

# Lecture Notes for Quantum Condensed Matter II

(Part of 4th Year Course C6 and Part of MMathPhys)

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## Preface

The first part of this course (which should be about 5 lectures) covers Landau theory of phases and phase transitions. This is the only part of my lectures which are required for C6. The lecture notes for this part of the course should be fairly thorough – and the course should be fairly similar to what has been taught in C6 in prior years. The notes may not be very well proofread at this point, since it is the first year they are being used.

The remainder of this course covers interesting quantum states of matter (Superfluids, Superconductors, Fermi Liquids, Quantum Hall Effects, etc). This is where condensed matter really starts to get bizarre — and therefore even more fun (at least in my opinion). C6 students are welcome and encouraged to attend all parts of the course, but only the phase transition part is on the syllabus. Others are also welcome to attend as well.

This “quantum states of matter” part of the course is mostly new for the MMathPhys course. (and it may be modified mid-stream for its first year.) There are no typed lecture notes for this part of the course yet (sorry!).

The official prerequisite for this course is the Michaelmas term Quantum Condensed Matter-I course (which is included in C6). QFT is also probably useful. However, I realize that possibly not everyone will have actually attended these courses (or possibly did attend, but didn’t pay attention), so I will try to make this course as self-contained as possible, while still making contact with what has been taught in QCMI.

Lets get started!



## Part I

# Landau Theory of Phases and Phase Transitions





# Chapter 1

## Phases and Phase Transitions

### 1.1 Some examples of phases diagrams and phase transitions

**Water:** We are all familiar with phase transitions. Water, probably the world's most familiar chemical, undergoes two transitions that we are all very familiar with: Freezing into solid ice, or boiling into gaseous vapor. The familiar phase diagram (See figure) shows the various phase transition lines – as well as the triple point and critical point (which will be of particular interest to us). At very high pressure there are many other phases of ice. In the main part of this figure

#### Phase Diagram for Water

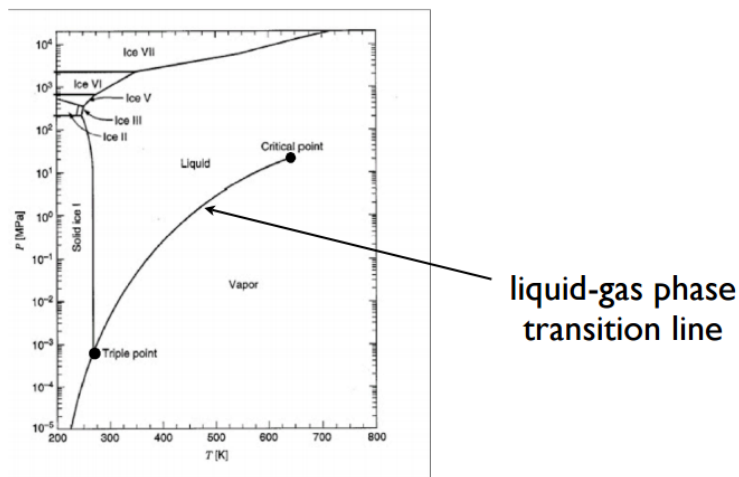


Figure 1.1: Phase Diagram of Water

(ignoring ultrahigh pressure), we have liquid, solid, and gas. Many materials have vaguely similar phase diagrams<sup>1</sup> – they melt and boil. Although this type of phase diagram is perhaps the most

<sup>1</sup>The slightly unusual thing about the water phase diagram is the negative slope of the freezing curve – which

familiar, it is actually one of the more difficult ones to understand in detail.

**Paramagnet-Ferromagnet:** Perhaps the most studied example of a phase transition is that of the para/ferromagnet. There are various ways to plot the phase diagram. We will show two here. On the left of the figure we plot the magnitude of magnetization as a function of

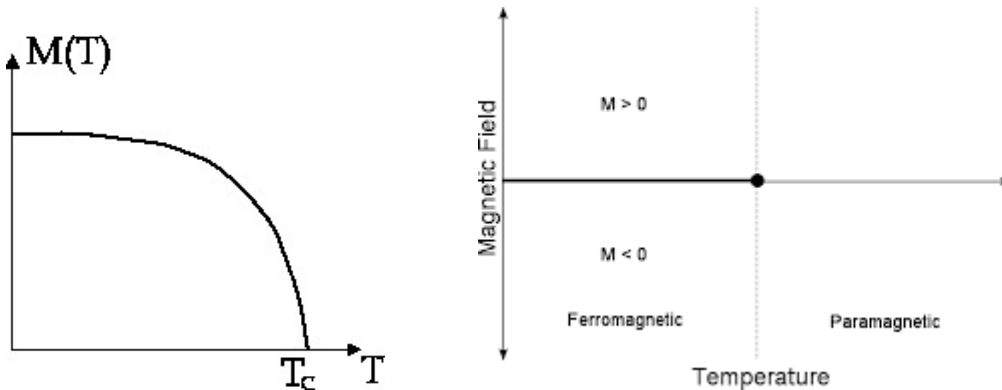


Figure 1.2: properties of a ferromagnet

temperature in zero applied magnetic field. Above the critical temperature  $T_c$ , the magnetization is zero, whereas below the critical temperature the magnetization becomes nonzero.

On the right is a phase diagram of a ferromagnet plotted in the Magnetic field-Temperature plane. Above the critical temperature the system is paramagnet and the magnetization approaches zero as the magnetic field is taken to zero. Below the critical temperature, the magnetization maintains a finite value even in zero applied magnetic field. Below the critical temperature, the dark line indicates a discontinuity — approaching the line from the two sides results in a different state. Below the critical temperature, approaching zero magnetic field from positive magnetic field side results in positive magnetization, whereas approaching from the negative magnetic field side results in a negative magnetization.

The paramagnet-ferromagnet scenario is repeated in a great number of systems. For example, one can have para/ferro-electrics. One need only replace magnetization  $M$  and magnetic field  $B$  by electric polarization  $P$  and electric field  $E$ , or one could have para/ferro-elastic where one replaces  $M$  by strain and  $B$  by stress.

**Bose Condensation:** Below a critical temperature, the lowest energy orbital (usually  $\mathbf{k} = 0$  if we think of plane wave orbitals) becomes macroscopically occupied — i.e., it becomes on the order of  $N$ , the number of bosons in the system. We call this a Bose-Einstein condensate (BEC). Above the critical temperature, the occupancy becomes essentially zero (smaller than order  $N$ ).

**Superconducting / Superfluid Transition:** Somewhat similar to the BEC, below a critical temperature, certain systems display dissipationless flow of current or of fluid mass. (We will spend a great deal of time later in the course discussing these two cases)

**High Energy Theory and Phase Transitions in the Early Universe:** One might think that phase transitions are only of interest to condensed matter physics. But in fact high energy theorists consider many different types of phase transitions as well. Just as one example, in the early universe (less than  $10^{-12}$  seconds after the big bang) the temperature of the universe

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(via the Clausius-Clapyeron equation) indicates that ice is actually a bit less dense than water.

was extremely hot and electromagnetism and the weak-interaction were fully unified. As the temperature cooled, a phase transition occurred that created these two different interactions.

**Structural Phase Transitions:** It is quite common in crystals to have phase transitions where above a certain temperature the crystal structure has one symmetry (say cubic) whereas below the temperature the structure has another symmetry (say tetragonal). One can also have a situation where the symmetry stays the same but there is nonetheless a sudden rearrangement of the atoms in the unit cell at a particular critical temperature.

**Liquid Crystal Transitions:** So called “liquid crystals” can display a huge range of phase transitions. In the figure we see two different phase transitions. At low temperature there is a phase transition from a true crystal to a so-called “nematic liquid crystal” where translational order is lost, but orientational order remains (i.e., all the sticks remain aligned, but are not periodically arranged). Then at higher temperature still there is a phase transition from the nematic to an isotropic liquid, where orientational order is lost.

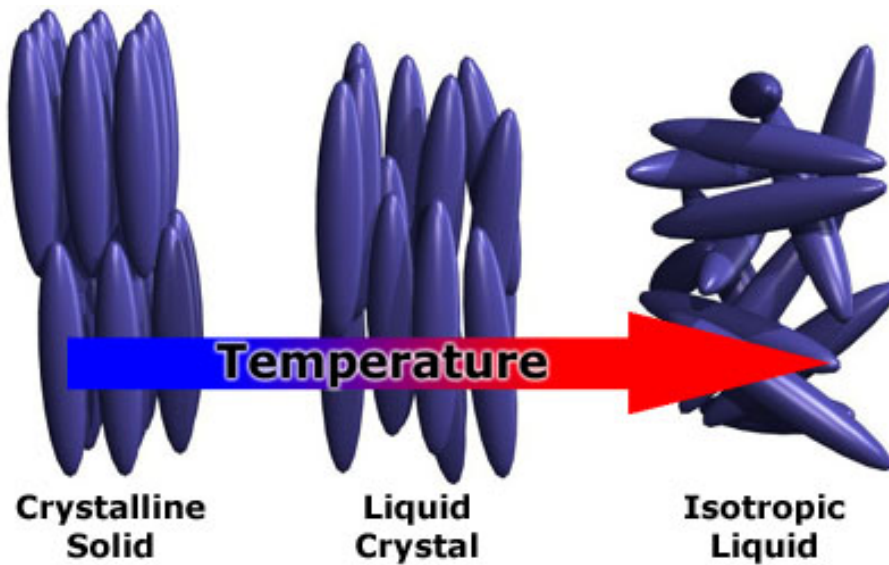


Figure 1.3: phase transitions in liquid crystals

**Phase Separation of Mixtures:** The so-called salad-dressing phase transition. Below a certain temperature two fluids (such as oil and vinegar) don’t mix, but above the temperature they do mix. (Actually, I suspect if you do this with a real salad dressing, they won’t mix at any temperature before the system boils, but nonetheless there are certainly plenty of cases of fluids that mix at high temperature but not at low temperature).

### 1.1.1 Nomenclature of Phase Transitions: First and Second Order

Paul Ehrenfest<sup>2</sup> tried to classify phase transitions in terms of singularities in the free energy of the system, or singularities of the derivatives of the free energy. Ehrenfest’s classification scheme has

<sup>2</sup>Ehrenfest was one of Boltzmann’s students, and one of the founding fathers of statistical mechanics in the early days. Like Boltzmann, despite being a genius (or perhaps because of it) he struggled with severe mental illness. He committed suicide at age 53, after shooting his younger son who had Down’s syndrome.

fallen into disfavor, but parts of his nomenclature remain. Note that different references do still disagree on the precise definition of some of these terms.

As we tune some parameter of the system (pressure, temperature, magnetic field) the free energies must always be continuous.

**First Order Phase Transition:** In this case a first derivative of the free energy is discontinuous at the phase transition point. Since derivatives of the free energy correspond to thermodynamic quantities, this means there is a jump in some measurable quantity. See for example the right hand side of Fig. 1.4. Often (but not always) there is a jump in the entropy, hence a latent heat associated with the phase transition. At a first order phase transition there may be two-phase coexistence.

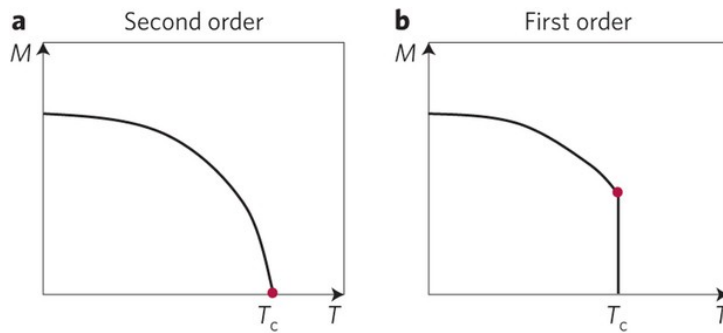


Figure 1.4: First and Second Order Phase Transition in a Ferromagnet

An example of a first order transition without latent heat (which, indeed, some references would object to it being called first order!) is the transition shown on the right hand side of Fig. 1.2. If you consider crossing the dark horizontal phase transition line from  $M > 0$  to  $M < 0$ , there is a jump in  $\mathbf{M}$  (it changes direction) but no change in  $|M|$  and also no latent heat.

**Second Order Phase Transition:** In this case there is a discontinuity in a higher order derivative of the free energy. There is no two-phase coexistence. We can think of this as the limit of a first order transition where the size of the jump in a parameter goes to zero. See the left hand side of Fig. 1.2.

In addition to these two categories, one should also be aware that we could have a “crossover” which is not a phase transition at all. For example, in Fig. 1.1, if we follow a path around the critical point from liquid to vapor, we have made a crossover, with no singularities in any derivatives of the free energy.

## 1.2 Why Do We Care So Much About Phase Transitions?

(Besides the fact that it is part of the syllabus?)

