{-1}}$$

Near the critical temperature, the susceptibility diverges and hence $\chi_{\mathrm{T}}^{-1} \to 0$. Now, there is no apriori reason to consider the same critical point as in the ϕ^2 theory. Denoting the new critical temperature as T^* and changing to polar coordinates,

$$\frac{a_2}{3a_4}(T_c - T^*) = k_{\mathrm{B}}T^* \cdot \frac{S_{\mathrm{d}}}{(2\pi)^d\gamma^2}\int_0^\Lambda \mathrm{d}k\; k^{d-3} = \left[\frac{S_{\mathrm{d}}k_{\mathrm{B}}}{(2\pi)^d\gamma^2}\cdot\frac{\Lambda^{d-2}}{d-2}\right]T^*$$

From here, we obtain the value of $T*$,

$$T^* = \left[\frac{3a_4 S_{\mathrm{d}}k_{\mathrm{B}}}{(2\pi)^d a_2\gamma^2}\cdot\frac{\Lambda^{d-2}}{d-2} + 1\right]^{-1} T_c \implies T^* < T_c \tag{86}$$

The transition temperature is depressed below that of the mean-field value. Also note that, as $d \to 2$, $T^* \to 0$. This gives us the concept of the *lower critical dimension*, below which the critical fluctuations become so violent that no phase transition at a finite temperature is possible. Hence for $d < d_{\mathrm{l}} = 2$, no phase transition is possible.

Lecture 22: Continuous Symmetry-I

Till now, we focussed on a scalar order parameter, with only one component. Previously we had mentioned in passing that order parameters can be of any type. Here, we discuss about systems with multicomponent order parameter. Consider the order parameter,

$$\boldsymbol{\phi}(\mathbf{x}) \equiv \begin{bmatrix}\phi_1(\mathbf{x})\\ \phi_2(\mathbf{x})\\ \phi_3(\mathbf{x})\\ \vdots\\ \phi_N(\mathbf{x})\end{bmatrix}$$

Since there are N components in the order parameter, the simplest way to impose symmetry is to consider a free energy which is invariant under $\mathrm{O}(N)$ transformation, that is,

$$\phi_\alpha \to \phi_\alpha = R^\beta{}_\alpha\phi_\beta \qquad R^\top R = \mathbb{1}$$

where $R \in \mathrm{O}(N)$, the orthogonal group. We have suppressed the position dependence in ϕ above, since this is an *internal symmetry*, where the spatial points are not varied under the symmetry transformation.

The free energy will be constructed out of *scalars* which are invariant under this transformation. The simplest such case is,

$$\mathcal{L}[\boldsymbol{\phi}(\mathbf{x})] = \int \mathrm{d}^d x \left[\frac{\gamma}{2} \underbrace{\boldsymbol{\nabla}\boldsymbol{\phi}\cdot\boldsymbol{\nabla}\boldsymbol{\phi}}_{\text{gradient part}} + \frac{a_2}{2} \underbrace{(T-T_c)(\boldsymbol{\phi}\cdot\boldsymbol{\phi}) + \frac{a_4}{4}(\boldsymbol{\phi}\cdot\boldsymbol{\phi})^2 + \dots}_{\text{homogenous part}} \right] \tag{87}$$

where $\boldsymbol{\nabla}\boldsymbol{\phi}\cdot\boldsymbol{\nabla}\boldsymbol{\phi} \equiv \partial_i\phi_j\partial_i\phi_j$ where the sum is over the repeated indices. The homogenous part is analogous to the 'potential energy' while the gradient part is analogous to the 'kinetic energy'. The Landau free energy is invariant under any $\mathrm{O}(N)$ transformation by construction, so the symmetry of $\mathcal{L}$ is $G \equiv \mathrm{O}(N)$.

The homogenous part depends only on $|\boldsymbol{\phi}|$ and hence if we minimise it with respect to the norm, we obtain:

$$\frac{\delta\mathcal{L}}{\delta|\boldsymbol{\phi}|} = 0 \implies a_2(T-T_c)|\boldsymbol{\phi}| + a_4|\boldsymbol{\phi}|^3 = 0$$

Thus we obtain $|\boldsymbol{\phi}| = 0$ for $T > T_c$ and $|\boldsymbol{\phi}| = \sqrt{\frac{a_2}{a_4}(T_c - T)}$ for $T < T_c$. Note that minimisation of the free-energy fixed the magnitude of $\boldsymbol{\phi}$, however, it still can have any orbitrary direction for $T < T_c$ (for $T > T_c$, $\boldsymbol{\phi} = 0$ since norm of a vector is zero iff the vector itself is zero). The minimisation condition gives us one constraint in the symmetry broken phase ($T < T_c$),

$$\phi_1^2 + \phi_2^2 + \dots + \phi_N^2 = \frac{a_2}{a_4}(T_c - T)$$

In other words, $\boldsymbol{\phi} \in \mathbb{S}^{N-1}$, the $(N-1)$ dimensional sphere embedded in the N dimensional order parameter space. What happens is, when $T < T_c$, the system 'chooses' a particular direction along the sphere, in which the ground state $\boldsymbol{\phi}$ points, which we call as *spontaneous symmetry breaking*. Let us choose the ground state to be $\boldsymbol{\phi}_0 = (m_0, 0, 0, 0, \dots)$ (any other point on the sphere would have been equivalent but the calculations would be messier). If H is the symmetry of the ground state, then for any $R \in H$ we would have the invariance, $R\boldsymbol{\phi}_0 = \boldsymbol{\phi}_0$. Now, note that:

$$(\underbrace{R\boldsymbol{\phi}_0}_{\boldsymbol{\phi}_0})^\top (\underbrace{R\boldsymbol{\phi}_0}_{\boldsymbol{\phi}_0}) = (\boldsymbol{\phi}_0)^\top (R^\top R)(\boldsymbol{\phi}_0) = (\boldsymbol{\phi}_0)^\top(\boldsymbol{\phi}_0)$$

which implies that R is a orthogonal matrix. Now, from our choice of $\boldsymbol{\phi}_0$ we have:

$$(\boldsymbol{\phi}_0)_j = (R\boldsymbol{\phi}_0)_j = \sum_k R_{jk}(\boldsymbol{\phi}_0)_k = R_{j1}m_0$$

From this we observe that if $j \neq 1$ then $R_{j1} = 0$ and for $j = 1$ we have $R_{11} = 1$. This implies that the first column of the matrix is just $(1, 0, 0, 0, \dots)^\top$. As R is an orthogonal matrix, then each row must also have unit norm. Since $R_{11} = 1$ already, the remaining elements of the first row must be all zeroes, to maintain a unit norm. Now we have the structure of the matrix as,

$$R \equiv \begin{pmatrix} 1 & \mathbf{0} \\ \mathbf{0} & \mathbb{M}_{(N-1)\times(N-1)} \end{pmatrix}$$

We now again use the orthogonality of R to obtain,

$$\begin{aligned} R^\top R = \begin{pmatrix} 1 & \mathbf{0} \\ \mathbf{0} & \mathbb{M}_{(N-1)\times(N-1)} \end{pmatrix}^\top \begin{pmatrix} 1 & \mathbf{0} \\ \mathbf{0} & \mathbb{M}_{(N-1)\times(N-1)} \end{pmatrix} &= \begin{pmatrix} 1 & \mathbf{0} \\ \mathbf{0} & \mathbb{M}^\top_{(N-1)\times(N-1)} \end{pmatrix} \begin{pmatrix} 1 & \mathbf{0} \\ \mathbf{0} & \mathbb{M}_{(N-1)\times(N-1)} \end{pmatrix} \\ &= \begin{pmatrix} 1 & \mathbf{0} \\ \mathbf{0} & \mathbb{M}^\top_{(N-1)\times(N-1)}\mathbb{M}_{(N-1)\times(N-1)} \end{pmatrix} \equiv \mathbb{1} \end{aligned}$$

which implies that $\mathbb{M}^\top\mathbb{M} = \mathbb{1}$ and hence $\mathbb{M} \in \mathrm{O}(N-1)$. This implies that the symmetry of the ground state $H = \mathrm{O}(N-1)$. Thus, the $\mathrm{O}(N)$ symmetry of the theory is spontaneously broken down to its $\mathrm{O}(N-1)$ subgroup.

Recall that the Ising model possessed $\mathbb{Z}_2$ symmetry where there were two degenerate ground states and the system had to choose one of them. In here, we have the ground state space to be the entire sphere, all having the same energy. Hence, there are *infinitely* many degenerate ground states to choose from in the symmetry broken phase.

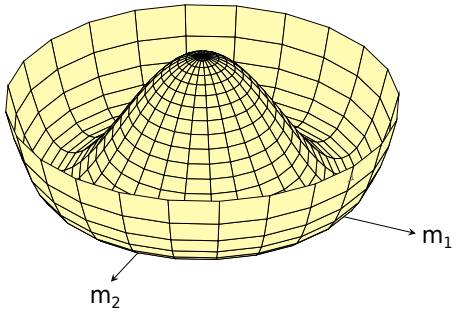


Figure 28: Homogenous part of the Landau functional for $n = 2$. This is the famous *Mexican hat potential*. The minima is spherically symmetric.

22.1. Fluctuations

Let us choose the particular ground state $\mathbf{m}_0 = (m_0\ 0\ 0\ \cdots\ 0)^\top$ and now we consider some fluctuating field $\boldsymbol{\psi}$ such that,

$$\boldsymbol{\phi} \equiv \mathbf{m}_0 + \boldsymbol{\psi} = \begin{bmatrix} m_0 + \psi_1 \\ \psi_2 \\ \vdots \\ \psi_N \end{bmatrix}$$

For simplicity, let us take $N = 2$ and thus we have $\mathbf{m} = (m_0 + \psi_1, \psi_2)$, where ψ_1 is *parallel* to m_0 while ψ_2 is in the *transverse* direction. Substituting this in the Landau functional and doing calculation for $T < T_c$, where $m_0^2 = -\frac{a_2}{a_4}(T - T_c)$ we have:

$$\begin{aligned}
\mathcal{L} &= \int \mathrm{d}^d x\ \Big[\frac{\gamma}{2}(\boldsymbol{\nabla}(m_0 + \psi_1, \psi_2))^2 + \frac{a_2}{2}(T - T_c)\big((m_0 + \psi_1)^2 + \psi_2^2\big) + \frac{a_4}{4}\big((m_0 + \psi_1)^2 + \psi_2^2\big)^2\Big] \\
&= \int \mathrm{d}^d x\ \frac{\gamma}{2}\big[(\boldsymbol{\nabla}\psi_1)^2 + (\boldsymbol{\nabla}\psi_2)^2\big] - \frac{1}{2}m_0^2 a_4\big(m_0^2 + \psi_1^2 + 2m_0\psi_1 + \psi_2^2\big) \\
&\qquad\qquad + \frac{a_4}{4}\big((m_0 + \psi_1)^4 + \psi_2^4 + 2(m_0 + \psi_1)^2\psi_2^2\big) \\
&= \int \mathrm{d}^d x\ \Big[\frac{\gamma}{2}\big[(\boldsymbol{\nabla}\psi_1)^2 + (\boldsymbol{\nabla}\psi_2)^2\big] + \frac{a_4}{4}\big[(m_0 + \psi_1)^4 + \cancel{2m_0^2\psi_2^2} - \big(2m_0^4 + 2m_0^2\psi_1^2 + 4m_0^3\psi_1 + \cancel{2m_0^2\psi_2^2}\big)\big]\Big] \\
&= \int \mathrm{d}^d x\ \Big[\frac{\gamma}{2}\big[(\boldsymbol{\nabla}\psi_1)^2 + (\boldsymbol{\nabla}\psi_2)^2\big] + \frac{a_4}{4}\big[(m_0^4 + \cancel{4m_0^3\psi_1} + 6m_0^2\psi_1^2) - \big(2m_0^4 + 2m_0^2\psi_1^2 + \cancel{4m_0^3\psi_1}\big)\big]\Big] \\
&= \int \mathrm{d}^d x\ \Big[\frac{\gamma}{2}\big[(\boldsymbol{\nabla}\psi_1)^2 + (\boldsymbol{\nabla}\psi_2)^2\big] + m_0^2 a_4\Big[\psi_1^2 - \frac{1}{4}m_0^2\Big]\Big] \\
&= \int \mathrm{d}^d x\ \Big[\frac{\gamma}{2}\big[(\boldsymbol{\nabla}\psi_1)^2 + (\boldsymbol{\nabla}\psi_2)^2\big] + \frac{1}{2}[2a_2(T_c - T)]\psi_1^2\Big] - \mathcal{L}_0
\end{aligned}$$

where $\mathcal{L}_0$ represents the ψ independent part of the functional. Except for the gradient, there is no quadratic term for ψ_2. We now write this in the Fourier space as before,

$$\mathcal{L} = \frac{1}{2V}\sum_{|\mathbf{k}|<\Lambda}\big[\gamma k^2 + 2a_2(T_c - T)\big]\Big|\widetilde{\psi}_{\mathbf{k}}^{(1)}\Big|^2 + \gamma k^2\Big|\widetilde{\psi}_{\mathbf{k}}^{(2)}\Big|^2 - \mathcal{L}_0 \tag{88}$$

We see that the coefficient of $\widetilde{\psi}_{\mathbf{k}}^{(1)}$ has a term $2a_2(T_c - T)$ other than the k^2 while no such thing occurs for $\widetilde{\psi}_{\mathbf{k}}^{(2)}$ term. We can find the correlation function in the parallel and transverse directions (using say the equipartition theorem),

$$\mathcal{G}_\parallel(\mathbf{k}) \sim \frac{1}{\gamma k^2 + 2a_2(T_c - T)} \qquad \mathcal{G}_\perp(\mathbf{k}) \sim \frac{1}{\gamma k^2} \tag{89}$$

The transverse correlation function $\mathcal{G}_\perp(r)$ in real-space is then the Coulomb potential ($\sim 1/r$) and hence has a power-law decay with infinite correlation length, while the paralle one $\mathcal{G}_\parallel(r)$ in real-space is the Yukawa potential, with an exponential decay and correlation length $\xi^{-2} = 2a_2(T_c - T)$.