(1) **True Phase Transitions (singularities in the free energy) can only occur in the thermodynamic limit** – i.e., when there are an infinite number of particles in the system. As such, the phase transition is somehow the “ultimate” example of collective phenomena — how many objects act together to give new physics.

**(2) In order to really understand a phase of matter, you should start by studying the phase transitions.** This is perhaps not so obvious. If you want to understand how liquid water is different from ice, understanding the phase transitions between the two forces you to fully understand exactly how these two differ in a very deep way. The history of modern physics tells us that studying these transitions is really the best way to learn about the phases. (OK, not obvious, but true).

**(3) Phase transitions have universality.** Phases of matter are so diverse that it is hard to even find a place to start when studying them. Many of the properties of these phases are "non-generic" — that is, they are not shared by any other systems. For example, there are ferromagnets whose critical temperature is 51 Kelvin and others whose critical temperature is 72 Kelvin and so forth and so on. Some have spin 3/2, some have spin 5/2, and so on. However, the types of phase transitions you can have turn out to fall into a relatively small number of classes known as "universality classes" which all behave the same as each other, despite being extremely different underlying systems. Although we will start to uncover this idea a bit, a full understanding of universality requires learning the "renormalization group" which is taught in trinity term. (More about universality in the next section).

**(4) The mathematical structure** that we build for studying phase transitions (the renormalization group) turn out to be THE fundamental way we understand MOST of physics. Whether we are studying high energy physics, or low temperature physics, the renormalization group provides the most complete modern understanding. (Alas, we will not get to this in these five lectures!).

## 1.3 Universality and Critical Exponents

Let me try to give an example of the universality of phase transitions.

Consider two different ferromagnets, Ferrous Fluoride,  $\text{FeF}_2$  and Cobalt Chloride Hexahydrate  $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ . The first has critical temperature around 78 K where the second has critical temperature around 2K. The two materials have very different crystal structure. They have different spin-spin interactions. How similar could they be?

**Magnetization exponent** If you look very close to the critical point between ferro and paramagnetism, many things start to look the same for the two materials. For example, near to the critical point for  $T < T_c$ , we can write<sup>3</sup>

$$M(T) \sim |T - T_c|^\beta$$

by which we mean

$$M(T) = C |T - T_c|^\beta +$$

Things that are smaller than  $|T - T_c|^\beta$  in the limit of small  $T - T_c$

i.e., in this case meaning they go to zero even faster in this limit.

for some prefactor  $C$ . See for example, the left hand side of Fig. 1.4 to see this behavior. The exponent  $\beta$  is an example of what is known as a "critical exponent" meaning that it defines the scaling behavior very close to the critical point.

Although the two ferromagnetic substances mentioned above have different  $C$  constant out front, and different  $T_c$ , they have the same value of  $\beta \approx .31$  to within experimental resolution (indeed, it is suspected that the value of  $\beta$  is exactly the same for the two materials).

<sup>3</sup>Do not confuse  $\beta$  for inverse temperature! Hopefully it would never be tempting to do so.

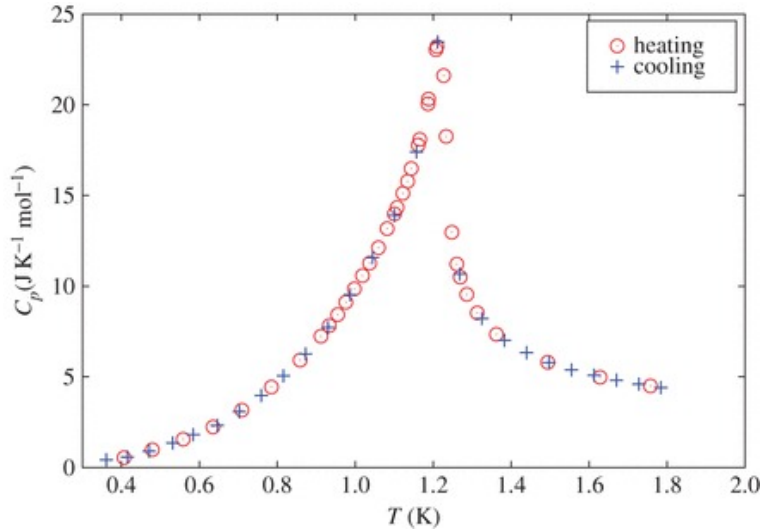


Figure 1.5: Specific heat of Ferromagnet near the transition temperature 1.2 K. Close to the phase transition we have  $C \sim |T - T_c|^{-\alpha}$ . (I stole the picture from the web, and I don't remember what the material is that is being measured in this picture. Sorry!)

**Heat capacity exponent** Another quantity we can examine is the specific heat of materials. For example, the specific heat of a particular magnet is shown near the ferro-para magnetic transition in Figure 1.5. Near the phase transition the the heat capacity diverges as

$$C(T) \sim \begin{cases} A_+(T - T_c)^{-\alpha_+} & T > T_c \\ A_-(T_c - T)^{-\alpha_-} & T < T_c \end{cases} \quad (1.1)$$

Again the symbol  $\sim$  means up to terms that are less important (in this case meaning they diverge less quickly than the leading term which we have written).

Given the general form written in Eq. 1.1, surprisingly it turns out that generally  $\alpha_+ = \alpha_-$  so we usually just call it  $\alpha$ , although  $A_+$  and  $A_-$  are usually different. Again,  $\alpha$  is known as a critical exponent (sometimes called the heat capacity exponent for obvious reasons).

As with the case of the magnetization above, we find some universality in the exponent. For example, for the two magnets we mentioned above Ferrous Fluoride,  $\text{FeF}_2$  and Cobalt Chloride Hexahydrate  $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ , the measured value of the exponent  $\alpha$  is the same in both cases  $\alpha \approx .11$  to within experimental precision.

There are many other critical exponents we can define as well.

**Susceptibility exponent:** For example, defining the magnetic susceptibility to an applied field  $H$

$$\chi = \lim_{H \rightarrow 0} \frac{\partial M}{\partial H}$$

(Note that  $M$  is nonzero below  $T_c$  but we can perfectly well define this susceptibility as the derivative nonetheless). Close to the critical point, we write

$$\chi \sim |T - T_c|^{-\gamma}$$

As with the heat capacity exponent, one might imagine that the exponent is different depending on whether you are above or below the critical temperature. In fact, it turns out that the exponent

is the same both above and below. As with the heat capacity case, the prefactor can differ depending on whether one is above or below  $T_c$ . For the two physical magnets we have discussed above  $\gamma \approx 1.23$ .

**another magnetization (order-parameter) exponent** Yet another critical exponent we can define is as follows. Imagine setting the temperature to precisely the critical temperature. We can then write

$$M(T = T_c, H) \sim H^{1/\delta}$$

where  $H$  is an applied magnetic field. The fact that  $\delta$  occurs downstairs in the exponent is just a definitional convention. For the two magnets discussed above we have  $\delta \approx 4.8$

**correnglation length exponent** A final important exponent that we will define depends on the spatial correlations in the material. If we are considering a system of spins, the magnetization  $M$  is related to  $\langle S_i \rangle$ . However, we can also consider correlations between spins some distance apart. Let us first consider the case where  $T > T_c$ . In this case it is useful to define

$$g(i, j) = \langle S_i S_j \rangle$$

This measures how correlated spin  $i$  and  $j$  are. In otherwords, if  $S_i$  is pointing up, how likely is it that  $S_j$  is also pointing up?. Another way to ask this is “how much does the spin  $S_i$  care about what the direction is of  $S_j$ ?”. At very high temperatures, we expect that the spins are fluctuatng independently so that  $g(i, j)$  will be close to zero for any  $i \neq j$ . However, for a material that is ferromagnetic, as temperature gets lower and we get closer to  $T_c$  we expect that spins will tend to point in the same direction as their neighbors, which means that  $g(i, j)$  will be nonzero if the position of  $i$  is close to the position of  $j$ . We generally expect that in the long distance limit, we should have<sup>4</sup>

$$g(i, j) \propto e^{-|\mathbf{r}_i - \mathbf{r}_j|/\xi} \quad (1.2)$$

where  $|\mathbf{r}_i - \mathbf{r}_j|$  is the physical distance between spins  $i$  and  $j$ , and  $\xi$  is known as the correlation length. Approaching  $T_c$  from above, the effects of the correlations get stronger and stronger (until they become infinite ranged when the system becomes a ferromagnet – the direction of all spins in the system are correlated in the ferromagnetic phase). We can write a relation

$$\xi \sim |T - T_c|^{-\nu} \quad (1.3)$$

indicating how this correlation length diverges. Crucially we note that the divergence of the correlation length tells us that all length scales are becoming correlated as we approach the critical point.<sup>5</sup>

Even below  $T_c$  there is a concept of a correlation length. Once we are below  $T_c$ , all of the spins in a ferromagnet are roughly aligned – hence giving infinite ranged correlations. However, if we look at the fluctuations of the spins around their average direction and magnitude we will see very similar effects to what we see above  $T_c$ . Spins will tend to fluctuate in the same directions as the spins that are nearby to them. Thus we more generally define

$$g(i, j) = \langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle$$

<sup>4</sup>If one is thinking about as system that is anisotropic, one might have different values of  $\xi$  depending on the orientation of the vector  $\mathbf{r}_i - \mathbf{r}_j$

<sup>5</sup>In one dimension, the system is not ferromagnetic for any temperature above  $T = 0$ , so we can think of the critical temperature as being  $T_c = 0$ . Using transfer matrix methods, it is a good exercise to calculate the correlation length as a function of temperature in 1d, and see that it does indeed diverge as one approaches  $T = 0$ . Is there a sensible exponent in this case?

For a uniform system this can be simplified to

$$g(i, j) = \langle S_i S_j \rangle - \langle S \rangle^2 = \langle (S_i - \langle S \rangle) (S_j - \langle S \rangle) \rangle$$

For spins which are far apart from each other  $g(i, j)$  will go to zero. Indeed, the correlations follow the same exponential form as in Eq. 1.2. Surprisingly, perhaps, the correlation length also diverges as we approach  $T_c$  from below, and Eq. 1.3 remains true. As in the case of the heat capacity exponent, the exponent  $\xi$  is the same both above and below  $T_c$ , although the prefactor will generally differ. For completeness we just comment that for both of the magnets we considered above  $\xi \approx .62$ .

### 1.3.1 Universality Beyond Simple Magnets (and the idea of an order parameter)

One might think "So what... some magnets seem to behave like each other". But in fact universality extends far beyond just magnets. Consider, for example, the critical points (temperature and pressure) of several fluids<sup>6</sup>.

Fluid	$T_c$ (K)	$P_c$ (MPa)
Argon	151	4.8
Xenon	290	5.8
Ethane	305	4.9

Although the critical temperatures and pressures are very different, the heat capacity shows universality at the transition. All three materials have

$$C_p \sim |T - T_c|^{-\alpha}$$

with the same feature that  $\alpha$  is the same both above and below the transition. More surprising still is that the measured value of  $\alpha$  is precisely the same as that measured for the magnet  $\alpha \approx .11$  (!).

One might wonder if there is an analog of some of the other exponents which don't have an obvious analogue in a fluid. For example, what is the analog of magnetization?

#### The idea of an Order Parameter (briefly)

The magnetization in a ferromagnet is zero above in one phase (paramagnetic phase) and nonzero in the other phase (ferromagnetic phase). We call such a quantity an "order parameter", as it keeps track of the new order that forms at the transition. In particular the existence of the nonzero magnetization breaks the symmetry of the paramagnetic phase (where up and down are equivalent) into the symmetry of the ferromagnetic phase (where the magnetization points only in one direction).

For a vapor-liquid transition, the order parameter is not so obvious — since the symmetry of the two phases are in fact the same (vapor-liquid transitions are among the hardest to understand!). Nonetheless, we can be brave and try to define a parameter that at least will go to zero at the critical point. Let us define

$$O = \rho - \rho_c$$

where  $\rho_c$  is the density right at the critical point. Rather surprisingly, we find that

$$O \sim |T - T_c|^\beta$$

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<sup>6</sup>Of course these numbers are approximations, the critical pressures and temperatures can be measured much more accurately



where  $\beta = .31$  *exactly the same as for the magnetic phase transitions we mentioned above!*

### Are all phase transitions exactly the same? (Spoiler: No)

Given that all of the critical points we have looked at so far seem to show identical behavior, we might be tempted to think that *all* phase transitions are identical. This is not true. Let us consider several other ferromagnet to paramagnet transitions.

Material	Type of Magnet	Crystal Structure	$T_c$ (K)
Fe (Iron)	Itinerant	FCC	1044
Ni (Nickel)	Itinerant	FCC	631
EuO	Local Moment	NaCl form	69
Sr <sub>2</sub> FeMoO <sub>6</sub>	Half-Metallic	tetragonal	415

Measurement of critical exponents for these compounds give markedly different results from those mentioned above. Instead of  $\beta = .31$  and  $\alpha = .11$  we obtain instead  $\beta = .36$  and  $\alpha = -.12$  for all of these materials (while the two possible values of  $\beta$  are close to each other, they are measurably different with some effort. The two values of  $\alpha$  have opposite sign and are easily distinguished).

### 1.3.2 Universality Classes and Symmetry

We divide all critical points into "universality classes". If two critical points are in the same universality class, they share all of the same critical exponents—for example, the ferromagnetic transitions of FeF<sub>2</sub>, and CoCl<sub>2</sub>·6H<sub>2</sub>O as well as the critical point of Argon liquid-vapor transition are all in the same universality class. Whereas Fe and Ni ferromagnetic transitions belong to a different universality class. Once we know which universality class a particular transition is in, we then know all of its critical exponents, and as a result we know an enormous amount about the details of the transition. There are relatively few such universality classes occurring in nature, so it behooves us to study them carefully.

A complete understanding of universality and universality classes requires the renormalization group, which we will not learn this term. (But you have an opportunity to learn next term!).

So why is it that FeF<sub>2</sub> ferromagnetic transition is in one class whereas Fe is in a different class? The answer turns out to be that they have different symmetries. You may recall two different simple models of magnets, the Ising model

$$\mathcal{H} = - \sum_{ij} J_{ij} S_i^z S_j^z$$

and the Heisenberg model

$$\mathcal{H} = - \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

FeF<sub>2</sub> is Ising-like whereas Fe is Heisenberg-like. This does not mean that Fe is precisely a Heisenberg model (it could have three or four spin interactions etc). What is crucial is that the Hamiltonian is left unchanged under any global rotation of all the spins in the system. For a Heisenberg-like model, the ordered state has all spins aligned, but it does not matter what direction the spins are pointing. On the other hand, FeF<sub>2</sub> is Ising-like. Again, this does not mean that it is precisely an Ising model. What is important is that the Hamiltonian is invariant under an inversion of all of the spins of the system ( $S_z \rightarrow -S_z$ ) but is not invariant under an arbitrary rotation. The key point here is that universality classes are defined by the symmetries of the system (as well as by the

dimension of space you are working in – for example, ferromagnets are quite different if they are restricted to be in 2 dimensions rather than in regular 3 dimensional space)! Once the symmetries (and the dimension of space) are determined, none of the details of the system matter if you are close enough to the critical point!

So you might ask why it is that the liquid-vapor critical point is in the Ising class along with  $\text{FeF}_2$ . This is a bit harder to understand. Imagine dividing up a physical system near the liquid-vapor transition into many small boxes. We declare each box to be filled either with liquid or vapor – and there is some tendency for neighboring boxes to be filled with the same state of matter. We realize that this is roughly equivalent to an Ising model – there are two possible states of each microscopic "box". While this seems like a rather rough analogy, since details don't matter close enough to a critical point, this rough analogy is enough to put the liquid-vapor transition in the Ising universality class.

## Chapter 2

# Warm Up: The Ising Model Mean Field Theory

In order to get warmed up in our study of phase transitions, it is useful to study one phase transition in some detail. The “hydrogen atom” of phase transitions is the Ising model — simple enough to work with, yet complex enough to show interesting behavior.

We consider spins  $\sigma_i$  on some lattice. The Ising Hamiltonian is

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - h \sum_i \sigma_i$$

Here the  $\langle i, j \rangle$  means we are summing over nearest neighbor pairs  $i, j$  with each pair counted exactly once. We are considering the ferromagnetic case so  $J > 0$  and  $h$  is the applied external magnetic field.<sup>1</sup>

Statistical mechanics problems often start by writing down a partition function from which we determine free energies and other thermodynamic quantities. So let us write

$$\begin{aligned} Z &= \sum_{\sigma_1=\pm 1} \sum_{\sigma_2=\pm 1} \dots \sum_{\sigma_N=\pm 1} e^{-\beta \mathcal{H}(\sigma_1, \dots, \sigma_N)} \\ &= \sum_{\{\sigma_i\}} e^{-\beta \mathcal{H}(\{\sigma_i\})} \end{aligned}$$

From this we would construct a free energy  $F = -k_B T \log Z$  and go from there. Note that actually performing this sum is exceedingly difficult in general<sup>2</sup>. However, it should be clear that the result, for any finite size system, (which is just a sum of finitely many exponentials) must be an analytic function of  $\beta$ ,  $h$  and  $J$ . As a result there cannot be any actual singularities or discontinuities in the free energy for any finite size system. We conclude singularities in a derivative of the free energy (which are the signature of phase transitions – see point 1 of section 1.2 ) only occur in the infinite system size limit!

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<sup>1</sup>Note that  $J$  and  $h$  both have dimensions of energy here. If you took B6 last year (or if you read The Oxford Solid State Basics – my favorite book!) we were very careful to keep track of factors of Bohr magneton and spin 1/2 if necessary. Here, to keep ourselves from notational nightmare, we will drop these factors, and assume you can figure out where to put them back in if you ever need to figure out what  $h$  is in units of Tesla.

<sup>2</sup>It can be done in 1d by transfer matrix method, and in 2d in the absence of magnetic field only. Amazingly just in the last few years certain critical exponents of the 3d Ising model have been calculated!

Since evaluating the partition function is too hard, we are going to have to make some approximations. Eventually the approximation we will use is a type of mean field theory.

## 2.1 Some standard thermodynamics and statistical mechanics

Although the following manipulations are standard in stat-mech and thermodynamics, it is worth reviewing them for comparison later.

To get ourselves prepared for this, let us rewrite our partition function

$$Z = \sum_m \sum_{\{\sigma_i\} | \sum_i \sigma_i = m} e^{-\beta H(\{\sigma_i\})}$$

Here what we have done is to divide up the full sum into a sum over all possible values of the total magnetic moment  $m$  which must be an integer, then each individual sum over the set of  $\sigma$ s are subject to the constraint that each individual sum adds up to  $m$ . We then define

$$e^{-\beta F(m)} = \sum_{\{\sigma_i\} | \sum_i \sigma_i = m} e^{-\beta H(\{\sigma_i\})}$$

and rewrite the partition function as

$$Z = \sum_m e^{-\beta F(m)}$$

where  $F$  is the free energy of the system with magnetic moment  $m$ . It is convenient now to change to magnetization  $M = m/V$  which is moment divided by volumen and also to consider free energy per volume  $f = F/V$ . We then can write

$$Z = \int dM e^{-\beta V f(M)}$$

with the assumption that for large enough volume, the magnetization becomes a continuous variable. The next step is a standard maneuver in statistical physics and thermodynamics. Note that the exponent has a large prefactor  $V$ , so to a good approximation, so the argument of the integral is extremely peaked around the point where  $f(M)$  reaches its minimum (so called steepest descent). Thus we have

$$Z \approx e^{-\beta V f(M_{min})}$$

or equivalently

$$\log Z = -\beta F(M_{min})$$

which is the thermodynamic definition of the free energy.

## 2.2 Bragg-Williams Approach

We now will be forced to make some mean-field approximations. The approach we will take is Bragg-Williams. It may look a bit familiar. Starting with

$$F = U - TS$$

we want to make some approximation for  $U$  and  $S$  which we cannot calculate exactly.

To estimate  $S$  we assume that all configurations with the same magnetization are equally likely. In this case, the entropy as a function of magnetization is just the log of the number of states with that magnetization. We write the magnetization  $m$  (here moment per site) as

$$m = \frac{N_{\uparrow} - N_{\downarrow}}{N} = \langle \sigma \rangle$$

which has a value between  $-1$  and  $1$ . The total number of up pointing spins is then

$$N_{\uparrow} = N \left( \frac{1+m}{2} \right)$$

and the total number of configurations with  $N_{\uparrow}$  up pointing spins is

$$\Omega = \binom{N}{N_{\uparrow}} = \frac{N!}{N_{\uparrow}!(N - N_{\uparrow})!}$$

For convenience, setting Boltzmann's constant to unity (which we will do frequently) we then have the entropy approximately given by  $S = \log \Omega$  and using Stirling's approximation we obtain

$$S/N \approx \ln 2 - \frac{1}{2}(1+m) \log(1+m) - \frac{1}{2}(1-m) \log(1-m)$$

Next, to obtain an estimate of the energy per site, we imagine replacing  $\sigma$  in the Hamiltonian on every site with  $m$  since  $\langle \sigma \rangle = m$ . We then obtain

$$U = -J \sum_{\langle i,j \rangle} m^2 - h \sum_i m$$

Defining  $z$  to be the coordination number (the number of neighbors each site has) we obtain

$$U/N = -\frac{Jzm^2}{2} - hm$$

Putting these together, the free energy per site is given by

$$\begin{aligned} f &= F/N = U/N - TS/N \\ &= -\frac{Jzm^2}{2} - hm - T \left[ \ln 2 - \frac{1}{2}(1+m) \log(1+m) - \frac{1}{2}(1-m) \log(1-m) \right] \end{aligned} \quad (2.1)$$

Extremizing the free energy with respect to  $m$  we obtain

$$\begin{aligned} 0 &= \frac{\partial f}{\partial m} \\ &= -Jmz - h - \frac{T}{2} \log \left( \frac{1+m}{1-m} \right) \end{aligned}$$

which, with a bit of algebra can be rewritten as

$$m = \tanh \left( \frac{Jmz + h}{T} \right)$$

This result is entirely the same as a Weiss mean field theory. One derives it by noting that a free spin in a field  $h_{eff}$  obtains a magnetization

$$m = \tanh(h_{eff}/T)$$

and then making a mean field approximation the effective field is given by

$$h_{eff} = Jmz + h$$

where the  $Jmz$  term is the effective field from the coupling to neighboring spins.

### Properties of the free energy

Now, instead of solving the self-consistency equations directly, it is quite useful to instead examine the properties of the free energy function in Eq. 2.1. Expanding for small values of  $m$ , we have

$$f = -T \log 2 - hm + \frac{m^2}{2}(T - Jz) + \frac{1}{12}Tm^4 + \dots \quad (2.2)$$

Let us restrict our attention for now to zero external field  $h = 0$ . Further, the term  $-T \log 2$  is a relatively uninteresting (albeit temperature dependent) constant, so we can just ignore it (putting it back should we ever need it – which we won't).

Truncating the expansion at order  $m^4$ , it is clear that there are two different possible behaviors depending on the sign of  $T - Jz$ . If  $T > Jz$  then the coefficient of both the quadratic and the quartic terms are positive. Then the free energy as a function of  $m$  is shaped like the left hand side of figure 2.1. In this case there is a single minimum at  $m = 0$ , which we identify as the paramagnetic phase. On the other hand for  $T < Jz$  then the quadratic term is negative, while the quartic term is positive. In this case, the curve looks like the right of Fig. 2.1, and the minimum of the free energy occurs at some nonzero value of the magnetization  $\pm m_0$ , which signals ferromagnetism. The fact that there are two possible solutions is simply the fact that the aligned spins can point either in the up or down direction. The transition between the two behaviors occurs<sup>3</sup> when the quadratic term changes signs, i.e., at  $T = T_c = Jz$ .

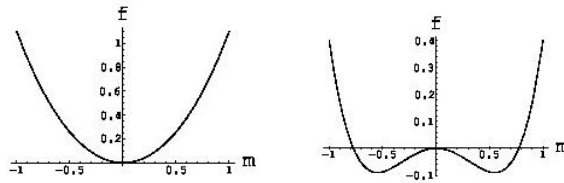


Figure 2.1: Free energies as a function of magnetization at different temperatures. (Left) At  $T > Jz$  the free energy has a unique minimum at  $m = 0$ . (Right) At  $T < Jz$  the free energy has to minimum at nonzero  $m$ . This signifies ferromagnetism. Note, the plots are both given with the  $T \log 2$  piece of the free energy dropped so that there is an extremum at  $f = 0$ .

<sup>3</sup>The actual critical temperature of the Ising model depends on the particular lattice and dimension we are considering (not just on the coordination number). For example, in 2D,  $T_c/(Jz)$  is approximately .57, .61, .51 on the square lattice, triangular lattice, and honeycomb respectively (exact solutions are known in these cases). In 3D,  $T_c/(Jz)$  is approximately .75 for the cubic lattice (numerically known).

### 2.2.1 Some Critical Exponents Calculated from Mean Field Theory

Although the Bragg-Williams approach is not exact (it is indeed equivalent to the Weiss Mean Field theory), we can nonetheless examine its predictions for critical exponents.

So long as we are close to the critical point, we can use the expansion, Eq. 2.2. To determine the value of the magnetization we extremize the free energy giving

$$0 = \frac{\partial f}{\partial m} = -h + m(T - T_c) + \frac{1}{3}Tm^3 \quad (2.3)$$

which we solve to find  $m$  near the critical point.