We also have a pole in $\mathcal{G}_\perp(k)$ at $k = 0$, which is called the *Goldstone mode* (which is *gapless*). If general for the O(N) model in the symmetry broken phase, if instead of 2 components, we had taken a general N, component order parameter, in each of the $(N-1)$ transverse components, we would have gotten transverse modes with infinite correlation length and only 1 mode with a finite correlation length. The mode with finite correlation length is called the *Higgs' mode* (which is *gapped*).

The above is the manifestation of *Goldstone's Theorem* which roughly says that to each broken generator corresponds a massless field [1]. Well, *broken generator* means those generators g of G which do not keep the ground state invariant, that is, g is not a generator of H. Since the number of generators of a group is equal to its dimension, we have the number of Goldstone bosons to be,

$$\mathfrak{n} = \dim\, G - \dim\, H = \dim\ \mathrm{O}(N) - \dim\ \mathrm{O}(N-1) = \frac{1}{2}N(N-1) - \frac{1}{2}(N-1)(N-2) = (N-1)$$

which is exactly what we found from the correlation function thing. Now, note that any broken generator will not keep the ground state invariant and will take to some other vector on the sphere. This new vector is also another ground state, since its magnitude is the same as before.

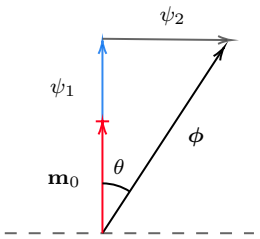
Thus, any broken generator shifts us from one ground state to another, without costing 'energy' (since the Goldstone modes are gapless). From this, we see that the dimension of the space of the ground state is equal to the number of Goldstone bosons. For example, the ground state belongs to $\mathbb{S}^{N-1}$ whose dimension is $(N-1)$ which is equal to the number of Goldstone bosons that we found.

Lecture 23: Continuous Symmetry-II

Let us understand the gapped and gapless modes more closely. For that, consider the fluctuation $\boldsymbol{\psi}$ to the ground state as defined before such that we can write,

$$\boldsymbol{\phi} = \begin{bmatrix} m_0 + \psi_1 \\ \psi_2 \end{bmatrix}$$

Instead of writing the fluctuation in terms of the transverse component $\psi_2(\mathbf{x})$, we write it as a local change in the direction.



We can define $\tan\theta = \frac{\psi_2}{m_0+\psi_1}$. Considering the fluctuations to be small, we can effectively take $\tan\theta \approx \theta$ and $|\psi_1| \ll |m_0|$ which gives us $\psi_2 \simeq m_0\theta$. Then the transverse fluctuation is completely characterised by θ. From Eq. (88), we can use the same *equipartition theorem* to find that,

$$V\mathcal{G}_\perp(k) = \left\langle \left|\widetilde{\theta}_{\mathbf{k}}\right|^2 \right\rangle = \frac{Vk_{\mathrm{B}}T}{\gamma m_0^2 k^2} \longrightarrow \mathcal{G}_\perp(k) = \frac{k_{\mathrm{B}}T}{\gamma m_0^2 k^2}$$

[1] This is in the context of QFT where propagators of a field have the form $D(k) \sim \frac{1}{k^2+m^2}$ where m is interpreted as the mass of the particle.

We now calculate the correlation function in real space, which gives us

$$\mathcal{G}_\perp(\mathbf{r}) = \int \frac{\mathrm{d}^d k}{(2\pi)^d} \frac{k_\mathrm{B}T}{\gamma m_0^2 k^2} e^{i\mathbf{k}\cdot\mathbf{r}} = -\frac{k_\mathrm{B}T}{\gamma m_0^2} C_d \tag{90}$$

where we defined this integral in terms of C_d which is the d-dimensional Coulomb potential for a unit charge at the origin, which can be easily seen, since it satisfies the Poisson equation,

$$\nabla^2 C_d(\mathbf{r}) = -\int \frac{\mathrm{d}^d k}{(2\pi)^d} \frac{1}{\cancel{k^2}} \cdot (-\cancel{k^2}) \cdot e^{i\mathbf{k}\cdot\mathbf{r}} = \delta^{(d)}(\mathbf{r}) \tag{91}$$

We can use Gauss' theorem to evaluate this.

$$1 = \int \mathrm{d}^d x \; \nabla^2 C_d(\mathbf{r}) = \int \mathrm{d}^d x \; \boldsymbol{\nabla} \cdot (\boldsymbol{\nabla} C_d(\mathbf{r})) = \oint_S \mathrm{d}\mathbf{S} \cdot \boldsymbol{\nabla} C_d(\mathbf{r}) \tag{92}$$

Since the source is at the origin, C_d must be spherically symmetric and hence the gradient is purely radial, that is,

$$\boldsymbol{\nabla} C_d = \frac{\mathrm{d}C_d}{\mathrm{d}r} \, \hat{\mathbf{r}}$$

Substituting this in the equation above and integrating over a hypersphere, we obtain

$$\oint_S \mathrm{d}S \hat{\mathbf{r}} \cdot \frac{\mathrm{d}C_d}{\mathrm{d}r} \hat{\mathbf{r}} = \frac{\mathrm{d}C_d}{\mathrm{d}r} \oint_S \mathrm{d}S = 1$$

Since $\frac{\mathrm{d}C_d}{\mathrm{d}r}$ on the surface of a hypersphere is a constant, as it is dependent only on r, so we pull it out of the integral. The remaining integral is just the surface area of the d-dimensional sphere given by $A_d = S_d r^{d-1}$ where S_d is the solid angle (or area of a unit sphere in d dimensions), which implies,

$$\frac{\mathrm{d}C_d}{\mathrm{d}r} = \frac{1}{S_d r^{d-1}} \;\longrightarrow\; C_d = \frac{1}{S_d} \int_{r_0}^{r} \mathrm{d}r' \frac{1}{(r')^{d-1}} = \begin{cases} \frac{1}{S_d(d-2)} \left[\frac{1}{r^{d-2}} - \frac{1}{r_0^{d-2}} \right] & d \neq 2 \\ \frac{1}{S_d} \ln\left(\frac{r}{r_0}\right) & d = 2 \end{cases} \tag{93}$$

where we imposed a lower cutoff to r, since the Landau-Ginzburg theory is a coarse-grained theory with a characteristic length scale below which correlations do not have any meaning. Since $\mathcal{G}_\perp \propto C_d$ we have the long-range behaviour ($r \to \infty$) of $\mathcal{G}_\perp(r)$ as,

$$\mathcal{G}_\perp(r) \sim \begin{cases} \frac{1}{r_0^{d-2}} & d > 2 \\ r^{2-d} \to \infty & d < 2 \\ \ln\left(r/r_0\right) \to \infty & d = 2 \end{cases} \tag{94}$$

For $d > 2$, the phase fluctuation is then finite while for $d \leq 2$, they become asymptotically large. As the phases $\theta \in [0, 2\pi)$, the divergence implies that long-range order of the phases is completely washed out for $d \leq 2$. This is the consequence of the *Mermin-Wagner Theorem* which states that systems with continuous symmetry cannot have long-range order in $d \leq 2$ at any finite temperature. Thus for such systems, the lower critical dimension is $d_c = 2$.

Now, let us examine the correlation function of the order parameter itself, that is, (*notcompleted*)

Lecture 24: Higgs' Mechanism

Instead of considering a two-component vector order parameter $\psi = (\psi_1, \psi_2)^\top$, we can equivalently consider a complex scalar field, $\psi = \psi_1 + i\psi_2 \equiv |\psi| e^{i\theta}$. Then the O(2) invariance under a global rotation changes to U(1) invariance of ψ under a global phase shift. Then the Landau functional becomes,

$$\mathcal{L} = \int \mathrm{d}^d x \left[\frac{\gamma}{2} (\boldsymbol{\nabla}\psi)^* (\boldsymbol{\nabla}\psi) + \frac{a_2}{2}(T - T_c)\psi^*\psi + \frac{a_4}{4}(\psi^*\psi)^2 \right] \tag{95}$$

We integrate the gradient term by parts, after which we write the Landau functional as,

$$\mathcal{L} = \int \mathrm{d}^d x\ \psi^* \Big[-\frac{\gamma}{2}\boldsymbol{\nabla}^2 + \frac{a_2}{2}(T - T_c) + \frac{a_4}{4}(\psi^*\psi) \Big] \psi \equiv \int \mathrm{d}^d x\ \psi^* \widetilde{H} \psi$$

where $\widetilde{H}$ is a non-linear Hamiltonian and $\mathcal{L}$ is just the expectation value of this Hamiltonian. Let us now move on to *superconductors*.

Technically, we can treat superconductors using the BCS theory, which is a *microscopic approach*, however, here we do a coarse-grained study using the Landau-Ginzburg theory. Till now, we had neutral fields, but since superconductors are basically condensates of electronic *Cooper pairs*, these are essentially charged and hence, will couple to electromagnetic fields.

To incorporate this, we impose a local gauge invariance and the gradient term is changed due to *minimal coupling*

$$\boldsymbol{\nabla} \to \boldsymbol{\nabla} - \frac{iq}{\hbar}\mathbf{A}$$

where q is the charge of the field and $\mathbf{A}(\mathbf{x})$ is the vector-potential (which introduces a magnetic field $\mathbf{h} = \boldsymbol{\nabla} \times \mathbf{A}$). We also get a contribution of $\frac{1}{\mu_0^2}(\boldsymbol{\nabla} \times \mathbf{A})^2$ from the vector potential. Thus, the modified Landau functional becomes,

$$\mathcal{L}[\psi, \mathbf{A}] = \int \mathrm{d}^d x\ \frac{\hbar^2}{2m} \Big[\Big\{ \Big(\boldsymbol{\nabla} - \frac{iq}{\hbar}\mathbf{A} \Big)\psi \Big\}^* \Big\{ \Big(\boldsymbol{\nabla} - \frac{iq}{\hbar}\mathbf{A} \Big)\psi \Big\} \Big] + \frac{a_2}{2}(T - T_c)(\psi^*\psi) + \frac{a_4}{4}(\psi^*\psi)^2 + \frac{1}{2\mu_0}(\boldsymbol{\nabla} \times \mathbf{A})^2 \tag{96}$$

where we now introduced a $\frac{\hbar^2}{2m}$ factor in place of γ, to make it look more quantum-mechanical. To find the equation of state, we vary $\mathcal{L}$ separately with respect to ψ (or better, ψ^*) and $\mathbf{A}$. Let us start with the gradient term which is the most complicated.

$$\begin{aligned}
\delta_{\psi^*} \int \Big[\Big\{ \Big(\boldsymbol{\nabla} - \frac{iq}{\hbar}\mathbf{A} \Big)\psi \Big\}^* \Big\{ \Big(\boldsymbol{\nabla} - \frac{iq}{\hbar}\mathbf{A} \Big)\psi \Big\} \Big] &= \int \Big\{ \Big(\boldsymbol{\nabla} - \frac{iq}{\hbar}\mathbf{A} \Big)\psi \Big\} \Big[\Big(\boldsymbol{\nabla} + \frac{iq}{\hbar}\mathbf{A} \Big)(\delta\psi^*) \Big] \\
&= \int \Big\{ \Big(\boldsymbol{\nabla} - \frac{iq}{\hbar}\mathbf{A} \Big)\psi \Big\} \cdot \boldsymbol{\nabla}(\delta\psi^*) + \Big\{ \Big(\boldsymbol{\nabla} - \frac{iq}{\hbar}\mathbf{A} \Big)\psi \Big\} \cdot \Big(\frac{iq}{\hbar}\mathbf{A} \Big)(\delta\psi^*) \\
&\xrightarrow{IBP} \int (\delta\psi^*) \Big[\Big\{ \Big(\boldsymbol{\nabla} - \frac{iq}{\hbar}\mathbf{A} \Big)\psi \Big\} \cdot \Big(\frac{iq}{\hbar}\mathbf{A} \Big) - \boldsymbol{\nabla} \cdot \Big\{ \Big(\boldsymbol{\nabla} - \frac{iq}{\hbar}\mathbf{A} \Big)\psi \Big\} \Big] \\
&= -\int \Big(\boldsymbol{\nabla} - \frac{iq}{\hbar}\mathbf{A} \Big)^2 \psi
\end{aligned}$$

The variation of the other terms are straight forward. Doing this, we obtain the equation of state:

$$(i\hbar\boldsymbol{\nabla} + q\mathbf{A})^2\psi + \frac{a_2}{2}(T - T_c)\psi + \frac{a_4}{2}|\psi|^2\psi = 0 \tag{97}$$

This equation handles the average behaviour of the order parameter. Let us now find the variation with respect to $\mathbf{A}$. Let us focus on the term,

$$\begin{aligned}
\delta_{\mathbf{A}} \int (\boldsymbol{\nabla} \times \mathbf{A})^2 &= 2 \int (\boldsymbol{\nabla} \times \mathbf{A}) \cdot (\boldsymbol{\nabla} \times \delta\mathbf{A}) \\
&= 2 \int (\boldsymbol{\nabla} \times \mathbf{A})_i (\epsilon_{ijk} \partial_j (\delta\mathbf{A})_k) \\
&= -2 \int \partial_j (\boldsymbol{\nabla} \times \mathbf{A})_i (\epsilon_{ijk} (\delta\mathbf{A})_k) \\
&= 2 \int \epsilon_{kji} \partial_j (\boldsymbol{\nabla} \times \mathbf{A})_i (\delta\mathbf{A})_k \\
&= 2 \int (\boldsymbol{\nabla} \times (\boldsymbol{\nabla} \times \mathbf{A})) \cdot (\delta\mathbf{A})
\end{aligned}$$

And the variation of the kinetic terms become:

$$\delta_{\mathbf{A}} \int \Big[\Big\{ \Big(\boldsymbol{\nabla} - \frac{iq}{\hbar}\mathbf{A} \Big)\psi \Big\}^* \Big\{ \Big(\boldsymbol{\nabla} - \frac{iq}{\hbar}\mathbf{A} \Big)\psi \Big\} \Big] = \int \frac{iq}{\hbar}(\psi^* \boldsymbol{\nabla}\psi - \psi \boldsymbol{\nabla}\psi^*) + \frac{q^2}{\hbar^2}|\mathbf{A}|^2|\psi|^2$$

Then what we get overall from the variation of the vector potential is,

$$\frac{1}{\mu_0}\boldsymbol{\nabla}\times\mathbf{B}+\frac{iq\hbar}{2m}(\psi^*\boldsymbol{\nabla}\psi-\psi\boldsymbol{\nabla}\psi^*)+\frac{q^2}{m}|\mathbf{A}||\psi|^2=0 \tag{98}$$

Let us define the current,

$$\mathbf{J}:=\frac{q\hbar}{2im}(\psi^*\boldsymbol{\nabla}\psi-\psi\boldsymbol{\nabla}\psi^*)-\frac{q^2}{m}|\mathbf{A}||\psi|^2$$

which gives us the equation in simplified form as,

$$\boldsymbol{\nabla}\times\mathbf{B}=\mu_0\mathbf{J}$$

This equation handles the electrodynamic degrees of freedom. Suppose we want an uniform solution with zero current. Then the gradients will vanish and also $\mathbf{J}=0$, which gives us $\mathbf{A}=0$ and from the equation of state we get,

$$|\psi_0|^2=-\frac{a_2}{a_4}(T-T_c)$$

24.1. Gaussian Fluctuations

24.2. Meissner Effect

Lecture 25: Scaling Relations

Till now, we have had numerous (apparently pointless) discussions on the critical exponents $\alpha,\beta,\gamma,\delta\ldots$ blah blah. There are so many of them and we are now interested in finding some relations between these exponents. It turns out that all these are not independent. Finding a few of them will help us to calculate of all them through relations called the *scaling laws*. These can be obtained from the *static scaling hypothesis* which treats thermodynamic quantities near the critical points to be *generalised homegenous functions*.