**order parameter exponent:** Recall the definition of the critical exponent  $\beta$ , which is given by  $m = |T - T_c|^\beta$  for  $T < T_c$ . Setting  $h = 0$  in Eq. 2.3 we obtain

$$0 = m(T - T_c) + \frac{1}{3}Tm^3$$

This equation has three roots. The first root is  $m = 0$  which is not a minimum (and thus is not the droid we are looking for). The other two roots are

$$m = \pm(3(T_c - T)/T)^{1/2} \quad (2.4)$$

Thus  $\beta = 1/2$ .

**another magnetization exponent** Recall the definition of the order parameter  $\delta$ , which is given by setting  $T = T_c$  and turning on the field  $h$  to get  $m \sim h^{1/\delta}$ . If we set,  $T = T_c$  in Eq. 2.3 we have

$$0 = \frac{\partial f}{\partial m} = -h + \frac{1}{3}Tm^3$$

giving

$$m = (3h/T)^{1/3}$$

hence  $\delta = 3$ .

**Susceptibility exponent:** Recall the susceptibility exponent  $\chi = \lim_{h \rightarrow 0} \partial m / \partial h \sim |T - T_c|^{-\gamma}$ . For  $T > T_c$ , our equation Eq. 2.3 is

$$0 = -h + m(T - T_c) + \dots$$

and since we are concerned with  $m$  and  $h$  limitingly small, we don't need to consider the additional terms. We thus obtain  $m = h(T - T_c)^{-1}$  or

$$\chi = |T - T_c|^{-1} \quad (2.5)$$

or the exponent  $\gamma = 1$ . On the other hand, for  $T < T_c$ , we have  $m > 0$  so we should keep the cubic term in Eq. 2.3. In the absence of  $h$  field, let us call the magnetization  $m_0$  which from Eq. 2.4 is given by  $m_0 = (3(T_c - T)/T)^{1/2}$ . Then we apply a small  $h$  and expand  $m(h) = m_0 + dm$ . Then our Eq. 2.3 becomes

$$\begin{aligned} 0 &= -h + (m_0 + dm)(T - T_c) + T\frac{1}{3}(m_0 + dm)^3 \\ &= -h + [m_0(T - T_c) + \frac{1}{3}Tm_0^3] + dm(T - T_c) + Tm_0^2 dm + \mathcal{O}(dm^2) \end{aligned}$$

Note that the term in the square bracket is precisely zero (see the definition of  $m_0$ ... this is not a coincidence, we have defined  $m_0$  to be such that the free energy would be at a minimum when  $h = 0$ !). The remaining terms then give

$$h = dm[(T - T_c) + Tm_0^2] = dm[(T - T_c) + 3(T_c - T)]$$

or the susceptibility  $\chi = \lim_{h \rightarrow 0} \partial m / \partial h = dm/h$  given by

$$\chi = \frac{1}{2}|T - T_c|^{-1} \quad (2.6)$$

So as expected, the exponent again is  $\gamma = 1$ , the same below  $T_c$  as above  $T_c$ . However, note that the prefactors are different in the two cases (compare Eq. 2.5 and Eq. 2.6).

**Heat Capacity Exponent:** Finally we turn to the heat capacity exponent, defined as  $c \sim |T - T_c|^{-\alpha}$ . First we must derive the heat capacity from the free energy. Note that our free energy has  $h$  as an independent variable, so we have  $df = -(S/N)dT - mdh$  we have  $S/N = -\partial f / \partial T|_h$ . Then heat capacity per particle is

$$c_{h=0} = -T \left. \frac{\partial(S/N)}{\partial T} \right|_{h=0} = -T \left. \frac{\partial^2 f}{\partial T^2} \right|_{h=0}$$

For  $T > T_c$  with  $h = 0$  we have  $m = 0$  in which case we have  $f(T) = -T \log 2$  and  $c_{h=0} = 0$ . Thus the exponent is  $\alpha = 0$ . On the other hand, for  $T < T_c$  and  $h = 0$  we have  $m$  given by Eq. 2.4. Plugging this into the free energy (and using  $T_c = Jz$ ), we obtain

$$\begin{aligned} f &= -T \log 2 - \frac{3}{2} \frac{(T - T_c)^2}{T} + \frac{9}{12} \frac{(T - T_c)^2}{T} \\ &= -T \log 2 - \frac{3}{4} \frac{(T - T_c)^2}{T} \end{aligned}$$

Differentiating to obtain

$$c_{h=0} = (3/2)(T_c/T)^2$$

which has no divergence or zero at  $T_c$  so the exponent is again  $\alpha = 0$ . Note however that the constant value which it approaches at  $T_c$  from below is different from the constant (0) that is approached from above.

**Correlation length exponent.** This exponent is much harder to calculate so we will defer its discussion to section 4.2 below.

The exponents we have calculated here are known (for obvious reasons) as "mean field" exponents. They are only approximate for most systems of physical interest (The exception to this being the superconducting phase transitions where they become extremely accurate when compared to most experiments). However, if we were to consider, for example, an Ising model in four dimensions, these mean field exponents actually become exact!



## Chapter 3

# Landau Theory of Phase Transitions

The Landau theory of Phase transitions, first described by the great (and very colorful) physicist Lev Landau in 1937 is a paradigm for describing both phases and the transitions between them. It is basically a generalization of the calculation we just did for the Ising model. The approach applies most generally in a regime near phase transitions where the order parameter is small. Thus, it can be applied for 2nd order transitions generally (which will be our main focus), and sometimes can be applied (with caution) to 1st order phase transitions, so long as the order parameter remains fairly small.

**Identify the Order Parameter** (or order parameters) which we often call  $\phi$  (although other notations are often used as well). Sometimes the order parameter may be a vector, or even a tensor. The order parameter typically goes to zero in the disordered phase and becomes nonzero in the ordered phase. For a second order transition, we would expect the order parameter to turn on continuously as we go through the transition.

For example, in the case of the Ising model which we considered above, we take the order parameter to be just the magnetization per site  $\phi = m$ . As in this case we should always think of the order parameter as being some sort of coarse grained or average of microscopic quantities.

**Expand the Free Energy** The next step is to write an expansion of the free energy (analogous to Eq. 2.2). We will generally write the free energy as a power series expansion in the order parameter  $\phi$  and also any external fields, such as  $h$ .

*Crucially* we will be able to determine what kinds of terms are allowed or not allowed in the expansion by examining the symmetries of the system. We write down all the terms that are allowed, but we do not generally try to calculate their precise values (that would require a real microscopic calculation of some sort – such as Bragg-Williams). The expansion coefficients (the prefactors of terms in the free energy expansion) are only allowed to vary smoothly with temperature.

**Minimize Free Energy and Calculate Exponents** The remaining step follows very similarly to what we did for the Ising model. We simply minimize the free energy and calculate anything we need from it. We will find that, in absence of precise knowledge of the expansion coefficients, we will not obtain precise expressions for the value of quantities such as the order

parameter, but we will nonetheless be able to extract exponents.

### 3.1 Example of Ising — Again

Instead of doing a "real" calculation to obtain the free energy (like we did in section 2.2, let us instead try to obtain the form of the free energy just by using the Landau approach — examine the symmetries and write down all allowed terms.

**In zero external field:** In the absence of any applied magnetic field, the free energy of the Ising model must be invariant under flipping all of the spins over. Just from this we know that

$$f(\phi, h = 0) = f(-\phi, h = 0)$$

So we can generally expand the free energy as<sup>1</sup>

$$f(\phi, h = 0) = \alpha_0(T) + \alpha_2(T) \phi^2 + \alpha_4(T) \phi^4 + \dots$$

We typically truncate the expansion at 4th order, and we assume that  $\alpha_4 > 0$  so that the free energy is bounded below. If we do run into a situation where  $\alpha_4 < 0$  then we must continue the expansion to 6th order such that the free energy does not go off to negative infinite energy!

As in the Ising case above, the behavior of this quartic function is different depending on whether  $\alpha_2$  is greater or less than zero. For  $\alpha_2 > 0$  the free energy as a function of  $\phi$  looks like the left of Fig. 2.1, and the minimum is at  $\phi = 0$  (meaning we are in the disordered phase). On the other hand for  $\alpha_2 < 0$  the free energy as a function of  $\phi$  looks like the right of Fig. 2.1 and there are two minima at some  $\pm\phi_0$  indicating an ordered phase. The transition between the two phases clearly occurs at  $\alpha_2 = 0$ . Since the expansion coefficients  $\alpha_n$  are assumed to be smooth functions of the temperature, we can expand  $\alpha_2$  around the critical temperature

$$\alpha_2(T) = a(T - T_c)$$

Given only this information, we can then extract exponents as we did above for the Ising case. For  $T < T_c$  we can solve for the minimum free energy

$$0 = \frac{\partial f}{\partial \phi} = 2a(T - T_c)\phi + 4\alpha_4\phi^3$$

which we solve for the minimum at

$$\phi = \left( \frac{a(T_c - T)}{2\alpha_4} \right)^{1/2} \sim |T - T_c|^{1/2} \quad (3.1)$$

meaning the exponent  $\beta = 1/2$ .

Similarly (and this calculation should look very familiar from the above Ising case) we can calculate the heat capacity. The free energy is generally given by

$$c = -T \frac{\partial^2 f}{\partial T^2}$$

---

<sup>1</sup>Note that there are various conventions that are used in different references. In particular, one might think it more natural to use  $\alpha_n \phi^n / n!$  written instead of  $\alpha_n \phi^n$ . Also it is often the case that one writes  $\alpha, \beta, \gamma$  instead of  $\alpha_0, \alpha_2, \alpha_4$ . This is perhaps the worst convention since  $\beta$  is used for inverse temperature, and in fact all of these symbols are also used for critical exponents as well! Finally, in some references the quantity  $\beta f$  is expanded rather than  $f$  (i.e., temperature is absorbed into the expansion coefficients).

above  $T_c$ , we have  $\phi = 0$  so the free energy is just  $f = \alpha_0(T)$ . Now while this may have a nonzero derivative and hence nonzero heat capacity, the assumption that the expansion coefficients are smooth tells us that there is no singularity in the derivatives and we conclude that the heat capacity exponent is  $\alpha = 0$ . For  $T < T_c$  we must plug the value of 3.1 into the free energy to obtain

$$f = \alpha_0(T) - \frac{a^2}{2\alpha_4(T)}(T - T_c)^2$$

compared to the  $T > T_c$  case, the second term is now extra. If we treat  $\alpha_4$  as being independent of temperature (which is often done as a shorthand<sup>2</sup>) we see that we obtain an extra term

$$\delta c = Ta^2/(2\alpha_4)$$

which has no singular behavior at  $T_c$  so that the critical exponent  $\alpha$  is again determined to be zero — although the value of the heat capacity jumps at  $T_c$ . Now if we are more careful, we will worry about treating the temperature dependence of  $\alpha_4(T)$ . However, it is clear that even if we include this, in our derivative we will not obtain any singularity<sup>3</sup> in the heat capacity at  $T_c$ .

**in finite external field:** Once an external field is applied we expect that the order parameter pointing up and down should give different free energies, so for  $h \neq 0$

$$f(\phi, h) \neq f(-\phi, h)$$

However, if we flip over both the spins (the order parameter) and the external field at the same time, the free energy should still remain the same

$$f(\phi, h) = f(-\phi, -h)$$

Thus we expand the free energy more generally as

$$\begin{aligned} f(\phi, h = 0) &= \alpha_0(T) + \alpha_2(T)\phi^2 + \alpha_4(T)\phi^4 + \dots \\ &\quad - h\phi - \alpha_{1,3}(T)h\phi^3 - \alpha_{3,1}(T)h^3\phi + \dots \end{aligned}$$

with the assumption that  $\alpha_2(T) = a(T - T_c)$ .

There are a few things to note about this free energy. First, we have set the coefficient of  $h\phi$  to unity. This is a convention for setting the magnitude of the order parameter (it defines what we call the order parameter!). Secondly, the other terms on the second line — we know they are in fact NOT present in the microscopic free energy that we derived for the Ising model (Eq. 2.2) above. However, these terms are not forbidden by symmetry, so in principle should be kept. Fortunately, they won't be important for any calculations that we will need to do.

Again, we simply follow the same procedure we used for the Ising case.

$$\frac{\partial f}{\partial \phi} = 0 = 2a(T - T_c)\phi + 4\alpha_4(T)\phi^3 + h + \dots \quad (3.2)$$

To calculate the critical exponent  $\delta$  we set  $T = T_c$  and then solve for  $\phi$  given small  $h$  to result in.

$$\phi = \left( \frac{h}{4\alpha_4} \right)^{1/3} \sim h^{1/\delta}$$

<sup>2</sup>From our above analysis of the Bragg Williams approximation for the Ising model, we might guess that  $\alpha_4$  is actually temperature independent, but this is just a result of the approximation we have used and might more generally not be so.