The beginning to all these was perhaps an attempt of exploratory data analysis, where we look for pattens in data and find an explanation for them. The ultimate basis for this is the OG *renormalisation group*, which we will deal with later.

25.1. Scaling for Magnetisation

From our previous discussions, we know that in the zero-field and for $T<T_c$, $m\sim(-t)^\beta$ (where $t=(T-T_c)/T_c$ is the reduced temperature) while at $T=T_c$, $m\sim h^{1/\delta}$. Let us now combine these into a single expressions, showing dependence of magnetisation on both T and h,

$$m(t,h)=\begin{cases}t^\beta\mathcal{F}_+\left(\frac{h}{t^\Delta}\right) & t>0\\ (-t)^\beta\mathcal{F}_-\left(\frac{h}{(-t)^\Delta}\right) & t<0\end{cases} \tag{99}$$

where Δ is a "new" exponent which is introduced and is often referred to as the *gap exponent*. $\mathcal{F}_\pm$ are well-behaved universal functions[1]. This is still a bit *ad hoc* and we need to justify writing this expression. However, let us come to what we can do, provided this expression is valid. Firstly from the experimental data, if we plot $m/|t|^\beta$ vs. $h/|t|^\Delta$, then we expect that all the data across various systems will fall on the same curve. This is called *data collapse* and is very useful for estimating the exponents (but we do have to "guess" the exponents for the collapse, since these are not known beforehand).

We can also extract information from various limits of this scaling. Let us first take $h\to0$ which gives us,

$$m(t,h)=\begin{cases}t^\beta\mathcal{F}_+(0) & t>0\\ (-t)^\beta\mathcal{F}_-(0) & t<0\end{cases}$$

[1]So, these functions will be same for every system belonging to the same *universality class*

Based on the previous discussions, we expect $\mathcal{F}_+(0) = 0$ and $\mathcal{F}_-(0) = \text{const.} \neq 0$. Now, let us take $t \to 0$ keeping h to be small but non-zero. Then $(h/t^\Delta) \to \infty$, but we want m to be finite in this limit and to follow $m \sim h^{1/\delta}$. This forces us to assume a power-law behaviour for $\mathcal{F}_\pm$ with some exponent ρ,

$$\mathcal{F}_\pm(x) \sim x^\rho \implies m \sim |t|^\beta \times \left[\frac{h}{|t|^\Delta}\right]^\rho = |t|^{\beta - \Delta\rho} h^\rho$$

The exponent of $|t|$ must cancel since we know $m \sim h^{1/\delta}$ and hence we can conclude $\beta = \Delta\rho$ and $\rho = \frac{1}{\delta}$. This gives $\boxed{\Delta = \beta\delta}$, which implies that Δ is not anything new, just the product of two previously obtained exponents.

Let us now move on to the derivatives, starting with susceptibility.

$$\chi \sim \frac{\partial m}{\partial h}\Big|_{h=0} = |t|^\beta \frac{\partial}{\partial h}\left[\mathcal{F}_\pm\left(\frac{h}{|t|^\Delta}\right)\right]_{h=0} \cdot \frac{1}{|t|^\Delta} = |t|^{\beta-\Delta}\mathcal{F}'_\pm(0)$$

Using the form $\chi \sim |t|^{-\gamma}$ we conclude that $\beta - \Delta = -\gamma \implies \boxed{\Delta = \beta + \gamma}$. Using the above two expressions for Δ, we obtain our first scaling relation,

$$\beta\delta = \beta + \gamma \tag{100}$$

which is known as the *Widom scaling law*. The validity of this relation is seen across multiple experiments for diverse systems. Moreover, the relation is independent of the dimension of the system. Even though the actual exponents differed from those predicted by the mean-field approach, the scaling law still seemed to be valid, which implies a more fundamental basis of scaling laws.

25.2. Scaling for Free Energy

Let us now try to find a similar thing for the free energy. For that, let us assume a scaling form of $F(t, h)$,

$$F(t, h) = t^\lambda \widetilde{\mathcal{F}}\left(\frac{h}{t^\Delta}\right)$$

We consider the scenario only for $t > 0$. Differentiating once with respect to the field gives us the magnetisation

$$m = -\frac{\partial F}{\partial h} \sim t^\lambda \widetilde{\mathcal{F}}'\left(\frac{h}{t^\Delta}\right) \cdot \frac{1}{t^\Delta}$$

Then this tells us that $\boxed{\lambda - \Delta = \beta}$, from the previous scaling form. Differentiating F once with respect to the temperature gives us,

$$\frac{\partial F}{\partial t} = \lambda t^{\lambda-1}\widetilde{\mathcal{F}}\left(\frac{h}{t^\Delta}\right) - t^\lambda \widetilde{\mathcal{F}}'\left(\frac{h}{t^\Delta}\right) \cdot h\Delta t^{-\Delta-1} = \lambda t^{\lambda-1}\left[\widetilde{\mathcal{F}}\left(\frac{h}{t^\Delta}\right) - ht^{-\Delta}\widetilde{\mathcal{F}}'\left(\frac{h}{t^\Delta}\right) \cdot \frac{\Delta}{\lambda}\right]$$

Differentiating again with respect to temperature,

$$\frac{\partial^2 F}{\partial t^2} = \lambda(\lambda-1)t^{\lambda-2}[\ \#\ ] + \lambda t^{\lambda-1}\left[-h\Delta\widetilde{\mathcal{F}}'\left(\frac{h}{t^\Delta}\right)t^{-\Delta-1} - h \times (\ldots)\right]$$

In the zero field case ($h = 0$), only the first term survives and the specific heat is then,

$$C_v \propto \frac{\partial^2 F}{\partial t^2} \sim t^{\lambda-2}$$

From this, we at once conclude that $\lambda - 2 = -\alpha \implies \boxed{\lambda = 2 - \alpha}$. From the above two expressions, we have $\alpha + \beta + \Delta = 2 \implies \alpha + \beta + (\beta + \gamma) = 2$. Using this, we get our second scaling relation,

$$\alpha + 2\beta + \gamma = 2 \tag{101}$$

which is known as the *Rushbrooke's scaling law*. Let us see whether these laws apply for the mean-field theory or not! For MFT, the critical exponents are:

$$\alpha = 0 \quad \beta = \frac{1}{2} \quad \gamma = 1 \quad \delta = 3$$

Then we have,

$$\text{Rushbrooke} : \alpha + 2\beta + \gamma = 0 + 1 + 1 = 2 \qquad \checkmark$$
$$\text{Widom} : \beta + \gamma = \frac{1}{2} + 1 = \frac{3}{2} = \frac{1}{2} \cdot 3 = \beta\delta \qquad \checkmark$$

Lecture 26: Further Scaling

The scaling forms used in the previous lectures all come by assuming that the thermodynamic quantities are generalised homogenous functions. So let us discuss a bit about homogenous functions in general. A function $f : \mathbb{R} \to \mathbb{R}$ is called *homogenous* if

$$f(\lambda x) = g(\lambda) f(x)$$

where $g(\lambda)$ is some function. A simple example is, $f(x) = x^2$ since $f(\lambda x) = \lambda^2 x^2 = \lambda^2 f(x)$, with $g(\lambda) = \lambda^2$. Note that, $g(\lambda)$ cannot be any arbitrary function, it must satisfy some properties. For this, note:

$$f(\lambda(\mu x)) = g(\lambda)g(\mu)f(x) = f((\lambda\mu)x) = g(\lambda\mu)f(x)$$

which imposes the condition $g(x)g(y) = g(xy)\ \forall\ x, y$. This eventually forces the form $g(x) = x^\rho$ which has an elegant proof, considering g to be differentiable.

Proposition 1:
If $g : \mathbb{R} \to \mathbb{R}$ is a *differentiable* function and $g(x)g(y) = g(xy)\ \forall\ x, y$ then for all x, either $g(x) = 0$ or $g(x) = x^\lambda$ for some λ

Proof. Let any arbitrary $y = y_0$. Differentiating both sides, we get:

$$g'(x)g(y_0) = y_0 g'(xy_0)\ \forall\ x \quad \xrightarrow{x=1} \quad \frac{g'(y_0)}{g(y_0)} = \frac{g'(1)}{y_0} \quad \xrightarrow{\text{Integrating}} \quad g(y_0) = A y_0^\lambda$$

where, after differentiation we have taken the g as a function of y_0 since y_0 was arbitrary and then replaced $g'(1) = \lambda$. The initial condition $g(1) = (g(1))^2 \implies g(1) = 0$ or $g(1) = 1$. If $g(1) = 0$ then this implies $A = 0$, implying that g is identically zero. Otherwise, if $g(1) = 1$ then $A = 1$ which gives us $g(x) = x^\lambda$

We can extend the definition of homogenity to arbitrary number of variables.

$$f(\lambda x_1, \lambda x_2 \dots \lambda x_n) = g(\lambda) f(x_1, x_2 \dots x_n) \implies f(\lambda \mathbf{x}) = \lambda^p f(\mathbf{x}) \quad \mathbf{x} \in \mathbb{R}^n$$

The cool thing with homogenous functions is that if we know the value of the function at one point, then we know it at every other point, since given $f(x_0) = c$, we can always choose $\lambda = \frac{y}{x_0}$ such that $f(y) = \left(\frac{y}{x_0}\right)^\lambda f(x_0)$. We now extend the definition of a homogenous function to generalised homogenous function (GHF); a function $f : \mathbb{R}^n \to \mathbb{R}^m$ is called a GHF if,

$$f(\lambda^{a_1} x_1, \lambda^{a_2} x_2, \dots, \lambda^{a_n} x_n) = \lambda^k f(x_1, x_2, \dots, x_n)$$

where $\{a_i\}$ and k are some arbitrary numbers. Note that these are not independent, since if we choose an arbitrary $\lambda = \mu^{1/k}$ then we have,

$$f(\mu^{a_1/k} x_1, \mu^{a_2/k} x_2, \dots, \mu^{a_n/k} x_n) = \mu f(x_1, x_2, \dots, x_n)$$

Then all $a_i \mapsto a_i/k$ which is just a rescaling. The GHF can thus be defined by always choosing $k = 1$ and hence the final definition,

$$f(\lambda^{a_1}x_1, \lambda^{a_2}x_2, \ldots, \lambda^{a_n}x_n) = \lambda f(x_1, x_2, \ldots, x_n)$$

Let us now focus only on the two variable case, which is $F(t, h)$. The static scaling hypothesis states that the thermodynamic potentials are GHFs near the critical point T_c. Then the free energy can be written as,

$$F(\lambda^{a_\mathrm{t}}t, \lambda^{a_\mathrm{h}}h) = \lambda F(t,h) \quad \longrightarrow \quad -\frac{\partial}{\partial h}[F(\lambda^{a_\mathrm{t}}t, \lambda^{a_\mathrm{h}}h)] = -\lambda\frac{\partial}{\partial h}[F(t,h)] \implies \lambda^{a_\mathrm{h}-1}m(\lambda^{a_\mathrm{t}}t, \lambda^{a_\mathrm{h}}h) = m(t,h)$$

Now, suppose we take $T > T_c$. Then we choose λ such that $\lambda^{a_\mathrm{t}} = -\frac{1}{t} \implies \lambda = (-t)^{-1/a_\mathrm{t}}$. Taking the zero-field limit we get:

$$(-t)^\beta \sim m(t,0) = (-t)^{-(a_\mathrm{h}-1)/a_\mathrm{t}}m(1,0) \implies \boxed{\beta = \frac{1-a_\mathrm{h}}{a_\mathrm{t}}}$$

Now, suppose we take $T = T_c$ and choose λ such that $\lambda^{a_\mathrm{h}} = \frac{1}{h} \implies \lambda = h^{-1/a_\mathrm{h}}$. Substituting this in the scaling form above, we get:

$$h^{1/\delta} \sim m(0,h) = h^{-(a_\mathrm{h}-1)/a_\mathrm{h}}m(0,1) \implies \boxed{\delta = \frac{a_\mathrm{h}}{1-a_\mathrm{h}}}$$

Solving these we get,

$$a_\mathrm{h} = \frac{\delta}{1+\delta} \qquad a_\mathrm{t} = \frac{1}{\beta(1+\delta)} \tag{102}$$

We get a_h and a_t in terms of the critical exponents (and vice versa). Now, differentiating m with respect to h gives us the susceptibility:

$$\lambda^{2a_\mathrm{h}-1}\chi(\lambda^{a_\mathrm{t}}t, \lambda^{a_\mathrm{h}}h) = \chi(t,h)$$

For $T > T_c$, taking $h = 0$ and choosing λ such that $\lambda^{a_\mathrm{t}} = \frac{1}{t}$, we get the following

$$t^{-\gamma'}\chi(t,0) = t^{-(2a_\mathrm{h}-1)/a_\mathrm{t}}\chi(1,0)$$

from which we can read off the exponent as,

$$\gamma' = \frac{(2a_\mathrm{h}-1)}{a_\mathrm{t}} = \frac{\frac{2\delta}{1+\delta}-1}{\frac{1}{\beta(1+\delta)}} = (\delta-1)\beta \implies \beta\delta = \beta + \gamma$$

which was the Widom's scaling law that we had earlier derived. One thing to note here is that, if we had taken $T < T_c$ then also the same calculation follows, which would give us the same expression for γ. Hence we can conclude that $\gamma = \gamma'$

Doing the same thing for the specific heat will lead to the Rushbrooke relation (which I skip since it has become very boring at this point of time!).