<sup>3</sup>This is so long as  $\alpha_4(s)$  is smooth and does not go through zero at  $T_c$ . However, we have already assumed that  $\alpha_4$  is positive, and furthermore if it does go through zero, there should be no reason that it does so exactly at the same point where  $\alpha_2$  goes through zero.

giving us, as above in the Ising case, the critical exponent  $\delta = 3$ . It is worth checking that the ... terms that we dropped from Eq. 3.2 don't matter at all.

Similarly, away from  $T_c$  we can calculate the susceptibility exponent (we won't belabor the point, since this is identical to the calculation of section 2.2.1 above) to obtain  $\gamma = 1$ . As with the heat capacity, the prefactor of the susceptibility is different depending on whether one approaches  $T_c$  from above or below.

**Summary of this Example:** The key point of this section is that in fact, we don't actually need any microscopic details in order to calculate exponents (at least at this Landau-theory-mean-field level). All we needed to know was the symmetry of the order parameter, that  $f(\phi, h) = f(-\phi, -h)$ . From there, a generic Taylor series expansion was all we needed, and we didn't even need to know much about the value of any of the expansion coefficients. One could have ferromagnets on any shaped lattice, with nearest neighbor interactions, with long range interaction, or any sort of microscopic physics, and still the same expansion pertains. Furthermore, we can translate this calculation to many other systems, such as ferroelectrics (where  $h$  is replaced by externally applied electric field) or even very different systems such as liquid-solid transitions, if one can argue that the necessary symmetry holds.

## 3.2 A Slightly More Complicated Example: Heisenberg Magnets (Briefly)

You may recall that definition of the Heisenberg model of a magnet, given by

$$H = - \sum_{\langle i,j \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

The key difference between this and the Ising model is that the Heisenberg Hamiltonian is rotationally invariant. The ground state of the model is to have all the spins aligned, but it doesn't matter in which direction they all line up.

We might again think of using the coarse-grained magnetization 3-vector  $\mathbf{M}$  as an order parameter. Since the model is invariant under rotation of all spins together, our order parameter expansion should only contain terms that are invariant under rotation. Rotation acts on the order parameter as

$$M_i \rightarrow \sum R_{ij} M_j$$

where  $R$  is a rotation matrix (I.e., an  $O(3)$  matrix, meaning it is a 3 dimensional real matrix and  $R^T R = R R^T = \mathbf{1}$ .)

What sort of expressions can we make from the order parameter  $\mathbf{M}$  (a vector) which are invariant under rotation? In fact, the only quantity you can make from a single vector that doesn't change under any rotation, is the vector's length (and then any function of the length as well). When writing down an expansion of the free energy, we should only have quantities that are analytic in  $\mathbf{M}$ , thus the expansion looks like

$$f = \alpha_0 + \alpha_2(T)(\mathbf{M} \cdot \mathbf{M}) + \alpha_4(T)(\mathbf{M} \cdot \mathbf{M})^2 + \dots$$

(Although terms like  $|\mathbf{M}|$  are rotationally invariant, they are not analytic, and therefore not allowed in an expansion. Thus we have only even powers of  $\mathbf{M}$ ).

We should expect much the same physics as in the Ising case. If  $\alpha_2 > 0$  then the lowest energy state is  $\mathbf{M} = 0$ , however, if  $\alpha_2 < 0$  then the minimum of the free energy occurs at a finite value of  $(\mathbf{M} \cdot \mathbf{M})$ . It is easy enough to calculate that exponents such as  $\beta$  and  $\alpha$  are the same for the Heisenberg magnets as they are for the Ising case.

### 3.3 Models with Less Symmetry

What happens if we have a free energy with less symmetry, perhaps where  $f(\phi) \neq f(-\phi)$ . We would then generally expect a free energy expansion with all powers of  $\phi$  in it. For example, we might have

$$f = \alpha_0 - h\phi + \alpha_2\phi^2 + \alpha_3\phi^3 + \alpha_4\phi^4 + \dots$$

where we assume  $\alpha_3 \neq 0$  (otherwise we would be back to the case considered above) and  $\alpha_4 > 0$  such that the free energy is bounded below for large  $\phi$ .

Let us imagine a case where we can set  $h = 0$  (say it is the external magnetic field) and for simplicity (and without loss of generality) let us assume  $\alpha_0 = 0$  as well. We now find the minimum of the free energy by

$$0 = df/d\phi = 2\alpha_2\phi + 3\alpha_3\phi^2 + 4\alpha_4\phi^3 \quad (3.3)$$

There is always one extremum of the free energy at  $\phi = 0$ , whose free energy is zero. For now, let us assume that  $\alpha_2 > 0$ . In this case, the extremum at  $\phi = 0$  is a local minimum of the free energy. There may additionally be two other extrema. If the roots of Eq. 3.3 are real. This happens if  $9\alpha_3^2 - 32\alpha_4\alpha_2 > 0$ . If there are additional extrema, one of these extrema will be a second local minimum and the other will be a local maximum. Now when two local minima exist, either of these two minima can be the global minimum – hence the global ground state.

Let us consider what happens as, for example,  $\alpha_2$  changes as a function of temperature. As shown in Fig. 3.3 one can see that the global minimum suddenly jumps between the two local minimum at some particular value of  $\alpha_2$ . This signals a first order transition as shown in the right of Fig. 1.4.

Calculating the value of  $\alpha_2$  where the first order transition occurs requires a bit of algebra. We want to have both  $df/d\phi = 0$  (because we want to be considering a minimum) and  $f = 0$  (because we want the minimum to have the same energy as the minimum at  $\phi = 0$ ), Thus we have

$$0 = \alpha_2\phi^2 + \alpha_3\phi^3 + \alpha_4\phi^4 \quad (3.4)$$

$$0 = 2\alpha_2\phi + 3\alpha_3\phi^2 + 4\alpha_4\phi^3 \quad (3.5)$$

Subtracting twice the first equation from the second and solving for  $\phi$  gives the solution

$$\phi = -\alpha_3/(2\alpha_4)$$

Plugging this back into Eq. 3.4 gives us

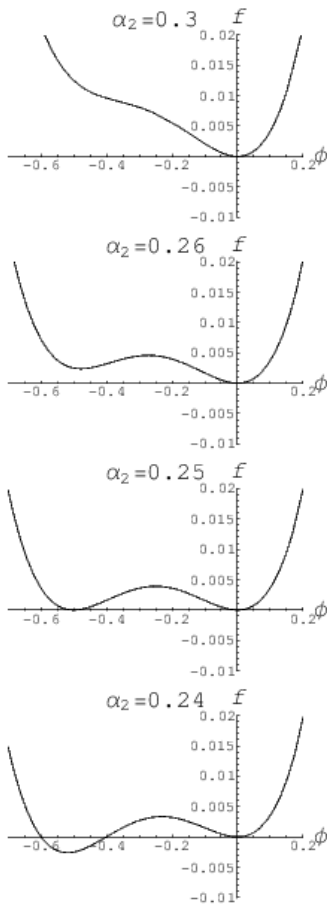
$$\alpha_2^{critical} = -\alpha_3^2/(4\alpha_4)$$

giving the critical value of  $\alpha_2$  where the first order transition occurs.

As with many first order transitions, it is possible to have hysteresis — where the system is stuck in a local minimum of the order parameter and does not manage to change to the global minimum. It is easy to determine the limits of  $\alpha_2$  for which one can have such so-called metastability. We only need to find out when the local minimum disappears. As mentioned above, the

local minimum away from  $\phi = 0$  does not exist for  $\alpha_2 > 9\alpha_3^2/(32\alpha_4)$ . And the minimum at  $\phi = 0$  does not exist once  $\alpha_2 < 0$ . Thus the limits of metastability are

$$0 < \alpha_2 < 9\alpha_3^2/(32\alpha_4)$$



Caption: As the value of the expansion parameter is changed, the shape of the free energy curve changes. These are plots of  $f = \alpha_2\phi^2 + \alpha_3\phi^3 + \alpha_4\phi^4$  with  $\alpha_3 = \alpha_4 = 1$  and  $\alpha_2$  varied between plots. For large  $\alpha_2 > 9\alpha_3^2/(32\alpha_4)$  there is only a single minimum in the free energy at  $\phi = 0$ . For smaller value of  $\alpha_2$  (bottom three plots) there is a second minimum at  $\alpha_2 \neq 0$ . For  $\alpha_2$  small enough (bottom plot), this second minimum at  $\phi \neq 0$  is the global minimum. At the critical value of  $\alpha_2 = \alpha_3^2/(4\alpha_4) = .25$  the ground state of  $\phi$  jumps from  $\phi = 0$  to  $\phi = -\alpha_3/(2\alpha_4) = -.5$  suddenly (plot second from bottom). This indicates a first order phase transition.

Figure 3.1:

One important note we should keep in mind. Our expansion of the free energy pre-supposes that the order parameter  $\phi$  is small. However, we have now used the expansion to describe what happens for finite values of  $\phi$ . This needs to be used with much caution. We should not expect to get any quantitatively accurate result unless the system is tuned so that  $\phi$  remains small enough that the higher terms in the expansion can be neglected.

### 3.3.1 An example where we get first order behavior: The $Z_3$ Potts model

Let us define the  $Z_3$  Potts model<sup>4</sup>. This is a natural generalization of the Ising model where the "spin" variable on each site can take one of *three* possible values  $\sigma_i = 1, 2, 3$ . We should think of these values as being like a vector that can point in three directions each at 120 degrees from the other two. We can write a Hamiltonian for this model as

$$H = -J \sum_{\langle i,j \rangle} \delta_{\sigma_i, \sigma_j} - h \sum_i \delta_{\sigma_i, 1}$$

and we assume  $J > 0$  and  $h \geq 0$ . The first term gives a lower energy if each site is aligned with (has the same  $\sigma$  value) as its neighbor. The second term gives a lower energy to sites that are pointing in the  $\sigma = 1$  direction (rather than 2 or 3)<sup>5</sup> Note that we have very intentionally maintained a symmetry between the 2 and 3 direction, which are equivalently disfavored.

It is fairly clear what this system will do at high and low temperatures. At high temperature, in the absence of  $h$ , all three directions will be equally populated – and due to the high temperature there will be a great deal of fluctuation of the value of the spin on each site. At very low temperature, however, the spins will align with their neighbors, and eventually at low enough temperature the spin value of the entire system will be aligned. If we add a small field  $h$  in a particular direction (here in the "1" direction) this will assure that the spins all align pointing in the "1" direction at low temperature, rather than in one of the other two directions.

We now need to construct an appropriate order parameter for the system. If there are  $N$  sites in the system and  $N_\alpha$  pointing in the  $\alpha$  direction ( $\alpha = 1, 2, 3$ ), we can write

$$\begin{aligned} m_1 &= (1/3 + x) = N_1/N \\ m_2 = m_3 &= (1/3 - x/2) = N_2/N = N_3/N \end{aligned}$$

where we have used the fact that we expect the symmetry between the 2 and 3 direction to remain at any temperature. Here  $x = 0$  corresponds to the high temperature situation where all of the spins directions are equally populated. Conversely the maximum value of  $x$  is  $x = 2/3$  where all of the spins point in the 1 direction. It is crucial to note that there is now *no symmetry* enforcing  $f(x) = f(-x)$ . These are physically different situations. Because of this we should expect there should be a cubic term in the free energy expansion, and hence we should have a first order transition between the ordered ("ferromagnetic") and disordered ("paramagnetic") phases. We can draw this conclusion only based on the symmetry of the model! Indeed, it is found to be true that the  $Z_3$  Potts model has a first order transition in three dimensions (we will see later in chapter 5 why Landau theory tends to fail in lower dimensions).

#### Bragg Williams approach to $Z_3$ Potts

We can check our assumption about the form of the free energy of the  $Z_3$  Potts model by doing a Bragg-Williams style calculation — simply following the same scheme as we did for the

<sup>4</sup>Renfrey Potts worked on this model for his DPhil at Oxford in 1951 . It was suggested to him by his supervisor Cyril Domb.

<sup>5</sup>There are some nice physical realizations of the  $Z_3$  Potts model. One nice example is the material  $\text{DyAl}_2$ . This is a ferromagnet with cubic anisotropy — the spin wants to point along one of the x,y or z coordinate axes of a cubic lattice (along  $[0, 0, \pm 1]$ ,  $[0, \pm 1, 0]$ ,  $[\pm 1, 0, 0]$ ). Now if we add a strong magnetic field along the diagonal of the cube (along the  $[111]$  direction) then only the  $[0, 0, +1]$ ,  $[0, +1, 0]$ ,  $[+1, 0, 0]$  directions are favored. This gives three possible directions, all equally favored. By adding an additional small field  $h$  in one of the three coordinate axis directions, we can favor one direction over the other two.