26.1. A small note

The scaling laws that we derived manifest as inequalities when derived from thermodynamic principles, considering stability of physical systems. Let us try to derive the Rushbrook (in)equality!

Consider the first law of thermodynamics for a magnetic system with field H and and magnetisation M:

$$\mathrm{d}U = T\mathrm{d}S - M\mathrm{d}H \implies T = \left(\frac{\partial U}{\partial S}\right)_H \quad M = -\left(\frac{\partial U}{\partial H}\right)_S \tag{103}$$

We can now define the specific heat at constant magnetisation and at constant field as,

$$C_H = T\left(\frac{\partial S}{\partial T}\right)_H \qquad C_M = T\left(\frac{\partial S}{\partial T}\right)_M$$

Lecture 27: Kadanoff's Block Spins

In the previous lecture, we used an *ad hoc* assumption of the thermodynamic quantitites being generalised homogenous functions. We now try to give a proper justification of why this turns out to be okay(ish)! For that, consider our favourite Ising model with N spins, given by the corresponding Hamiltonian,

$$\mathscr{H} = -J\sum_{\langle ij\rangle}\sigma_i\sigma_j - h\sum_i \sigma_i$$

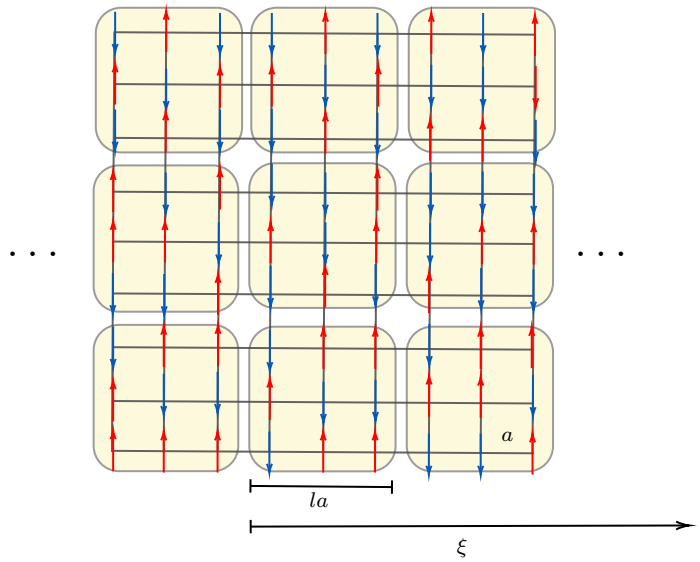


Figure 29: Kadanoff's block-spin construction

Let the system be defined on a d dimensional lattice, with lattice spacing a. Now consider an arbitrary number, $l \gg 1$ and partition the lattice into cells of dimension la. Hence, in a single cell there are l^d spins which implies there are $N' = N/l^d$ such blocks. For each such block I, define the *block spin* as,

$$S_{\text{I}} = \frac{1}{|m_l|}\frac{1}{l^d}\sum_{i\in I}\sigma_i \tag{104}$$

where m_l denotes the average magnetisation of block I and is given by:

$$m_l = \frac{1}{l^d}\sum_{i\in I}\langle\sigma_i\rangle \tag{105}$$

What we are doing is essentially a coarse-graining procedure, where we are treating a *block* of linear dimension la, to be an *effective spin* S_{I}. The total number of spins then decreases from N to Nl^{-d}. Since all spins within the correlation length will be correlated, we assume that $la \ll \xi$, so that each block will behave as an effective single correlated chamber, with all of the spins pointing in the same direction on average.

We now make a bold assumption that the block spins $\{S_{\text{I}}\}$ also follow the same Hamiltonian, which is not apriori evident. The new Hamiltonian for the block spins will have the same form but with different coupling constants, say J_l and h_l

$$\mathscr{H}_l = -J_l\sum_{\langle IJ\rangle} S_{\text{I}}S_{\text{J}} - h_l\sum_I S_{\text{I}}. \tag{106}$$

For this 'block' Hamiltonian, the lattice spacing is la and this also has fewer spins than the original Hamiltonian. Let ξ_1 denote the correlation length in units of a while ξ_l denote the same in units of la. Since the actual physical correlation length ξ is unchanged, we have

$$\xi = \xi_1 a = \xi_l(la) \implies \xi_l = \xi_1 l^{-1} < \xi_1$$

This says that the block spins are further away from criticality than the original system, which implies that the system is now at a new effective reduced temperature t_l.

Since the block spin Hamiltonian is of the same form, the total free energy should also be the same for both. Note that we consider only the singular part of the free energy (which actually determines the critical behaviour).

$$Nf(t,h) = N'f(t_l,h_l) = Nl^{-d}f(t_l,h_l) \implies f(t,h) = l^{-d}f(t_l,h_l) \tag{107}$$

where $f(t,h)$ is the free energy per spin. We now assume that the new couplings are related to the original ones by,

$$\begin{aligned} t_l &= tl^{y_t} \\ h_l &= hl^{y_h} \end{aligned} \tag{108}$$

where $y_t, y_h > 0$ are some positive numbers. Substituting this in the free energy equation above, we get:

$$f(tl^{y_t}, hl^{y_h}) = l^d f(t,h) \quad \xrightarrow{l\to l^{1/d}} \quad f(l^{y_t/d}t, l^{y_h/d}h) = lf(t,h) \tag{109}$$

The equation above seems to be the definition of a generalised homogenous function, however, there's a subtlety; to be a GHF, we need the parameter λ to be arbitrary. However, in this case, $\lambda = l$, which is constrained by $1 \ll l \ll \frac{\xi}{a}$. However, let us do away with this and just say that l can take any values. Hence, f becomes a GHF and the rest of the procedure to relate the exponents y_t and y_h to critical exponents follows as before.

27.1. Correlation Function

We now analyse the correlation function for the block spins,

$$\mathcal{G}(r_l,t_l) = \langle S_{\text{I}} S_{\text{J}} \rangle - \langle S_{\text{I}} \rangle \langle S_{\text{J}} \rangle$$

where $r_l = |\mathbf{r}_{\text{I}} - \mathbf{r}_{\text{J}}|$ in units of la. Since the physical distance remains the same, we have $r_l = r/l$. Let us substite the definition of the block spins in the correlation function,

$$\mathcal{G}(r_l,t_l) = \frac{1}{|m_l|^2 l^{2d}} \sum_{i\in I}\sum_{i\in J} \langle \sigma_i\sigma_j\rangle - \langle\sigma_i\rangle\langle\sigma_j\rangle \tag{110}$$

Now let us find some relation between the couplings and m_l. For that, note from the definition of the block spins,

$$h\sum_i \sigma_i = h\sum_I\sum_{i\in I}\sigma_i = h|m_l|l^d\sum_I S_{\text{I}} \equiv h_l \sum_I S_{\text{I}}$$

We can thus make an equivalence, $h|m_l|l^d = h_l \implies |m_l| = (h_l/h)l^{-d} = l^{y_h - d}$. Substituting this in the correlation function we get:

$$\mathcal{G}(r_l,t_l) = l^{-2y_h}\sum_{i\in I}\sum_{i\in J}\langle\sigma_i\sigma_j\rangle - \langle\sigma_i\rangle\langle\sigma_j\rangle \simeq l^{-2y_h}l^d\cdot l^d\langle\sigma_i\sigma_j\rangle - \langle\sigma_i\rangle\langle\sigma_j\rangle = l^{2(d-y_h)}\mathcal{G}(r,t)$$

where we assumed that if we take σ_i in the I^{th} block and σ_j in the J^{th} block, then for all such (i,j), the correlator will be same and equal to $\mathcal{G}(r,t)$. Let us also introduce the factor for field, which gives us finally

$$\mathcal{G}\Big(\frac{r}{l}, l^{y_t}t, l^{y_h}h\Big) = l^{2(d-y_h)}\mathcal{G}(r,t,h)$$

Let us choose l such that $lt^{y_t} = 1$ which gives us,

$$\mathcal{G}\Big(rt^{1/y_t}, 1, t^{-y_h/y_t}h\Big) = t^{-2(d-y_h)/y_t}\mathcal{G}(r,t,h)$$

Define a new function $\widetilde{\mathcal{F}}$ such that,

$$\mathcal{G}\Big(rt^{1/y_t}, 1, t^{-y_h/y_t}h\Big) \equiv (rt^{1/y_t})^{-2(d-y_h)}\widetilde{\mathcal{F}}\Big(rt^{1/y_t}, 1, t^{-y_h/y_t}h\Big)$$

Substituting this above, we get:

$$(rt^{1/y_t})^{-2(d-y_h)}\widetilde{\mathcal{F}}\Big(rt^{1/y_t}, 1, t^{-y_h/y_t}h\Big) = t^{-2(d-y_h)/y_t}\mathcal{G}(r,t,h) \implies \mathcal{G}(r,t,h) = r^{-2(d-y_h)}\widetilde{\mathcal{F}}\Big(rt^{1/y_t}, t^{-y_h/y_t}h\Big) \tag{111}$$

We know that near T_c, $\mathcal{G}(r) \sim r^{-(\eta+d-2)}$ and thus we expect that,

$$2(d-y_h) = \eta + d - 2 \implies y_h = \frac{d+2-\eta}{2}$$

Now, rt^{1/y_t} should be dimensionless and define $\xi \equiv t^{-1/y_t}$ and we also know that $\xi \sim t^{-\nu}$. From this we get $y_t\nu = 1$. We can also get something with the exponent γ. For that, note that $\mathcal{G}(r) \sim r^{-(\eta+d-2)}$ and,

$$t^{-\gamma} = \chi_{\mathrm{T}} \sim \int_{V_\xi} \mathrm{d}^d r\ \mathcal{G}(r) \sim \int_0^\xi \mathrm{d}r\ r^{d-1}\cdot r^{-(\eta+d-2)} = \int_0^\xi \mathrm{d}r\ \cdot r^{1-\eta} \sim \xi^{2-\eta} \sim t^{-(2-\eta)\nu}$$

Equating this, we get $\gamma = (2-\eta)\nu$ which is another scaling relation. We can derive a *hyperscaling relation*, which is explicitly dependent on the dimension d of the system. For this, consider Eq. (107)

$$f(t,h) = l^{-d}f(tl^{y_t}, hl^{y_h}) \implies C_v(t,h) = l^{-d}\cdot l^{2y_t}C_v(tl^{y_t}, hl^{y_h})$$

Choosing $tl^{y_t} = 1 \to l = t^{-1/y_t}$ we get,

$$C_v(t,h) = t^{(d-2y_t)/y_t}C_v\Big(\frac{h}{t^{y_h/y_t}}\Big) \xrightarrow{h\to 0} C_v(t) = t^{(d-2y_t)/y_t}C_v(0) \implies \alpha = \frac{2y_t - d}{y_t}$$

And from the correlation function we saw that $y_t = \frac{1}{\nu}$. Then, substituting this we finally obtain,

$$\alpha = \nu\cdot\left(\frac{2}{\nu} - d\right) = 2 - d\nu \implies d\nu = 2 - \alpha$$

which is called the *Josephson scaling law* and is dependent on the dimension d of the system. Note that, for the mean field exponents, $\alpha = 0$ and $\nu = \frac{1}{2}$, we have $d = 4$ and hence, this is not valid for any d. The thing is, Josephson relation does not hold good for $d > d_c$ where d_c is the upper critical dimension (note that mean field exponents are valid only for $d > d_c$ and hence the hyperscaling law does not hold for the mean field exponents). Let us summarise all the scaling laws that we had found so far:

- $\alpha + 2\beta + \gamma = 2$ (Rushbrooke)
- $\beta + \gamma = \beta\delta$ (Widom)
- $d\nu = 2 - \alpha$ (Josephson)
- $\gamma = (2-\eta)\nu$ (Fisher)

Lecture 28: Introduction to RG

We will have a sketchy introduction to the enlightening concept of the *renormalisation group*. RG can explain universality (why vastly different models seem to have same critical exponents) and can also predict these exponents. RG is an approach to approximately calculate the sums involved in the partition function.

Renormalisation basically means doing certain transformations or reparameterisation, in the hope that it will make the theory easier. It is called 'group' since two such transformations leads to a third

transformation (composition rule). First let us use this for the 1D Ising model. Consider N Ising spins on a 1D lattice with periodic boundary condition (*i.e.* $\sigma_1 \equiv \sigma_{N+1}$) with the following Hamiltonian,

$$\mathcal{H} = -J\sum_{i=1}^{N}\sigma_i\sigma_{i+1}$$

For this case, we take the zero field condition. We define $K := \beta J$ and using this, the partition function becomes,

$$\mathcal{Z} = \sum_{\sigma_1=\pm1}\sum_{\sigma_2=\pm1}\cdots\sum_{\sigma_N=\pm1} e^{K\sum_i \sigma_i\sigma_{i+1}} \equiv \sum_{\sigma_1=\pm1}\sum_{\sigma_2=\pm1}\cdots\sum_{\sigma_N=\pm1} e^{K(\sigma_1\sigma_2+\sigma_2\sigma_3+\sigma_3\sigma_4\ldots\sigma_N\sigma_1)}$$

Note that the even spins, say σ_2, appears in two consecutive terms. We can first do the trace over the even spins then, which gives us,

$$\begin{aligned}\mathcal{Z} &= \sum_{\sigma_1=\pm1}\sum_{\sigma_3=\pm1}\sum_{\sigma_5=\pm1}\cdots\sum_{\sigma_N=\pm1}\prod_{j=1}^{N/2}\left(e^{K(\sigma_{2j-1}+\sigma_{2j+1})}+e^{-K(\sigma_{2j-1}+\sigma_{2j+1})}\right)\\ &\equiv \sum_{\sigma_1=\pm1}\sum_{\sigma_3=\pm1}\sum_{\sigma_5=\pm1}\cdots\sum_{\sigma_N=\pm1}\prod_{j=1}^{N/2}\left[2\cosh(K(\sigma_{2j-1}+\sigma_{2j+1}))\right]\end{aligned} \tag{112}$$

Next, if we assume that there exist some function $f(K)$ and K' such that

$$2\cosh(K(\sigma_{2j-1}+\sigma_{2j+1})) = f(K)e^{K'\sigma_{2j-1}\sigma_{2j+1}} \qquad \forall\ j \tag{113}$$

then the partition function will take the following form,

$$\mathcal{Z} = (f(K))^{N/2}\sum_{\sigma_1=\pm1}\sum_{\sigma_3=\pm1}\sum_{\sigma_5=\pm1}\cdots\sum_{\sigma_N=\pm1}\prod_{j=1}^{N/2}e^{K'\sigma_{2j-1}\sigma_{2j+1}} \tag{114}$$

If we forgo the indexing, the red colour is exactly the partition function for a 1D Ising chain with $N/2$ spins and coupling constant K'. Thus, the partition function with N spins and coupling K follows,

$$\mathcal{Z}_{\rm N}(K) = (f(K))^{N/2}\mathcal{Z}_{\rm N/2}(K') \tag{115}$$

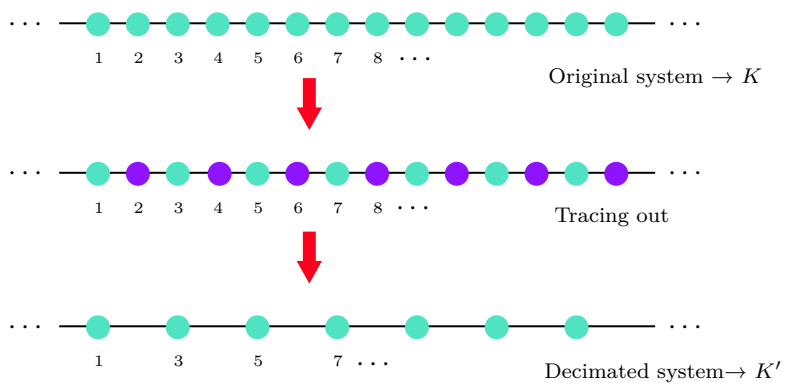


Figure 30: The process of decimation by taking partial traces of few spins, leading to a renormalised model.

Now, let us focus on our claim about the existence of this transformation. Eq. (113) is valid for all possibilities of $\sigma_{2j\pm1} \in \{+1,-1\}$. From this, we get:

$$2\cosh(2K) = f(K)e^{K'} \qquad f(K)e^{-K'} = 2$$

Dividing and multiplying the two expressions above give us,

$$\cosh(2K) = e^{2K'} \qquad 4\cosh(2K) = f^2(K) \implies K' = \frac{1}{2}\ln\cosh(2K) \qquad f(K) = 2\sqrt{\cosh(2K)}$$

Now, we know that the free energy $-\beta F = \ln Z_N \sim N \equiv N\zeta$ where ζ is the free-energy per spin (or atleast its singular part, which actually contributes to criticality). Using this in Eq. (115), we have

$$N\zeta(K) = \frac{N}{2}\ln f(K) + \frac{N}{2}\zeta(K') \implies \zeta(K) = \frac{1}{2}\ln f(K) + \frac{1}{2}\zeta(K') \implies \boxed{\zeta(K') = 2\zeta(K) - \ln\left[2\sqrt{\cosh 2K}\right]} \tag{116}$$

This is a recursion equation (or a map). So starting from a value of K, we can find a *decimated* system with coupling K'. Now, doing the same procedure again we get K'' and this continues,

$$K \to K' \to K'' \to \cdots$$

Also, note one thing. We have $2K' = \ln\cosh(2K)$ from which we get:

$$\begin{aligned} 2K' = \ln e^{2K} + e^{-2K} - \ln 2 &= \ln e^{2K}(1 + e^{-4K}) - \ln 2 \\ &= 2K + \ln\left(1 + e^{-4K}\right) - \ln 2 \\ \implies K' &= K + \frac{1}{2}\ln\left(1 + e^{-4K}\right) - \ln 2 \leq K \end{aligned}$$

From this, we see that the decimated coupling constant is less than the original coupling. Since we defined $K = \beta J$, this means that the new coupling is all the way farther from the critical point.

The opposite recursion relation (obtaining K from K') is given by,

$$K = \frac{1}{2}\cosh^{-1}(e^{2K'}) \qquad \zeta(K) = \frac{1}{2}\ln f(K) + \frac{1}{2}\zeta(K') = \frac{1}{2}(\ln 2 + K') + \frac{1}{2}\zeta(K')$$
$$\implies \boxed{\zeta(K) = \frac{1}{2}(\ln 2 + K') + \frac{1}{2}\zeta(K')} \tag{117}$$

Now, when K' is reall really small (so T is very high), then the contribution from the interaction is negligible since $\beta\mathcal{H} = K\sum\cdots \to 0$. Then the system effectively acts as a collection of non-interacting spins. So suppose we have N' spins in this case of very small K', then the partition function is simply $2^{N'}$ which implies that $\beta F = N' \ln 2$, hence $\zeta(K') = \ln 2$.

Starting from say $K_0 = 0.01$, we have $\zeta(K_0) \approx \ln 2$ and we put this in Eq. (117) to get the new value of K. Now we take this to be K' and put it again in Eq. (117).

Now, one thing which can probably happen is that, the transformation gives the same output as the input. Then the process will continue in a loop and will be essentially terminated. This situation occurs when we encounter a *fixed point* of the map. The fixed point K^* is then given by the condition, $2K^* = \ln\cosh(2K^*)$, which has solutions $K = 0$ ($T \to \infty$) and $K \to \infty$ ($T = 0$).

Hence, starting from any value of K_0, we will always land to $K = 0$. Thus, for a finite K_0 we never arrive at an ordered state *viz.* there is no phase transition in 1D Ising model. Only for $K \to \infty$ do the spins order.

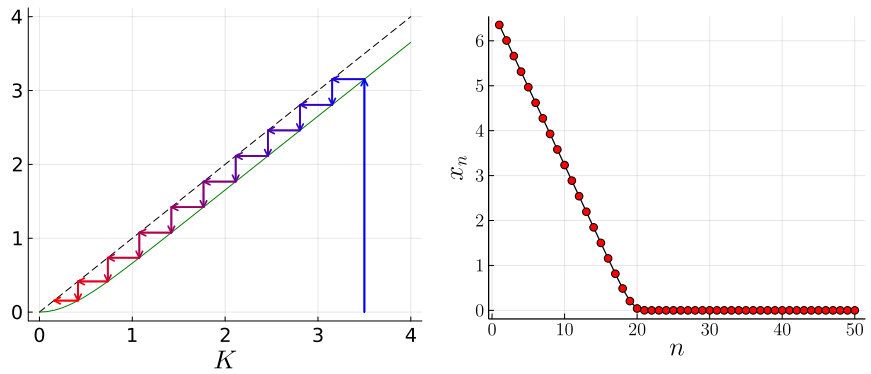


Figure 31: The decimation process. (a) Starting from $K_0 = 3.5$, we map it onto the curve $K' = \frac{1}{2}\ln\cosh 2K$ and repeat the process. The black dashed line represents $K' = K$ line while the green line represents $K' = \frac{1}{2}\ln\cosh 2K$ line. The process converges to $K^* = 0$. This type of diagram is called the *cobweb* diagram (b) x_n vs. the iteration n. We see that x_n converges to 0 after around 20 iterations.

Lecture 29: Stability Analysis

In the previous lecture, we saw a map over which we iterate our system to perform the decimation. This map resulted in two fixed points, $K^* = 0$ and $K^* \to \infty$ for the 1D Ising model case. $K^* = 0$ was a stable fixed point and hence starting the process from any $K_0 > 0$ resulted in convergence to zero, which denoted the infinite temperature, non-interacting case.

29.1. Stability in Non-Linear Systems

Let us proceed to understand a general procedure to analyse the stability of these kind of maps. We will focus on the *logistic map*, given by:

$$x_{n+1} = \mu x_n(1 - x_n) \qquad x_n \in [0, 1] \tag{118}$$

Consider the function $f(x) = \mu x(1-x) = -\mu\Big[\big(x - \frac{1}{2}\big)^2 - \frac{1}{4}\Big]$. It has a maxima of $\frac{\mu}{4}$ at $x = \frac{1}{2}$. Hence, if $\mu > 4$ then the maxima goes beyond 1 and then Eq. (118) no longer maps $[0, 1]$ to itself. And we should always be positive. Hence, we keep the control parameter $0 < \mu \leq 4$.

Let us now calculate the fixed points. Let x^* be the fixed point which implies,

$$f(x^*) = x^* \implies \mu x^*(1 - x^*) = x^* \implies x^* = 0 \quad \text{or} \quad x^* = 1 - \frac{1}{\mu} \tag{119}$$

Now, we calculate the stability of these fixed points. "Stability" refers to the situation that if we start at some point around x^*, then do we fall into x^* or go away from x^*. For this, consider a sequence ϵ_n such that,

$$x_n = x^* + \epsilon_n$$

Then, the fixed point condition $x^* = f(x^*)$ gives us,

$$x^* + \epsilon_{n+1} = x_{n+1} = f(x_n) = f(x^* + \epsilon_n) \xrightarrow{Taylor} f(x^*) + \epsilon_n f'(x^*) = x^* + \epsilon_n f'(x^*)$$

The above condition implies $|f'(x^*)| = \left|\frac{\epsilon_{n+1}}{\epsilon_n}\right|$ and this tells us a lot. From the map, we have $f'(x^*) = mu(1 - 2x^*)$. For $x^* = 0$ we have $f'(0) = \mu$ and for $x^* = 1 - \frac{1}{\mu}$ we have $f'(x^*) = 2 - \mu$. For stability, we need the sequence $\{|\epsilon_n|\}$ to be decreasing, that is, $|\epsilon_{n+1}| < |\epsilon_n| \implies |f'(x^*)| < 1$.

▷ **Stability of $x^* = 0$**

If $|f'(0)| = |\mu| < 1$ then $x^* = 0$ is a stable fixed point. Thus, for $0 < \mu < 1$ we have $x^* = 0$ is a *stable point* of the map. This means that starting from any value of x_0, we will eventually converge to 0.

▷ **Stability of $x^* = 1 - \frac{1}{\mu}$**

If $|f'(x^*)| = |2 - \mu| < 1$ then $x^* = 0$ is a stable fixed point. The condition leads to,

$$-1 < 2 - \mu < 1 \implies -3 < -\mu < -1 \implies 1 < \mu < 3$$

Thus, for $1 < \mu < 3$ we have $x^* = 1 - \frac{1}{\mu}$ is a *stable point* of the map. This means that starting from any value of x_0, we will eventually converge to $1 - \frac{1}{\mu}$. Note that the point of convergence will now depend on the value of μ.

Beyond $\mu = 3$, none of the fixed points are stable and there are some other complicated things like period-doubling and chaos going on. It can be shown that for $3 < r < 1 + \sqrt{6}$, there is a stable *period-2 orbit*, which means that instead of $f(x^*) = x^*$ we have $f(f(x^*)) = x^*$.

Similarly for $1 + \sqrt{6} < \mu < 3.54409\ldots$ we have a *period-4 orbit*. This way, period-2^n occurs for different μ_n (μ_n is the value where the first bifurcation occurs). Successive bifurcations come faster and faster and ultimately μ_n converges to μ_∞ (≈ 3.569946 for the logistic map). For $\mu > \mu_\infty$, the dynamics become *chaotic*.

These behaviour can be demonstrated using the *orbit diagram*, generated numerically. What we do is,

we choose a particular value of μ and then, choosing some initial value, we iterate the map for quite some generations (to kill of the initial transient behaviour). Then, we plot x_n for multiple successive iterations.

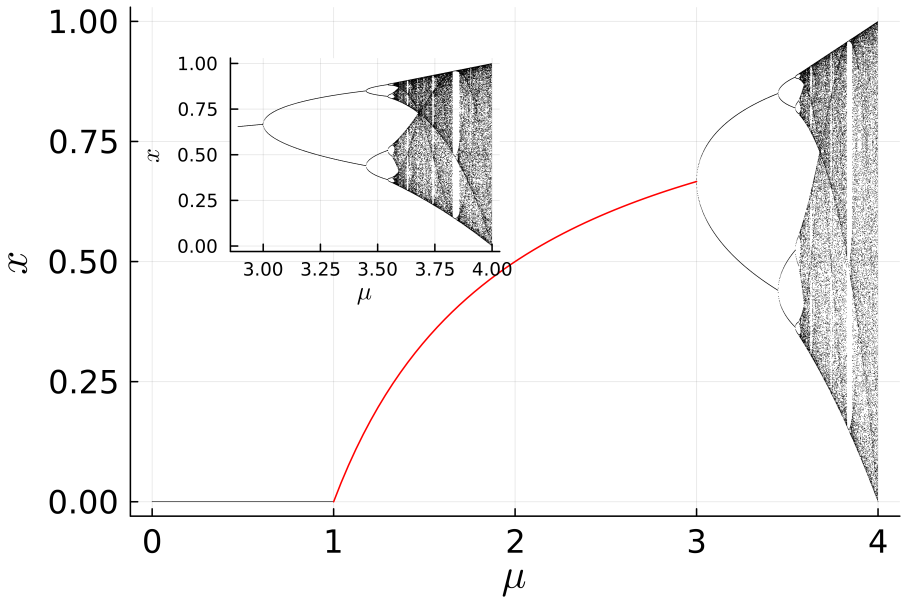


Figure 32: Orbit diagram for logistic map. We see that at $\mu = 1$, there is a bifurcation. At $\mu = 3$, there is another bifurcation (period doubling) and so on. The inset shows a zoomed in region between $3 < \mu < 4$ which shows further bifurcations. The red line shows the $x = 1 - \frac{1}{\mu}$ line.

Now, finally let us plot the cobweb diagrams for different values of μ which will make the case a bit more clear.