Ising case. Assuming all states equally occupied, the entropy of the system is

$$S = \log \left( \frac{N!}{N_1!N_2!N_3!} \right)$$

which we expand using stirling's approximation. The energy per site is

$$U/N = \frac{-Jz}{2}(m_1^2 + m_2^2 + m_3^2) - hm_1$$

where  $z$  is the coordination number. Substituting in our expressions into  $F = U - TS$  we obtain

$$f = \alpha_0 - hx + x^2 \left( \frac{9T}{4} - \frac{3Jz}{4} \right) - x^3 \frac{9T}{8} + x^4 \frac{81T}{32} + \dots$$

and we see the cubic terms as predicted<sup>6</sup>.

### 3.3.2 Nematic and Isotropic Liquid Crystals

One final example we will consider is the nematic to isotropic liquid crystal transition. As shown in Fig. 1.3 the molecules in this system are long rod-like objects. In the so-called nematic phase (center of Fig. 1.3) the rods are mostly oriented in the same direction, although the position of the rods are random, like a liquid. In the isotropic phase (right of Fig. 1.3) the orientation of the rods is also completely random.

The challenge here is to come up with an appropriate order parameter to describe this transition (an order parameter that will be nonzero in the nematic phase and zero in the disordered phase). We might be tempted to consider a unit vector  $\mathbf{v}$  which points in the direction of the rod. We might then imagine using a locally averaged vector  $\langle \mathbf{v} \rangle$  as our order parameter, which points in the (on average) in the direction of the rods in some given area of the system. Unfortunately, this is not the correct order parameter. The reason is that flipping the rods over (turning them 180 degrees) gives back exactly the same physical situation, but turns over the order parameter vector. In other words, we need an order parameter that is invariant under  $\mathbf{v} \rightarrow -\mathbf{v}$ .

A better idea is to try to construct an order parameter from the vector  $\mathbf{v}$  which would be invariant under this inversion. Let us consider a tensor order parameter

$$\tilde{Q}_{ij} = \langle v_i v_j \rangle$$

Being quadratic in the vector  $\mathbf{v}$  this is indeed invariant under inversion of the vector. This is almost correct, but still not quite right. The problem here is that this order parameter would be nonzero even in the isotropic phase when all of the rods point randomly. To see this, let us integrate this order parameter over all possible directions (we are imagining an isotropic system where the rods point equally in all directions). We then calculate

$$\tilde{Q}_{ij} = \frac{1}{4\pi} \int d\mathbf{v} v_i v_j$$

---

<sup>6</sup>We can also use this result to predict the critical temperature of the  $Z_3$  potts model. Solving  $\alpha_2 = \alpha_3^2/(4\alpha_4)$  we obtain  $T_c = 6Jz/17 \approx .353Jz$ . For a 3d system on cubic lattice (coordination number 6) numerical simulation gives the exact result  $T_c \approx .303$ . Here we have ignored the caution that our expansion is only valid for small values of the order parameter! We can check in retrospect that higher order terms in the expansion are not \*too\* large. If we are not happy with this, we can do a full solution of the Bragg-Williams approximation without expanding the free energy, where we obtain  $T_c \approx .361Jz$  (try this!).



where the integration is over all directions the unit vector can point. Writing

$$\begin{aligned} v_z &= \cos \theta \\ v_x &= \sin \theta \cos \phi \\ v_y &= \sin \theta \sin \phi \end{aligned}$$

it is easy to check that<sup>7</sup>

$$\tilde{Q}_{ij} = \frac{1}{4\pi} \int_0^{2\pi} d\phi \int_0^\pi d\theta \sin \theta v_i v_j = \delta_{ij}/3$$

Note that the trace of  $\tilde{Q}$  is unity. It is easy to see that this must be the case independent of the direction the  $\mathbf{v}$  points since

$$\sum_i Q_{ii} = \sum_i \langle v_i^2 \rangle = \langle |\mathbf{v}|^2 \rangle = 1$$

Given this we can now construct an order parameter which is both symmetric under inversion, and goes to zero in the isotropic phase

$$Q_{ij} = \langle v_i v_j \rangle - \frac{1}{3} \delta_{ij}$$

Independent of the direction  $\mathbf{v}$  points, this is a symmetric traceless rank 2 tensor.

Note that we can choose the measure  $Q_{ij}$  in any basis we wish (i.e., we can point the  $x, y, z$  axes in any directions so long as  $x, y, z$  are orthogonal). We might as well choose to point them in a direction for which  $Q$  is a diagonal matrix — let us choose the local direction of our  $z$ -axis to conveniently point in the direction that the rods point. In this case we can generically write

$$Q = \begin{pmatrix} -\frac{1}{3}S + T & 0 & 0 \\ 0 & -\frac{1}{3}S - T & 0 \\ 0 & 0 & \frac{2}{3}S \end{pmatrix} \quad (3.6)$$

$$Q_{ij} = S(n_i n_j - \delta_{ij}/3) + T(m_i m_j - l_i l_j) \quad (3.7)$$

here,  $\mathbf{n}$  is the director field of the rod, and  $\mathbf{m}$  is perpendicular to  $\mathbf{n}$  with  $\mathbf{l} = \mathbf{n} \times \mathbf{m}$  (all three of these vectors being unit vectors).

When  $T = 0$  the system is known as a “uni-axial nematic”. This means that one axis is special (the director field, or axis that the rods are aligned along). When  $T \neq 0$ , which is known as a “biaxial nematic”, this means that there is another special axis  $\mathbf{m}$  which is perpendicular to the first director field. For rod-like molecules it is somewhat hard to imagine how one could obtain a second special axis — although this can happen if an external field is applied. In fact all rod-like liquid crystals are uniaxial nematics — the molecule may even lack a rotational symmetry along its axis and nonetheless one almost always obtains  $T = 0$ . (It required a bit of a search to find a biaxial nematic!)

For now, let us remain general. We now aim to write the most general free energy consistent with the symmetries of our system. What are the symmetries? Well, like the Heisenberg model we discussed above, the free energy must be invariant under rotations. We thus need to think about

<sup>7</sup>In fact it is easy to see this without even doing the integration! By symmetry  $\langle v_i v_j \rangle = 0$  unless  $i = j$ . Then  $\langle v_i^2 \rangle = C$  should be the same for  $i = x, y, z$ . Finally  $3C = \langle v_x^2 + v_y^2 + v_z^2 \rangle = \langle |\mathbf{v}|^2 \rangle = 1$  giving us  $Q_{ij} = \delta_{ij}/3$  directly.

how the order parameter  $Q$  transforms under rotations. Recall that  $\mathbf{v}$  is a vector so under rotation it transforms as

$$v_i \rightarrow \sum_j R_{ij} v_j$$

where  $R$  is a 3-dimensional rotation matrix  $RR^T = R^T R = \mathbf{1}$ . Since  $Q$  is made from vectors  $\mathbf{v}$  we should have

$$Q_{ij} \rightarrow \sum_{pq} R_{ip} R_{jq} Q_{pq}$$

or equivalently

$$Q \rightarrow RQR^T$$

Next we need to ask what quantities we can create from powers of  $Q$  which remain invariant under these rotations? Clearly we can generatly construct

$$\text{Tr}[Q^n]$$

for any  $n \geq 2$  (for  $n = 1$  this quantity vanishes since  $Q$  is defined to be traceless – Check that all of the rotation matrices cancel out in the product of many  $Q$ 's in a row). In fact this is all we construct that is invariant under rotation.<sup>8</sup> So generically, we expect to write our free energy as

$$f = \alpha_0 + a_2 \text{Tr}[Q^2] + a_3 \text{Tr}[Q^3] + a_{4,1} \text{Tr}[Q^4] + a_{4,2} \text{Tr}[Q^2]^2 + \dots \quad (3.8)$$

If we now specialize to the case of the uniaxial nematic, we then have

$$f = \alpha_0 + \alpha_2 S^2 + \alpha_3 S^3 + \alpha_4 S^4 + \dots$$

Seeing that there is a cubic term here, we expect that the transition from isotropic to nematic should be first order. Indeed, this is what is observed experimentally!

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<sup>8</sup>Furthermore, most of the quantities we have constructed are redundant. Only the first two quantities

$$\text{Tr}[Q^2] \quad \text{and} \quad \text{Tr}[Q^3]$$

are actually independent. All higher powers can be made up from combinations of these. This is not surprising being that  $Q$  can be expressed in terms of only two independent parameters  $S$  and  $T$ . So for example the two fourth order terms in Eq. 3.8 are actually proportional to each other  $\text{Tr}[Q^2]^2 = 2\text{Tr}[Q^4]$  – so there is really only one term at fourth order.

S



## Chapter 4

# Ginzburg-Landau Theory

Landau theory is terrific for understanding phase transitions globally, but it gives us no information about the spatial structure of physical systems. For example, in our favorite ferromagnetic Ising model, we expect that as we go to lower temperatures — even above the phase transition — the spins will become correlated with each other at longer and longer distances. At very high temperature a spin is almost entirely independent of all its neighbors. As we cool it down, it starts to become correlated with its near neighbors (i.e., it tends to point in the same direction as its neighbor) and then at lower temperature still it becomes correlated with very large groups of spins until we hit the phase transition where the direction of all of the spins in the system are then correlated with each other. As we discussed in section 1.3 the correlation length of the spins diverges as we approach the phase transition — but this is something that we have not been able to describe with simple Landau theory since it does not describe anything about the spatial structure of the system.

In order to address such issues, we are going to upgrade our Landau theory to something that is spatially dependent. Instead of writing the free energy  $F(M)$  as a function of the magnetization, we will write the free energy as a *functional* of the magnetization, which itself is a function of position. So we are instead writing<sup>1</sup>

$$F[M(\mathbf{x})]$$

### 4.0.3 Interlude: Justification of Ginzburg-Landau Idea

There are various formal approaches to deriving the form of the Ginzburg-Landau functional. For our purposes it suffices to give a rough justification of what we are essentially doing. For simplicity we again return to the case of the Ising model for inspiration.

Let us imagine dividing our system into  $N$  small cells (or boxes) — we want the cells to be large on a microscopic scale, but still very small on compared to lengths of interest (i.e., we want to be able to take averages within the cells). We can then divide our partition function into

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<sup>1</sup>Often we will use the notation of a general order parameter  $\phi$  but here, since we are back to thinking about magnets as an example, it is probably useful to talk in the language of magnetization.

sums over the  $N$  individual cells

$$\begin{aligned} Z &= \sum_{\sigma} e^{-\beta H\{\sigma\}} \\ &= \sum_{M_1} \sum_{M_2} \dots \sum_{M_N} \sum_{\{\sigma \mid \sum_{i \text{ in cell } k} \sigma_i = M_k\}} e^{-\beta H\{\sigma\}} \end{aligned}$$

The last sum here is restricted such that the sum over all the spins in box  $k$  is equal to the magnetization  $M_k$ . We then define a free energy *given* the values of the magnetizations in the different boxes

$$Z = \sum_{M_1} \sum_{M_2} \dots \sum_{M_N} e^{-\beta F[M_1, M_2, \dots, M_N]} \rightarrow \int dM_1 dM_2 \dots dM_N e^{-\beta F[M_1, M_2, \dots, M_N]} \quad (4.1)$$

Compare this construction to what we did in section 2.1 above. In each case we are defining a free energy which is a function of a magnetization – the only difference is that here our free energy is a function of the free energy in all of the different cells. Here the sum over cells has been converted into integrals (since the cells are large enough that the averaged magnetization is essentially continuous) and then the integration over all of the small cells is essentially what we mean by a *functional integral*

$$Z = \int \mathcal{D}M(\mathbf{x}) e^{-\beta F[M(\mathbf{x})]} \quad (4.2)$$

where we can describe the free energy functional as an integral over a local energy functional

$$F[M(\mathbf{x})] = \int d\mathbf{x} f[M(\mathbf{x})]$$

Here we have made an assumption that the free energy functional is essentially local — an assumption that is usually true if there are no long ranged interactions and we think of the microscopic boxes as being larger than the interaction length scale.

Functional integrals of the form of Eq. 4.2 are familiar from the path integral formulation of quantum mechanics<sup>2</sup>. If the idea of the functional integral is frightening though, we can always fall back on the idea that we are just doing integrals over the magnetization in all of the cells in the system as given by Eq. 4.1.

## 4.1 The Ginzburg Landau Functional Form

As with Landau theory, our general strategy will be to guess the form of the free energy functional without doing any real calculation. We expect that the Ginzburg Landau functional should be of the form

$$\begin{aligned} f &= f_0 + \alpha_2 M^2 + \alpha_4 M^4 + \dots \\ &\quad + \kappa |\nabla M|^2 + \dots \end{aligned} \quad (4.3)$$

<sup>2</sup>You may recall the Feynman propagator expression for single particle motion

$$\langle x_{final} | e^{-\beta H} | x_{init} \rangle = \int \mathcal{D}x(\tau) e^{-S_E[x(\tau)]/\hbar}$$

where  $S_E$  is the euclidean action.