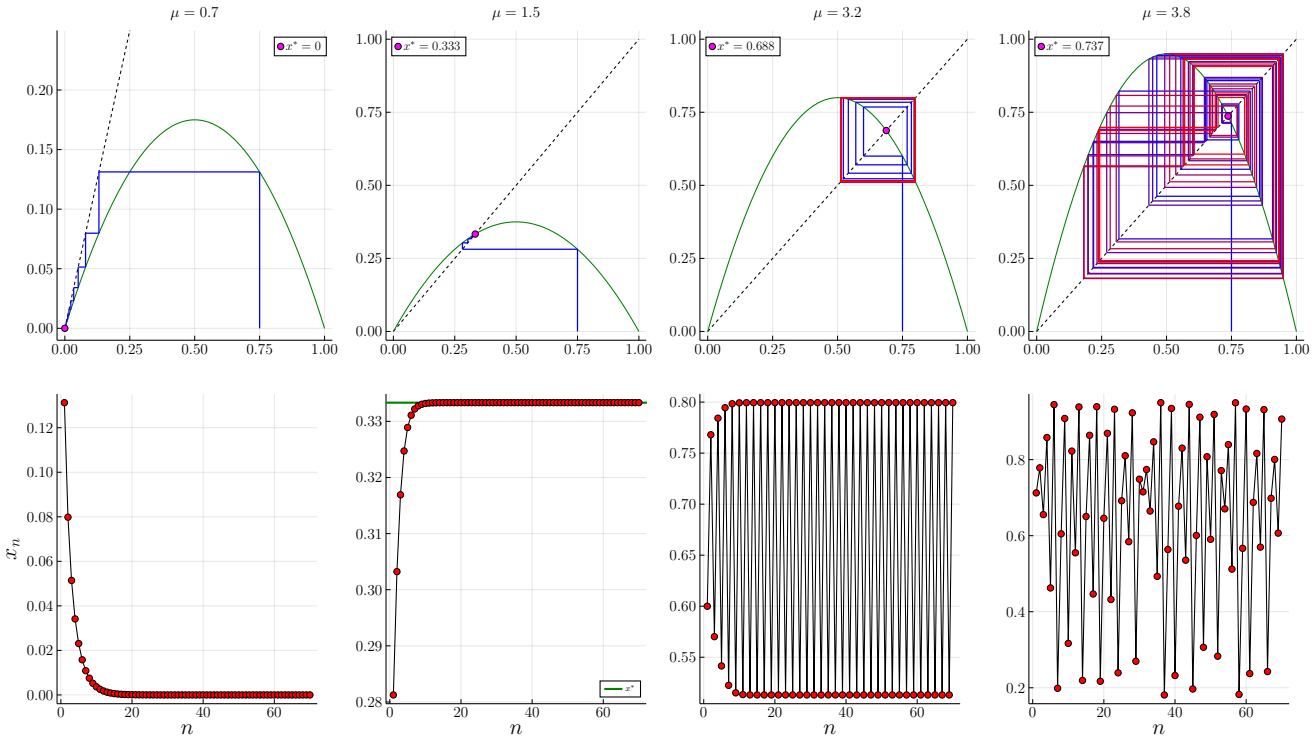


Figure 33: Cobweb diagram for different μ. The upper panel shows the cobweb diagram of the logistic map for different values of μ while the lower panel shows the corresponding convergence of the map under successive iterations. For the third panel, there is no convergence but there is a periodic orbit with period 2 and in the last panel, there is no pattern as such, the evolution is *chaotic*.

29.2. Stability in RG

As seen in the previous discussions, the recursion relations, like say Eq. (116), are called *RG transformations* and for a general system with a set of coupling constants $\mathbf{K} \equiv [K]$, is denoted by

$$[K'] = R_l[K] \qquad l > 1$$

where R_l is the non-linear transformation defining a "flow" from $\mathbf{K}$ to $\mathbf{K}'$. The subscript l refers to the change in length scale after such transformation. Like in Fig. 30, if the initial spacing between two spins was a, after decimation, the spacing between two spins become $a' = 2a$. The physical length remains same, which implies $A = a = \frac{a'}{2}$, hence $l = 2$ in this case.

There cannot be an inverse transformation in general, because we are tracing out degrees of freedom after each decimation step and there is no way to get that information back again. If we do successive transformations R_{l_1} and R_{l_2}, we get

$$[K'] = R_{l_1}[K] \qquad [K''] = R_{l_2}[K'] = R_{l_2} \cdot R_{l_1}[K] \equiv R_{l_1 l_2}[K]$$

Hence, product of two transformations is equal to another transformation and thus exhibits a 'semi-group' structure (it's not a group since the inverse does not exist in general). Also note that it doesn't matter whether we perform R_{l_1} first or R_{l_2} first, so these transformations commute.

If there is a fixed point $[K^*]$ for the RG transformation, then $[K^*] = R_l[K^*]$. Under R_l, the length scales are reduced by factor l and the correlation length of the rescaled couplings will be $\xi[K'] = \xi[K]/l$. For the fixed point,

$$\xi[K^*] = \frac{\xi[K^*]}{l} \implies \xi[K^*] = 0 \quad \text{or} \quad \xi[K^*] \to \infty$$

The fixed point where $\xi \to \infty$ is called the *critical fixed point* (since correlation diverges at the critical point) while those with $\xi = 0$ will be called the *trivial fixed point*.

Let us consider the fixed point $\mathbf{K}^* \equiv (K_1^*, K_2^*, \cdots)$ and some deviation $\boldsymbol{\delta K} = (\delta K_1, \delta K_2, \ldots)$ from this fixed point. We now Taylour expand the quantity:

$$K_n'(\{K_n\}) = K_n'(\{K_n^* + \delta K_n\}) = K_n^* + \sum_m \left.\frac{\partial K_n'}{\partial K_m}\right|_{K_m^*} \cdot \delta K_m + \Theta((\delta K)^2)$$

Now we can also write $K_n' = K_n^* + \delta K_n'$ in the vicinity of the fixed point. Equating both we get,

$$\delta K_m' = \sum_n M_{mn} K_n \qquad \text{where } M_{mn} \equiv \left.\frac{\partial K_m'}{\partial K_n}\right|_{\mathbf{K}^*} \tag{120}$$

The matrix $M^{(l)} \equiv [M_{mn}]$ is the linearised RG transformation where the superscript now denote the length scale of the transformation. Let us focus only only one coupling for the moment. Then the matrix M becomes just a scalar number, let us denote it by $\Lambda^{(l)}$. Using the semi-group property, we have:

$$\Lambda^{(l)}\Lambda^{(l')} = \Lambda^{(ll')} \tag{121}$$

This is a functional equation in l and l'. To solve it, let us first differentiate the above equation w.r.t l' for a fixed l and then put $l' = 1$,

$$\Lambda^{(l)} \frac{\mathrm{d}\Lambda^{(l')}}{\mathrm{d}l'} = \frac{\mathrm{d}\Lambda^{(ll')}}{\mathrm{d}(ll')} \cdot \frac{\mathrm{d}(ll')}{\mathrm{d}l'} \implies c \cdot \Lambda^{(l)} = l \frac{\mathrm{d}\Lambda^{(ll')}}{\mathrm{d}(ll')} = l \frac{\mathrm{d}\Lambda^{(l)}}{\mathrm{d}l}$$

where $c = \frac{\mathrm{d}\Lambda^{(l')}}{\mathrm{d}l'}$ at $l' = 1$. In the last step, we replaced the variable $ll' \to l$, since the function and derivative are both w.r.t the variable (ll'). Doing this we obtain the differential equation,

$$c \cdot \frac{\mathrm{d}l}{l} = \frac{\mathrm{d}\Lambda^{(l)}}{\Lambda^{(l)}} \implies \ln \Lambda^{(l)} = c \ln l + d \implies \Lambda^{(l)} = \Lambda_0^{(l)} l^c$$

The condition in Eq. (121) implies that $\Lambda_0^{(l)} = 1$ for non-trivial result and hence we obtain that $\Lambda^{(l)} = l^c$ where c is a number independent of l and we will see its implications later.

Lecture 30: RG for 2D Ising Model

Let us continue our discussion on RG and focus on some other things. Previously we saw that, for a *critical* fixed point $\mathbf{K}^*$, we should have the correlation length ξ^* either zero or infinite. However, we know that under successive RG transformations with say R_l, the correlation length only *decreases* (since $l > 1$) from $\xi \to \xi' = \xi/l$. This implies that, starting from $\mathbf{K}_0$ and on successive transformations, $\xi^* \to \infty$ at $\mathbf{K}^*$ can only happen if $\xi \to \infty$ also at $\mathbf{K}$ (and also in any intermediate point of flow from $\mathbf{K}$ to $\mathbf{K}^*$).

This constitutes a surface, called the *critical surface* (or a *critical manifold*, if we want to sound cool!), say $\mathcal{C}$, such that if $\mathbf{K} \in \mathcal{C}$ then $\mathbf{K}$ converges to $\mathbf{K}^*$. Any $\mathbf{K} \notin \mathcal{C}$ will move away from $\mathbf{K}^*$ (even if initially it moves towards it).

What it physically means is that, there are infinite directions in which, if we start, then we will not converge to the fixed point. Only starting on the particular *critical* surface will lead us to the fixed point.

Now, let us rediscuss about the linearisation of RG, from Eq. (120). Let us denote the eigenvalue and eigenvector set of M with $\{\lambda_\sigma, \hat{\mathbf{e}}_\sigma\}$. Negating all pathologies, we assume that the eigenvectors form a complete set and hence we can expand any vector in terms of these eigenvectors, using which we get:

$$\boldsymbol{\delta K} = \sum_\sigma u_\sigma \hat{\mathbf{e}}_\sigma \qquad \boldsymbol{\delta K}' = \sum_\sigma u'_\sigma \hat{\mathbf{e}}_\sigma \tag{122}$$

Substituting this in Eq. (120) we get,

$$\sum_\sigma u'_\sigma \hat{\mathbf{e}}_\sigma = M\left[\sum_\sigma u_\sigma \hat{\mathbf{e}}_\sigma\right] = \sum_\sigma \lambda_\sigma u_\sigma \hat{\mathbf{e}}_\sigma$$

Since the eigenvectors are complete, these form a linearly independent set from which we get $u'_\sigma = \lambda_\sigma u_\sigma$. The quantities $\{u_\sigma\}$ are called *scaling fields* of the given problem and are crucial to understand critical behaviour. Under successive transformations, $u_\sigma \mapsto [\lambda_\sigma]^n u_\sigma$

Since u_σ is directly related to $\boldsymbol{\delta K}$ then we can have three possibilities:

- ▷ If $|\lambda_\sigma| > 1$ then u_σ grows under successive transformations and hence $\boldsymbol{\delta K}$ "increases" along these directions, denoting the flow away from the fixed point. The scaling field is then referred to as *relevant*.
- ▷ If $|\lambda_\sigma| < 1$ then u_σ decays under successive transformations and the scaling field is referred to as *irrelevant*.
- ▷ If $|\lambda_\sigma| = 1$ then $u_\sigma \sim \mathcal{O}(1)$ and remains mostly constant, upto the linear approximation. It does not affect the 'critical behaviour' much but can introduce logarithmic factors. We then called this *marginal* scaling field.

On the critical surface, we have all the relevant variables equal to zero and hence, everything flows to the fixed point. Thus, only the irrelevant eigenvectors span this space.

Away from the critical surface, we have both relevant and irrelevant fields; the former drive the system away from the fixed point while the latter bring it closer to the fixed point. The net result is an initial approach to the fixed point but a final recession away from it.

The number of relevant eigenvalues is called the *codimension* of the critical surface, denoted by c and is equal to the difference in the dimension of the coupling constant space and the dimension of the critical surface.

30.1. RG for 2D Ising Model on square lattice

Let us see RG in play for the zero-field 2D Ising model, whose Hamiltonian is given by

$$-\beta\mathcal{H} = K \sum_{\langle ij \rangle} \sigma_i \sigma_j \tag{123}$$

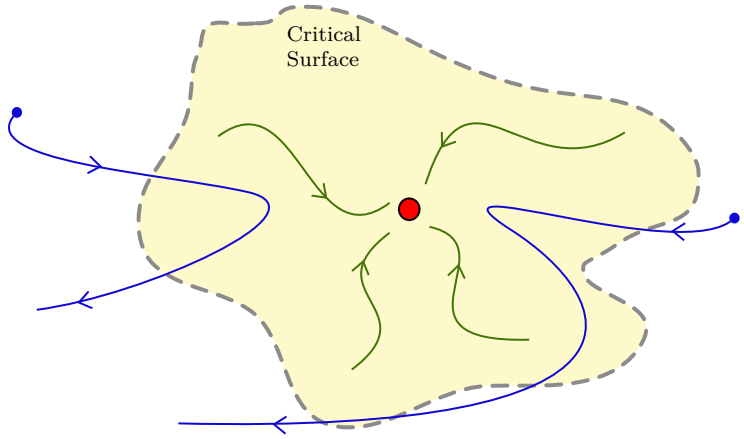


Figure 34: RG flow in K-space. The blue arrows denote the relevant flows, outside of the critical surface while the green arrows show the irrelevant flows towards the fixed point (red marker), on the critical surface. The critical surface is denoted by the yellow region.

where $K = \beta J$. Then the partition function becomes,

$$\mathcal{Z} = \sum_{\{\sigma_k\}} \exp\left[K \sum_{\langle ij \rangle} \sigma_i \sigma_j\right] = \sum_{\{\sigma_k\}} \prod_{\langle ij \rangle} \exp\left[K \sigma_i \sigma_j\right]$$

As before, let us take a particular spin, say $\sigma_{(i,j)}$ (where (i,j) represents the coordinate on the lattice), and then trace it out. The term $\sigma_{(i,j)}$ appears in:

$$\begin{aligned}\mathcal{Z}_N &= \left\{ \sum_{\substack{\sigma_{p\neq i,\, q\neq j} \\ =\pm 1}} \right\} \sum_{\substack{\sigma_{(i,j)} \\ =\pm 1}} \cdots \exp\left[K\sigma_{(i,j-1)}\sigma_{(i,j)}\right] \cdot \exp\left[K\sigma_{(i,j+1)}\sigma_{(i,j)}\right] \cdot \exp\left[K\sigma_{(i,j)}\sigma_{(i-1,j)}\right] \cdot \exp\left[K\sigma_{(i,j)}\sigma_{(i+1,j)}\right] \cdots \\ &= \sum_{\sigma_{p\neq i, q\neq j}=\pm 1} \cdots \cdot \left[2\cosh\left(K(\sigma_{(i,j+1)} + \sigma_{(i,j-1)} + \sigma_{(i+1,j)} + \sigma_{(i-1,j)})\right)\right] \cdots\end{aligned}$$

Again, we need to convert the resulting expression in the form of the original Hamiltonian with respect to these spins, as much as we can. Note that this will not be that much easy as in the case of the 1D counterpart, since there are now a total of 16 possibilities for the terms in $\left[2\cosh\left(K(\sigma_{(i,j+1)} + \sigma_{(i,j-1)} + \sigma_{(i+1,j)} + \sigma_{(i-1,j)})\right)\right]$. Note that all the 16 possibilities will not yield a unique sum, some will be repeated. Only 4 cases turn out to be non-equivalent:

- When all are equal, *i.e.* $\sigma_{i-1,j} = \sigma_{i+1,j} = \sigma_{i,j+1} = \sigma_{i,j-1}$.
- When one is -1, *i.e.* $\sigma_{i-1,j} = \sigma_{i+1,j} = \sigma_{i,j+1} = -\sigma_{i,j-1}$.
- When two are -1, which has two cases,
  - ▷ $\sigma_{i-1,j} = \sigma_{i+1,j} = -\sigma_{i,j+1} = -\sigma_{i,j-1}$
  - ▷ $\sigma_{i-1,j} = -\sigma_{i+1,j} = -\sigma_{i,j+1} = \sigma_{i,j-1}$

Now, if we want the decimated system to be of the form of the original Hamiltonian *viz.* the nearest-neighbour 2D Ising model, then the term in the partition function involved with these spins would be,

$$e^{A} \cdot e^{B\left(K(\sigma_{(i,j+1)} + \sigma_{(i,j-1)} + \sigma_{(i+1,j)} + \sigma_{(i-1,j)})\right)}$$

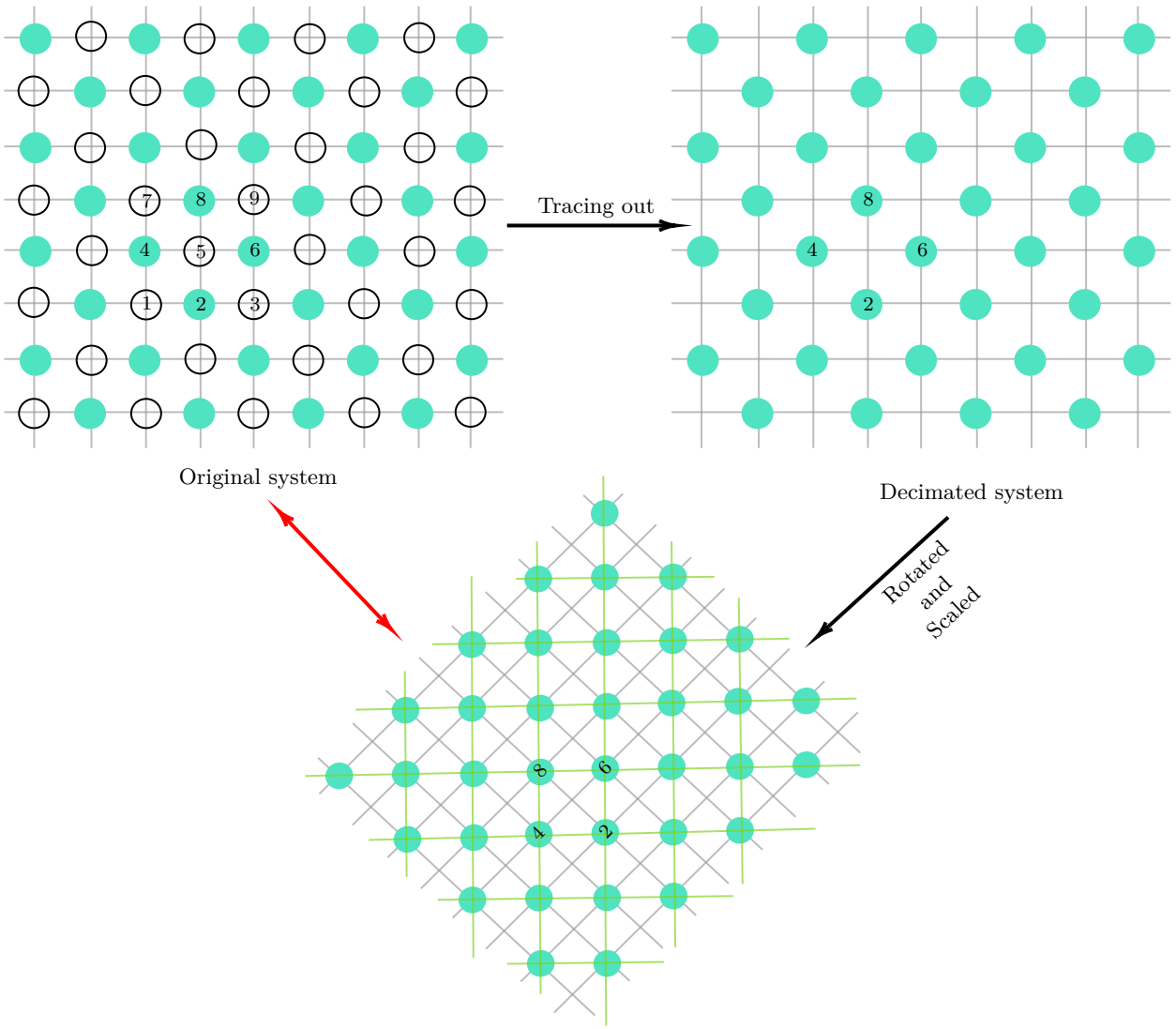


Figure 35: Decimation of the 2D Ising model. The hollowed out spins are the ones traced out, leaving behind a decimated system, which when rotated by $\frac{\pi}{4}$ and scaled appropriately, resembles the original system, specially in the thermodynamic limit.

which will be an issue since the given 4 possibilities of these spins exceed the number of parameters A and B to fix. We can make this work by considering higher order interactions, giving us,

$$\begin{aligned} 2\cosh\Big(K(\sigma_{(i,j+1)}+\sigma_{(i,j-1)}+\sigma_{(i+1,j)}+\sigma_{(i-1,j)})\Big) = e^{K_0'}\exp\Bigg[\frac{K'}{2}\Big(&\sigma_{(i,j-1)}\sigma_{(i-1,j)}+\sigma_{(i,j-1)}\sigma_{(i+1,j)} \\ &+\sigma_{(i-1,j)}\sigma_{(i,j+1)}+\sigma_{(i,j+1)}\sigma_{(i+1,j)}\Big) \\ &+L'\Big(\sigma_{(i+1,j)}\sigma_{(i-1,j)}+\sigma_{(i,j-1)}\sigma_{(i,j+1)}\Big) \\ &+M'\,\sigma_{(i-1,j)}\sigma_{(i+1,j)}\sigma_{(i,j+1)}\sigma_{(i,j-1)}\Bigg] \end{aligned}$$

where L' and M' are new couplings which are introduced. Imposing the spin possibilities gives us four equations relating the new and old couplings,

$$\begin{aligned} 2\cosh(4K) &= e^{K_0'+2K'+2L'+M} & 2\cosh(2K) &= e^{K_0'-M} \\ 2 &= e^{K_0'-2K'+2L'+M'} & 2 &= e^{K_0'-2L'+M'} \end{aligned} \tag{124}$$

After a few manipulations, we would obtain:

$$\begin{aligned} K'_0 &= \ln 2 + \frac{1}{2}\ln\cosh 2K + \frac{1}{8}\ln\cosh 4K \qquad & M' &= \frac{1}{8}\ln\cosh 4K - \frac{1}{2}\ln\cosh 2K \\ K' &= \frac{1}{4}\ln\cosh 4K & L' &= \frac{1}{8}\ln\cosh 4K \end{aligned} \tag{125}$$

Now take another value of the spin to trace over, say $\sigma_{(i+2,j)}$, and repeat the process. The process continues till all $N/2$ spins are summed over. Note that, the nearest neighbour interaction term $\sigma_{(i+1,j)}\sigma_{(i,j+1)}$ with coupling K' will appear when we trace out spins $\sigma_{(i,j)}$ and also when we trace out $\sigma_{(i+1,j+1)}$. This terms then appear exactly twice in the decimation process and hence we had taken $\frac{K'}{2}$ when we wrote the new couplings. Doing the decimation process until $N/2$ spins are traced out, will give us a partition funciton of the form,

$$\mathcal{Z}_N = e^{N'K'_0}\sum_{\sigma'}\exp\left[K'\sum_{\langle jk\rangle}\sigma'_j\sigma'_k + L'\sum_{\langle\langle jk\rangle\rangle}\sigma'_j\sigma'_k + M'\sum_{\text{plaquette}}\sigma'_j\sigma'_k\sigma'_l\sigma'_m\right]$$

with $N' = N/2$ and $\langle\langle\cdot\rangle\rangle$ denoting the nearest neighbour coupling and *plaquette* sum denoting the four spin interaction over a square plaquette. There is no exact correspondence between this and Eq. (123). The latter has only nearest neighbour terms while the former has all sort of complicated things going on. Things will only get worse when we do another round of decimation, such that $N' \to N/4$, leading to higher order spin interaction terms.

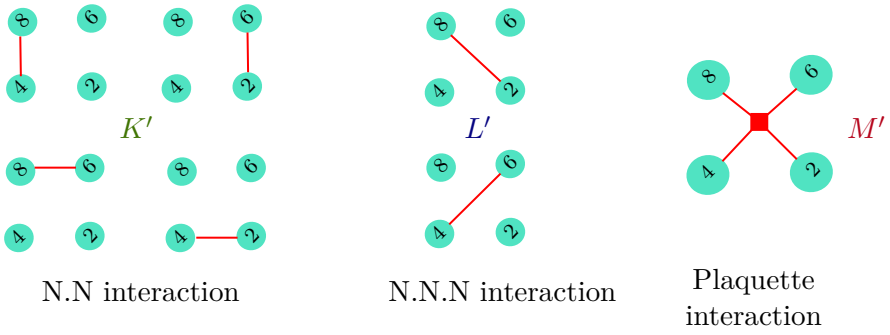


Figure 36: Type of interactions generated after one round of decimation.

To make a way around this problem of not having a correspondence with the original Hamiltonian, we assume that the initial Hamiltonian was also of the same form, with all these interactions, but the corresponding couplings were 0. So $L = M = 0$ for the original system. Then we can write,

$$\mathcal{Z}_N(\{K,0,0\}) = e^{N'K'_0}\mathcal{Z}_{N'}(\{K',L',M'\}) \implies \zeta(\{K,0,0\}) = -\frac{1}{2}K'_0 + \frac{1}{2}\zeta(\{K',L',M'\})$$

The number of parameters will increase after each round of decimation and the problem will become intractable unless we do what we *love* to do: take weird approximations! In here, we will assume that only the nearest (K) and the next-nearest neighbour interactions (L) are important and further, that these are very small (so $\cosh(x) \approx 1 + \frac{x^2}{2}$ and $\ln\left(1+\frac{x^2}{2}\right) \approx \frac{x^2}{2}$), which changes Eq. (125) to,

$$K' = 2K^2 \qquad L' = K^2$$

Furthermore, let us suppose that $L \neq 0$ in the beginning. Then, considering this we would have obtained the transformations as

$$K' = 2K^2 + L \qquad L' = K^2$$

Now, we need to find the fixed point of these transformations.

$$L^* = K^{*2} \qquad K^* = 2K^{*2} + L^* = 3K^{*2}$$

This gives us two set of fixed points, $(K^*, L^*) = (0, 0)$ and $(K^*, L^*) = (1/3, 1/9)$. The first one is the trivial fixed point, corresponding to infinite temperature, while the second one is the one of our interest.

Considering deviations from the fixed point, $K = K^* + \delta K$ and $L = L^* + \delta L$, we get:

$$K^* + \delta K' \equiv K' = 2(K^* + \delta K)^2 + (\delta L + L^*) = 2K^{*2} + 4K^*\delta K + \delta L + L^* = K^* + 4K^*\delta K + \delta L$$
$$L^* + \delta L' \equiv L' = K^{*2} + 2K^*\delta K = L^* + 2K^*\delta K$$

From this, we get the following in matrix form,

$$\begin{pmatrix}\delta K'\\ \delta L'\end{pmatrix} = \begin{pmatrix}4K^* & 1\\ 2K^* & 0\end{pmatrix}\begin{pmatrix}\delta K\\ \delta L\end{pmatrix} \quad \longrightarrow \quad \boxed{\begin{pmatrix}\delta K'\\ \delta L'\end{pmatrix} = \begin{pmatrix}4/3 & 1\\ 2/3 & 0\end{pmatrix}\begin{pmatrix}\delta K\\ \delta L\end{pmatrix}} \tag{126}$$

Before the transformation, we have the lattice spacing as a and after transformation, the lattice spacing becomes $a' = a\sqrt{2}$ which implies that $l = \sqrt{2}$. The linearised RG is thus,

$$\mathrm{M}^{(\sqrt{2})} \equiv \begin{pmatrix}4/3 & 1\\ 2/3 & 0\end{pmatrix}$$

Lecture 31: More on RG

As a final thing, we will find the eigenvalues of the linearised RG matrix around the fixed point $\mathbf{K} = (1/3, 1/9)$. Let us diagonalise the matrix,

$$\det\left(\mathrm{M}^{(\sqrt{2})} - \lambda\mathbb{1}\right) = 0 \implies \det\begin{pmatrix}4/3 - \lambda & 1\\ 2/3 & -\lambda\end{pmatrix} = 0 \implies \lambda\left(\lambda - \frac{4}{3}\right) = \frac{2}{3} \implies 3\lambda^2 - 4\lambda - 2 = 0$$

which gives us $\lambda_\pm = \frac{1}{6}\left(4 \pm \sqrt{40}\right) \approx 1.7207, -0.3874$. Thus, $|\lambda_+| > 1$ and hence it is a *relevant* eigenvalue, while $|\lambda_+| < 1$, rendering it *irrelevant*. The corresponding eigenvectors are,

$$\boldsymbol{u}_+ = \begin{pmatrix}1\\ \frac{\sqrt{10}-2}{3}\end{pmatrix} \approx \begin{pmatrix}1\\ 0.387\end{pmatrix} \qquad \boldsymbol{u}_- = \begin{pmatrix}1\\ -\frac{\sqrt{10}+2}{3}\end{pmatrix} \approx \begin{pmatrix}1\\ -1.7207\end{pmatrix}$$