The first line is familiar from (spatially independent) Landau theory in zero external field that we have previously discussed. The second term gives the functional some spatial dependence.

Let us try to justify this form. As above, we want to expand the free energy in powers of  $M$ . In addition here we want to expand the free energy in increasing powers of derivatives. The justification for this is that we expect spatial changes to be rather long length scales, so increasing number of derivatives will be increasingly small. In more detail our functional needs to be a scalar, so no terms linear in  $\nabla M$  can enter<sup>3</sup>. We also expect the ground state should be the case where  $M$  is spatially uniform — and this is true so long as  $\kappa$  is positive.

One way to understand this  $|\nabla M|^2$  term is to see that it is disfavoring any domain walls in the system. If  $M$  is pointing in some particular direction, then it should want to point the same direction nearby. (Perhaps this is even more obviously correct in the case of Heisenberg magnets where we can imagine  $\mathbf{M}$  rotating just a little bit from place to place).

We note that in a phase where  $\langle M \rangle$  is nonzero, it often makes more sense to define an order parameter as the expansion of  $M$  around its average

$$\phi(\mathbf{x}) = M(\mathbf{x}) - \langle M \rangle$$

so that  $\phi$  remains a small parameter. For example, in the ferromagnetic phase of the Ising model ( $\alpha_2 < 0$ ), we have

$$\langle M \rangle = \sqrt{\frac{-\alpha_2}{2\alpha_4}}$$

so writing  $M(x) = \phi + \langle M \rangle$  and plugging back into the free energy functional we obtain

$$\begin{aligned} f &= \alpha_0 + \alpha_2(\phi + \langle M \rangle)^2 + \alpha_4(\phi + \langle M \rangle)^4 + \dots + \kappa|\nabla\phi|^2 + \dots \\ &= \alpha_0 - 2\alpha_2\phi^2 + \dots + \kappa|\nabla\phi|^2 + \dots \end{aligned} \quad (4.4)$$

Note that here  $\alpha_2 < 0$  so the form of this functional is similar<sup>4</sup> to the form of the the free energy above  $T_c$  where we expand  $M$  around zero (Eq. 4.3).

## 4.2 Correlation Functions

OK, let us now try to determine something about the spatial structure of the system. In particular we will be interested in the correlation functions. This is a hard calculation, but it the result is pretty important so it is worth going through the details.

We are generally interested in correlations of the form

$$G(\mathbf{x}, \mathbf{x}') = \langle \phi(\mathbf{x})\phi(\mathbf{x}') \rangle$$

By this we mean something slightly different above versus below  $T_c$ . Above  $T_c$  we mean

$$G(\mathbf{x}, \mathbf{x}') = \langle M(\mathbf{x})M(\mathbf{x}') \rangle$$

and below  $T_c$  we mean

$$G(\mathbf{x}, \mathbf{x}') = \langle [M(\mathbf{x}) - \langle M \rangle][M(\mathbf{x}') - \langle M \rangle] \rangle = \langle M(\mathbf{x})M(\mathbf{x}') \rangle - \langle M \rangle^2$$

<sup>3</sup>If we applied a external field of some sort, it might be possible to construct scalar terms  $\mathbf{h} \cdot \nabla M$ .

<sup>4</sup>Actually below  $T_c$  there is a cubic term in the free energy because there is no symmetry around  $\phi = 0$ , since we are expanding around some nonzero magnetization anyway. This cubic term does not cause trouble since we are already (by definition) in a ferromagnetic phase, it does not effect any phase transition.

In either case, we will be working with essentially the same free energy (either Eq. 4.3 or 4.4). In fact, we will only need these free energies to quadratic order, so they are of identical form. Let us write the general form that we will work with

$$f = \alpha\phi(\mathbf{x})^2 + \kappa|\nabla\phi(\mathbf{x})|^2 - h(\mathbf{x})\phi(\mathbf{x})$$

where we have dropped the constant term (it is uninteresting) and higher order terms as well (for  $T < T_c$  we have  $\alpha = -2\alpha_2$  and  $T > T_c$  we have  $\alpha = \alpha_2$ ). We have also added back in an external field  $h$ , which we will eventually set to zero, but is useful here to use as a "source term" or generating term.

We thus write our partition function as

$$Z = \int \mathcal{D}\phi(\mathbf{x}) e^{-\beta \int \mathbf{d}\mathbf{x} [\alpha\phi^2 + \kappa|\nabla\phi|^2 - h\phi]}$$

and we want to calculate the correlation function

$$\begin{aligned} G(\mathbf{x}_1, \mathbf{x}_2) = \langle \phi(\mathbf{x}_1)\phi(\mathbf{x}_2) \rangle &= \frac{1}{Z} \int \mathcal{D}\phi(\mathbf{x}) \phi(\mathbf{x}_1)\phi(\mathbf{x}_2) e^{-\beta \int \mathbf{d}\mathbf{x} [\alpha\phi^2 + \kappa|\nabla\phi|^2 - h\phi]} \\ &= \frac{\delta^2 \log Z}{\delta h(\mathbf{x}_1)\delta h(\mathbf{x}_2)} \end{aligned}$$

where these derivatives are now *functional* derivatives<sup>5</sup>.

To evaluate our functional integral, it is useful to convert to Fourier space. Let us define the Fourier transform

$$\begin{aligned} \phi(\mathbf{x}) &= \frac{1}{V} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}} \phi_{\mathbf{k}} \\ \phi_{\mathbf{k}} &= \int \mathbf{d}^D\mathbf{x} e^{i\mathbf{k}\cdot\mathbf{x}} \phi(\mathbf{x}) = \phi_{-\mathbf{k}}^* \end{aligned}$$

where the last equality comes from the fact that  $\phi(\mathbf{x})$  is real. We will use similar definitions for any other quantity we want to Fourier transform.

Now let us write the free energy (the exponent of the exponential) in terms of these fourier modes

$$\begin{aligned} \beta F &= \beta \int \mathbf{d}\mathbf{x} [\alpha\phi^2 + \kappa|\nabla\phi|^2 - h\phi] \\ &= \frac{1}{V} \sum_{\mathbf{k}} \beta [(\alpha + \kappa|\mathbf{k}|^2)|\phi_{\mathbf{k}}|^2 - h_{\mathbf{k}}\phi_{-\mathbf{k}}] \end{aligned}$$

Which is a version of Parseval's theorem.

We can now convert the functional integral into something more familiar

$$\int \mathcal{D}\phi(\mathbf{x}) = \prod_{\mathbf{k}} \int d\phi_{\mathbf{k}}$$

Recall that the point of the functional integral is to integrate over all possible values of the function at all points in space (see Eq. 4.1). Here we will achieve the same thing by integrating over all

<sup>5</sup>These may sound scary but are no more difficult than regular derivatives!



possible functions in Fourier space (since any function in real space corresponds to a function in Fourier space). Here it is conceptually somewhat simpler since there is no arbitrary division of space into cells — the Fourier modes are naturally discrete (a discrete set of possible  $\mathbf{k}$  values).

We are now just about in a position to evaluate the path integral. First it is useful to "complete the square" in the free energy. Defining

$$\tilde{\phi}_{\mathbf{k}} = \phi_{\mathbf{k}} - \frac{h_{\mathbf{k}}}{\alpha + \kappa|\mathbf{k}|^2}$$

Note that the Jacobian for this transformation is trivial so that

$$\int \mathcal{D}\phi(\mathbf{x}) = \int \mathcal{D}\tilde{\phi}(\mathbf{x})$$

In terms of this new variable we have we then have

$$\begin{aligned} \beta F &= \frac{1}{V} \sum_{\mathbf{k}} \beta [(\alpha + \kappa|\mathbf{k}|^2)|\phi_{\mathbf{k}}|^2 - h_{\mathbf{k}}\phi_{-\mathbf{k}}] \\ &= \frac{1}{V} \sum_{\mathbf{k}} \beta \left[ (\alpha + \kappa|\mathbf{k}|^2)|\tilde{\phi}_{\mathbf{k}}|^2 - \frac{|h_{\mathbf{k}}|^2}{(\alpha + \kappa|\mathbf{k}|^2)} \right] \end{aligned}$$

Giving us

$$Z = \left[ \int \mathcal{D}\tilde{\phi}(\mathbf{x}) e^{-\frac{\beta}{V} \sum_{\mathbf{k}} (\alpha + \kappa|\mathbf{k}|^2)|\tilde{\phi}_{\mathbf{k}}|^2} \right] e^{-\frac{\beta}{V} \sum_{\mathbf{k}} \frac{h_{\mathbf{k}}h_{-\mathbf{k}}}{2(\alpha + \kappa|\mathbf{k}|^2)}}$$

The term in brackets gives just an overall constant which we will call  $\mathcal{N}$ . Admittedly, this is an important constant since it determines the free energy when one includes fluctuation corrections. The term of interest here is the term outside of the brackets, we thus have

$$\begin{aligned} Z &= \mathcal{N} e^{-\frac{\beta}{V} \sum_{\mathbf{k}} \frac{h_{\mathbf{k}}h_{-\mathbf{k}}}{2(\alpha + \kappa|\mathbf{k}|^2)}} \\ &= \mathcal{N} e^{-\frac{1}{2} \int \mathbf{d}\mathbf{x} \int \mathbf{d}\mathbf{y} h(\mathbf{x})\mathcal{G}(\mathbf{x}-\mathbf{y})h(\mathbf{y})} \end{aligned}$$

where

$$\mathcal{G}(\mathbf{x}) = \beta \int \frac{\mathbf{d}\mathbf{k}}{(2\pi)^D} \frac{e^{-i\mathbf{k}\cdot\mathbf{x}}}{(\alpha + \kappa|\mathbf{k}|^2)}$$

Now recall that we are interested in the correlation function

$$G(\mathbf{x}_1, \mathbf{x}_2) = \langle \phi(\mathbf{x}_1)\phi(\mathbf{x}_2) \rangle = \frac{\delta^2 \log Z}{\delta h(\mathbf{x}_1)\delta h(\mathbf{x}_2)}$$

taking the derivatives we see<sup>6</sup>

$$G(\mathbf{x}_1, \mathbf{x}_2) = \mathcal{G}(\mathbf{x}_1 - \mathbf{x}_2)$$

<sup>6</sup>Quite generally if we have a free energy (without external field) of the form

$$F \sim \sum_{\mathbf{k}} s(k)|\phi_{\mathbf{k}}|^2$$

we will have a correlation function

$$\langle \phi_{\mathbf{k}}\phi_{\mathbf{k}'} \rangle \sim \delta_{\mathbf{k}+\mathbf{k}'} s(k)^{-1}$$

This huge shortcut is essentially a version of the equipartition theorem. This gives immediately that

$$\langle \phi(x)\phi(0) \rangle \sim \int \frac{\mathbf{d}\mathbf{k}}{(2\pi)^D} e^{-i\mathbf{k}\cdot\mathbf{x}} s(k)^{-1}$$

At exactly  $T_c$  we have  $\alpha = 0$  in which case our integral is just<sup>7</sup>

$$\mathcal{G}(x) \sim \int d^D k \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{|k|^2} \sim \frac{1}{|x|^{D-2}} \quad (4.5)$$

for  $D > 2$  and the integral goes as  $\log|x|$  in  $D = 2$ . The power-law behavior shows us that at the critical point, all length scales are important. The precise value of this power law (yet another critical exponent!) gives us the so-called "naive scaling dimension" of the field  $\phi$  at the critical point. Just by dimension counting, if the dimension of a field  $\phi$  is

$$[\phi] = x^{(D-2)/2}$$

we might expect that a correlation function of two  $\phi$  fields would vary as given in Eq. 4.5. (In fact this is only a mean field hand-waving argument and it falls apart when examined more carefully. Nonetheless, the terminology is useful).

At  $T \neq T_c$  we have a much harder *nasty integral* to do (which we will defer for just a moment). The result, however, is that<sup>8</sup>

$$\mathcal{G}(x) \sim e^{-x\sqrt{\alpha/\kappa}} \quad (4.6)$$

meaning that the correlation length is

$$\xi = \sqrt{\kappa/\alpha(T)}$$

with  $\alpha = a(T - T_c)$  above  $T_c$  and  $\alpha = 2a(T_c - T)$  below  $T_c$  as discussed above, either way we have

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

or a critical exponent  $\nu = 1/2$ .