$\boldsymbol{u}_+$ is a relevant direction while $\boldsymbol{u}_-$ is an irrelevant direction which defines the critical surface. Suppose we start initially at the point (K_0, L_0) and successively apply the recursion formula. Upto linear approximation, we can expand the deviation $(K_0 - K^*, L_0 - L^*)$ in terms of the eigenvectors, that is,

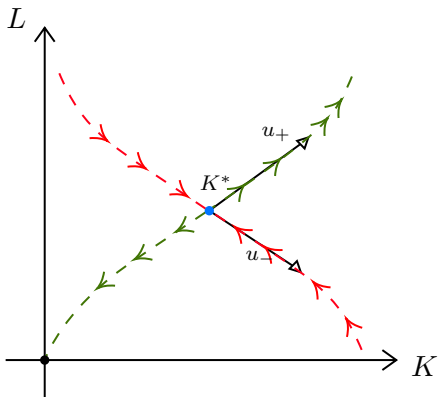
$$\begin{pmatrix}K_0\\ L_0\end{pmatrix} = \begin{pmatrix}K^*\\ L^*\end{pmatrix} + c_+\boldsymbol{u}_+ + c_-\boldsymbol{u}_- \quad \xrightarrow{l \text{ transformations}} \quad \begin{pmatrix}K_l\\ L_l\end{pmatrix} = \begin{pmatrix}K^*\\ L^*\end{pmatrix} + \lambda_+^l c_+\boldsymbol{u}_+ + \lambda_-^l c_-\boldsymbol{u}_- \tag{127}$$

Now, suppose that after l transformations, we want to reach the fixed point as much as possible. This cannot happen if c_+ is non-zero to begin with, as then, after the transformations, the deviation will grow along u_+.

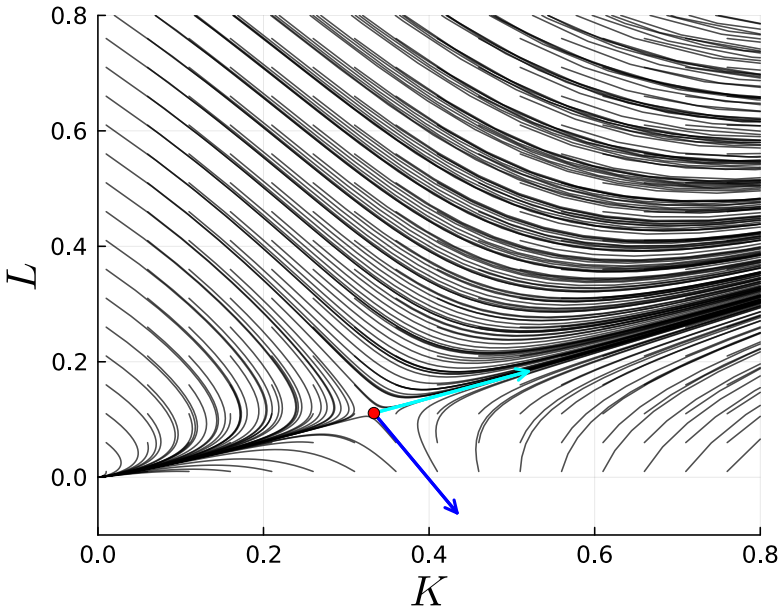
As an example, consider the original Ising model with nearest neighbour interaction only, that is, $L_0 = 0$. We start from some $K_0 = K_c \neq 0$ and we have to take $c_+ = 0$ (since we want to go to the fixed point eventually). Then the above equation tells us,

$$\begin{pmatrix}K_c\\ 0\end{pmatrix} = \begin{pmatrix}1/3\\ 1/9\end{pmatrix} + 0 \cdot \boldsymbol{u}_+ + c_-\begin{pmatrix}1\\ -(\sqrt{10}+2)/3\end{pmatrix}$$

From which we obtain $c_- = \frac{1}{3\left(2+\sqrt{10}\right)}$ which implies $K_c = \frac{1}{3} + \frac{1}{3\left(2+\sqrt{10}\right)} \approx 0.3979$. This is the critical point for the nearest neighbour 2D Ising model, however, this is quite off from Onsager's exact solution $K_c = 0.4406$. Then starting from $(K_c, 0)$ we will always go to the fixed point.



Now, suppose we have $K_0 \neq K_c$ which implies that, after l transformations we no longer go to the fixed point.



Appendices

From the first law we have the energy conservation equation,

$$\mathrm{d}U = T\mathrm{d}S - P\mathrm{d}V + \mu\mathrm{d}N$$

and thus the internal energy is a function of S, V and N. We know that the internal energy is a homogenous function of degree 1, on physical grounds, since if we scale the system variables by λ, U is also appropriately scaled (extensitivity)

$$U(\lambda S, \lambda V, \lambda N) = \lambda U(S, V, N)$$

Now, from Euler's theorem of homogenous functions, we know that any homogenous function f of degree k can be written as,

$$kf(x_1, x_2 \dots x_n) = \sum_{i=1}^{n} x_i \frac{\partial f}{\partial x_i}$$

Using this theorem for U, we have

$$U = S\frac{\partial U}{\partial S} + V\frac{\partial U}{\partial V} + N\frac{\partial U}{\partial N}$$

Substituting the values from the first law, we obtain $U = TS - PV + \mu N$

A. Legendre Transformation

From classical mechanics, we know that the Legendre transformation is used to convert Lagrangian $L(x, \dot{x})$ to the Hamiltonian $H(x, p)$ and vice versa. Note how we switch $\dot{x}$ in L for p in H. We will call the variable that we want to switch to as the 'conjugate' of the variable we are switching. The Legendre transformation of the Lagrangian gives us the Hamiltonian,

$$H(x, p) = p\dot{x} - L$$

A function $f(x)$ with the Legendre transform $f^*(p)$ satsifies $f(x) + f^*(p) = xp$. We will use this for thermodynamic quantities also, however we will use an alternate definition using minus sign, $f(x) - f^*(p) = xp$. From the first law, we know that,

$$U = T\mathrm{d}S - P\mathrm{d}V + \mu\mathrm{d}N$$

As clearly seen, the conjugate variable pairs are (S, T), $(V, -P)$, (N, μ). We will consider the starting point as the internal energy $U(S, V, N)$ which is a function of S, V, N from the statement of the first law. However, in any experiment, keeping these as control parameters are way too hard. Think about this, controlling entropy of a system is an arduous task but controlling its conjugate variable, T, is easy-peasy.

We get four different 'potentials' by just Legendre transformation (which is basically multiplying the conjugate variables together and subtracting from the function) of the internal energy, switching between the different conjugate variables.

- **Helmholtz Free Energy**: switching $S \leftrightarrow T$

$$F(T, V, N) = U - TS \implies \mathrm{d}F = -S\mathrm{d}T - P\mathrm{d}V + \mu\mathrm{d}N$$

- **Enthalpy**: switching $V \leftrightarrow -P$

$$H(S, P, N) = U + PV \implies \mathrm{d}H = T\mathrm{d}S + V\mathrm{d}P + \mu\mathrm{d}N$$

- **Gibb's Free Energy**: switching both $S \leftrightarrow T$ and $V \leftrightarrow -P$

$$G(T, P, N) = U - TS + PV \implies \mathrm{d}G = -S\mathrm{d}T + V\mathrm{d}P + \mu\mathrm{d}N$$

- **Grand Potential**: switching both $S \leftrightarrow T$ and $N \leftrightarrow \mu$

$$\Phi(T, V, \mu) = U - TS - \mu N = -PV \implies \mathrm{d}\Phi = -S\mathrm{d}T - P\mathrm{d}V - N\mathrm{d}\mu$$

B. 1D Solution of Ising Model

In 1D, the Ising model is given by,

$$\mathcal{H} = -J\sum_{i}^{N}\sigma_i\sigma_{i+1} - h\sum_i \sigma_i$$

where we have assumed periodic boundary conditions. The second term can be written as a symmetric sum, utilisng the translation invariance. Hence the Hamiltonian becomes,

$$\mathcal{H} = -J\sum_{i}^{N}\sigma_i\sigma_{i+1} - \frac{h}{2}\sum_i(\sigma_i + \sigma_{i+1}) \equiv \sum_i \mathcal{E}(\sigma_i, \sigma_{i+1})$$

where $\mathcal{E}(\sigma_i, \sigma_{i+1}) = -J\sigma_i\sigma_{i+1} - \frac{B}{2}(\sigma_i + \sigma_{i+1})$. Note that $\mathcal{E}(+,+) = -(J+h), \mathcal{E}(-,-) = -(J-h), \mathcal{E}(+,-) = \mathcal{E}(-,+) = J$. The contribution of each configuration is,

$$P(\{\sigma_i\}) \propto e^{-\beta\mathcal{H}(\{\sigma_i\})} = \exp\left(-\beta\sum_j \mathcal{E}(\sigma_j, \sigma_{j+1})\right) \equiv \prod_{i=1}^{N}\exp(-\beta\mathcal{E}(\sigma_i, \sigma_{i+1}))$$

Let us define $t_{\sigma_i\sigma_{i+1}} = \exp(-\beta\mathcal{E}(\sigma_i, \sigma_{i+1}))$ which is an entry of a matrix t called the *transfer matrix*:

$$t_{\sigma_i\sigma_j} \equiv \langle\sigma_i|t|\sigma_j\rangle$$

The transfer matrix is just a notational trick and is assumed to be an operator of the Hilbert space spanned by $|+1\rangle$ and $|-1\rangle$.

$$\begin{aligned} \langle+|t|+\rangle &= e^{\beta(J+h)} \qquad \langle+|t|-\rangle = e^{-\beta J} \\ \langle-|t|-\rangle &= e^{\beta(J-h)} \qquad \langle-|t|+\rangle = e^{-\beta J} \end{aligned}$$

The partition function can then be written as,

$$\begin{aligned} \mathcal{Z} = \sum_{\{\sigma_i\}} e^{-\beta\mathcal{H}(\{\sigma_i\})} &= \sum_{\sigma_1}\sum_{\sigma_2}\cdots\sum_{\sigma_N} t_{\sigma_1\sigma_2}t_{\sigma_2\sigma_3}\ldots t_{\sigma_N\sigma_1} \\ &= \sum_{\sigma_1}\sum_{\sigma_2}\cdots\sum_{\sigma_N} \langle\sigma_1|t|\sigma_2\rangle\langle\sigma_2|t|\sigma_3\rangle\langle\sigma_3|t|\sigma_4\rangle\ldots\langle\sigma_N|t|\sigma_1\rangle \end{aligned} \tag{128}$$

From the resolution of identity, $\sum_\sigma |\sigma\rangle\langle\sigma| = \mathbb{1}$ and hence all the inner spin sums vanish. We are left with,

$$\mathcal{Z} = \sum_{\sigma_1}\langle\sigma_1|t^N|\sigma_1\rangle = \mathrm{Tr}(t^N) = \lambda_+^N + \lambda_-^N = \lambda_+^N\left(1 + \left(\frac{\lambda_-}{\lambda_+}\right)^N\right)$$

where $\lambda_- < \lambda_+$ are the eigenvalues of the transfer matrix. In the limit $N \to \infty$, $\mathcal{Z} \to \lambda_+$. The eigenvalues of the transfer matrix are given as,

$$t \equiv \begin{pmatrix} e^{\beta(J+h)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-h)} \end{pmatrix} \implies \boxed{\lambda_\pm = e^{\beta J}\left[\cosh(\beta h) \pm \sqrt{\sinh^2(\beta h) + e^{-4\beta J}}\right]}$$

In the thermodynamic limit, the free energy $F = -k_\mathrm{B}T\ln\mathcal{Z} = -Nk_\mathrm{B}T\ln\lambda_+$ and then the magnetisation is given as,

$$\begin{aligned} M = -\frac{\partial F}{\partial h} &= Nk_\mathrm{B}T\frac{\partial}{\partial h}\left[\beta J + \ln\left(\cosh(\beta h) + \sqrt{\sinh^2(\beta h) + e^{-4\beta J}}\right)\right] \\ &= Nk_\mathrm{B}T\frac{\beta\sinh(\beta h) + \frac{2\beta\sinh(\beta h)\cosh(\beta h)}{2\sqrt{\sinh^2(\beta h)+e^{-4\beta J}}}}{\left(\cosh(\beta h) + \sqrt{\sinh^2(\beta h) + e^{-4\beta J}}\right)} \\ &= N\cancel{(k_\mathrm{B}T)}\cancel{\beta}\frac{\sinh(\beta h)\left[\sqrt{\sinh^2(\beta h) + e^{-4\beta J}} + \cosh(\beta h)\right]}{\left(\sqrt{\sinh^2(\beta h) + e^{-4\beta J}}\right)\left(\cosh(\beta h) + \sqrt{\sinh^2(\beta h) + e^{-4\beta J}}\right)} \\ &= \frac{N\sinh(\beta h)}{\sqrt{\sinh^2(\beta h) + e^{-4\beta J}}} \end{aligned}$$

The magnetisation per spin is then,

$$\boxed{m = \frac{\sinh(\beta h)}{\sqrt{\sinh^2(\beta h) + e^{-4\beta J}}}}$$

For $T > 0$ and $h \neq 0$, m is a well-behaved function with no singularity. For $h \to 0$, we get $m \to 0$ for all $T > 0$. Thus, temperature is not sufficient to produce a finite magnetisation without an external field. For $T \to 0$, we have $m \to 1$ and hence we can say that the phase transition to ferromagnetic behaviour in the 1D Ising model is at $T_c = 0$. This is the reason why Ising said that there is no phase transition in 1D case (and incorrectly generalised it to higher dimensions too)!

C. Gaussian Integration

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