### 4.2.1 Nasty Integrals

Finally we attack the above mentioned *nasty integral*. First, we set  $\tilde{\alpha} = \alpha/\kappa$  so that we have

$$\mathcal{G}(\mathbf{x}) = \int d^D k \frac{e^{-i\mathbf{k}\cdot\mathbf{x}}}{|\mathbf{k}|^2 + \tilde{\alpha}}$$

This function doesn't care what direction  $\mathbf{x}$  is in, so let us write

$$\mathbf{x} = (x_1, x_2, \dots, x_D) = (x, 0, \dots, 0, 0)$$

and

$$\mathbf{k} = (k_1, k_2, \dots, k_D) = (k_1, \mathbf{k}_\perp)$$

where  $\mathbf{k}_\perp$  is a  $D - 1$  dimensional vector. We then have

$$\mathcal{G}(x) = \int d^{D-1} k_\perp \left[ \int dk_1 \frac{e^{-ik_1 x}}{k_1^2 + |\mathbf{k}_\perp|^2 + \tilde{\alpha}} \right]$$

<sup>7</sup>If this result isn't obvious, try rescaling the integral by defining  $x' = vx$  and  $k' = k/v$ . Note also that for small  $x$  one strictly speaking should impose a cutoff on the  $k$  integral at large  $k$  which represents the inverse of the lattice spacing.

<sup>8</sup>There is a powerlaw  $x^{-(D-1)/2}$  prefactor which we ignore for the moment.

The integral in the brackets can be done most easily by method of contours, to give<sup>9</sup>

$$\mathcal{G}(x) \sim \int d^{D-1}k_{\perp} \frac{e^{-x\sqrt{|\mathbf{k}_{\perp}|^2 + \tilde{\alpha}}}}{\sqrt{|\mathbf{k}_{\perp}|^2 + \tilde{\alpha}}}$$

Now going to radial coordinates we have

$$\mathcal{G}(x) \sim \int_0^{\infty} dk k^{D-2} \frac{e^{-x\sqrt{k^2 + \tilde{\alpha}}}}{\sqrt{k^2 + \tilde{\alpha}}}$$

This can be approximated accurately by steepest descents (for the limit where  $x$  is large). So we write this as

$$\mathcal{G}(x) \sim \int_0^{\infty} dk e^{-f(k)}$$

where

$$f(k) = x\sqrt{\tilde{\alpha} + k^2} - (D-2)\log k + \log \sqrt{\tilde{\alpha} + k^2}$$

For large  $x$  the maximum of this function occurs at the position

$$k_{min}^2 \approx \frac{D-2}{x} \sqrt{\tilde{\alpha}}$$

Thus the value of the integral is roughly<sup>10</sup>

$$\mathcal{G}(x) \sim e^{-f(x_{min})} \sim e^{-x\sqrt{\tilde{\alpha}}}$$

implying that

$$\xi \sim \sqrt{\tilde{\alpha}}$$

as claimed.

---

<sup>9</sup>Perhaps easier is to do the inverse Fourier transform  $\int dx e^{ikx} e^{-x/b} \sim 1/(k^2 + b^2)$ .

<sup>10</sup>Being more careful there is, as mentioned in a footnote above, a prefactor proportional to  $x^{-(D-1)/2}$ . If you are interested in trying this as a fun exercise, you have to actually do the gaussian integration to get this right.



# Chapter 5

## Upper and Lower Critical Dimensions

The Landau approach to mean field theory is both simple and powerful, but we may wonder when (if ever!) it is accurate, and further whether it even makes sense at all!<sup>1</sup>

### 5.1 When is Mean Field Theory Valid?

Considering the mean field approximations that we have made we need to understand what has been left out. Perhaps this is easiest when we think in terms of Weiss (or Bragg-Williams) mean field theory. Here, we have averaged some microscopic quantity to make some sort of coarse-grained order parameter. For example, in the case of the Ising mean field theory, we replace  $\sigma_i$  with  $\langle \sigma_i \rangle = m = \phi$  which we use as the order parameter. What this leaves out is fluctuations around this average value – i.e., not all sites have exactly the average value of the magnetization. Some have more, some have less. The question we need to ask is whether these fluctuations matter or not. Hopefully, at least in some cases, near the critical point, where physics becomes "universal" we will be able to argue that these fluctuations can be thrown away.

Ginzburg came up with a criterion for determining when mean field theory is valid. We must have

$$\text{Free Energy Associated with Fluctuations} \ll \text{Mean Field Free Energy} \quad (5.1)$$

This seems sensible enough. We need the part that we discard in mean field theory (the left hand side) to be much less than the part we keep (the right).

Let us try to determine the size of the terms in Eq. 5.1. Assuming an expansion for, say, the Ising model, on the right, the mean field energy is simple to calculate. We have

$$F_{\text{mean-field}}/V \sim \alpha_2 \phi^2 + \alpha_4 \phi^4$$

where  $\alpha_2 \sim (T - T_c)$ . Minimizing the free energy, for  $T < T_c$  we obtain (as we have many times before now)  $\phi_{\text{min}}^2 = -\alpha_2/(2\alpha_4)$ , which we plug back into the free energy to obtain

$$F_{\text{mean-field}}/V \sim \alpha_2^2/(4\alpha_4) \sim (T - T_c)^2$$

---

<sup>1</sup>Spoiler alert: Yes, it makes sense — at least sometimes!

On the left side of Eq. 5.1 we need to estimate the fluctuations in free energy. Near the critical point we should think of regions of size  $\xi$  all fluctuating as a large block (recall that  $\xi$  is the length over which spins are correlated). If we have a large block fluctuating as a single large-spin we should estimate that it has a total fluctuation energy of order  $k_b T$ . Thus the energy density associated with fluctuations is

$$F_{fluctuation}/V \sim k_b T / \xi^D \sim |T - T_c|^{D/2}$$

where we have used our calculation of the correlation length

$$\xi \sim |T - T_c|^{-1/2} \quad (5.2)$$

Thus the criterion Eq. 5.1 that allows us to neglect fluctuations becomes

$$|T - T_c|^{D/2} \ll |T - T_c|^2$$

which is obviously satisfied close enough to the critical point for

$$D > 4.$$

Indeed, it turns out that the critical exponents we derive from Landau theory are actually exact in  $D > 4$ . We say that  $D = 4$  is the *upper critical dimension*.

### 5.1.1 Some Comments on Upper Critical Dimension

- It should be understood that we have done this derivation only for a particular Landau expansion (the expansion appropriate for the Ising model — where we have quadratic and quartic terms, but no cubic terms). If the Landau expansion is different (for example, at a tricritical point where there is no quartic term in the expansion) then we will find that the upper critical dimension can change as well.
- For the “Ising” universality class (the calculation we have just done), the critical exponents, are the mean field exponents only in  $D \geq 4$ . For  $D < 4$  the critical exponents of the Ising universality class are different from what one calculates in mean-field theory.
- Amazingly enough, for the superconducting transition<sup>2</sup>, most experiments typically measure mean field exponents even in  $D = 3$  despite the fact that the upper critical dimension is  $D = 4$ . This behavior can be understood by looking back at Eq. 5.1 more carefully. It will remain true that the fluctuations (the left hand side of Eq. 5.1) will scale as  $|T - T_c|^{D/2}$ , and it will also be true that the right hand side will scale as  $|T - T_c|^2$ . So *close enough* to  $T_c$ , the left hand side will be smaller only for  $D > 4$ . However, as it turns out, in most superconductors, the prefactor in Eq. 5.2 is huge, so that fluctuations per unit volume will remain tiny unless  $|T - T_c|$  is tiny. Thus, Eq. 5.1 will remain satisfied (and hence mean-field behavior will remain valid) unless one can control the temperature extremely precisely to get  $T$  to be exceptionally close to  $T_c$  where one can see that mean field theory does indeed fail, as predicted by the Ginzburg criterion.

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<sup>2</sup>As we will see below, the Ginzburg Landau expansion for superconductors will have a quadratic and a quartic term, so the calculation of upper critical dimension will look the same as for the Ising model that we just did.

## 5.2 Spontaneous Symmetry Breaking and Goldstone Modes

### 5.2.1 Symmetry Breaking

The general rule of 2nd order phase transitions in Landau theory is that the ordered phase breaks a symmetry of the disordered state<sup>3</sup>. For example, in the Ising model, there is a symmetry of the system, that the up and down directions are equivalent — in the disordered phase, there is nothing to distinguish the two directions. However, in the ordered phase, the net magnetization must choose to point in either the up or in the down direction — it doesn't matter which one, but one direction must be chosen. As we cool the system below the critical temperature, one of the two directions will be chosen — we say that the direction is chosen "spontaneously", or we say that the symmetry is broken spontaneously.

In the Ising model, the broken symmetry is *discrete* — meaning there are a countable number of equivalent ground states (in this case there are two — magnetization pointing up and magnetization pointing down).

For the Heisenberg model, the magnetization vector  $\mathbf{M}$  can point in any direction — it is a *continuous* symmetry — meaning that there are an infinite number of possible equivalent ground states<sup>4</sup>.

Just to give another example, consider freezing of a liquid into a solid. The liquid has both translational and rotational symmetry, whereas the solid has neither. These symmetries have been broken by the structure of the solid crystal. The orientation and position of the crystal lattice has been chosen arbitrarily — symmetry has been broken spontaneously.

Crucially note that whenever symmetry is broken spontaneously — when a ground state is chosen arbitrarily — changing the choice of ground state should cost no energy. For example, for the Heisenberg model the ground state



and the ground state



must have the same energy.

### 5.2.2 Goldstone Modes

In cases where a continuous symmetry is broken, we expect to be able to have the system reorient slowly in space with very low energy cost. Locally one is in a ground state with all spins locally aligned, but as one moves over long distances, the direction of magnetization changes a little bit. In the language of our Ginzburg-Landau theory, one should only pay the gradient energy  $\kappa|\nabla\mathbf{M}|^2$ ,

<sup>3</sup>There are exceptions! — such as the liquid-gas critical point, liquid and gas have the same symmetries!

<sup>4</sup>More mathematically, we speak of the *symmetry group* of the disordered phase — which in the Ising case is  $Z_2$  corresponding to exchanging ups with downs, whereas in the Heisenberg case is  $SO(3)$ , corresponding to continuous rotations of all spins.

and if the change occurs over a large enough distance scale, the energy cost of reorienting the spins is extremely low.

A more precise statement of this physics is known as *Goldstone's Theorem*, which we paraphrase as follows:

If the Hamiltonian (or free energy or Lagrangian) is finite ranged, and if a continuous symmetry is spontaneously broken, then there exist gapless (or “massless”) excitations associated with the local reorientation of the broken symmetry.

**Comments:**

- The massless excitations are known as *(Nambu)-Goldstone bosons*.
- If the symmetry is explicitly broken weakly (say, for example, a small external magnetic field is added to the Heisenberg model thus picking out one particular direction) then the Goldstone bosons become finite energy (“gapped” or “massive”).
- In theories with *gauge symmetry* the situation is different. Goldstone bosons can get “eaten” by a gauge boson to develop a mass.

Some examples of Goldstone modes are the long wavelength spin waves in a Heisenberg model (as we have been discussing, see Fig. 5.1) or the acoustic phonons in a crystal lattice (recall that the symmetry of the translational position of the atoms in a crystal is spontaneously broken when the system freezes from a liquid).



Figure 5.1: The long wavelength goldstone mode of a Heisenberg ferromagnet. In each location the spins are very close to being exactly aligned with their neighbors – hence the energy of this excitation is extremely low.

### 5.3 $O(n)$ model and the Mermin-Wagner Theorem

Let us consider a generalized Heisenberg ferromagnet. We imagine a system where the spin is a  $n$ -dimensional vector  $\mathbf{S}$  of fixed length (the dimension of the physical space can be anything). This is generally known as the  $O(n)$  model since the symmetry group is  $O(n)$  — meaning the rotations of  $n$ -dimensional space.

- $n = 1$ . In this case,  $\mathbf{S}$  is simply a scalar of fixed magnitude that points either up or down – it is equivalent to the Ising model. There is no continuous symmetry and therefore no Goldstone mode.
- $n = 2$ . Here  $\mathbf{S}$  is a 2-vector of fixed length that lives in a plane. It is known as the *XY-model* and it turns out (as we will see below) to be relevant for superconductor and superfluids. There is a continuous symmetry associated with rotations of the spins in the XY-plane, hence there is a Goldstone mode.
- $n = 3$ . This is just the regular Heisenberg model that we’ve been discussing above (hence a Goldstone mode) where  $\mathbf{S}$  is a 3-vector of fixed length.



In all of these cases, we can write the Ginzburg-Landau free energy per unit volume as

$$f = \alpha_0 + \alpha_2 |\mathbf{M}|^2 + \alpha_4 |\mathbf{M}|^4 + \dots \\ + \kappa |\nabla \mathbf{M}|^2 + \dots$$

where  $\mathbf{M}$  is the order parameter (coarse-grained average spin) and where by the term with coefficient  $\kappa$  we mean

$$\kappa \sum_{i=1}^d \sum_{j=1}^n \left| \frac{\partial M_j}{\partial x_i} \right|^2$$

The ground state has uniform  $\mathbf{M}$  (costing no gradient energy). Minimizing the free energy with respect to  $\mathbf{M}$  we obtain (as we have many times before)

$$|\mathbf{M}|^2 = \alpha_2 / (2\alpha_4)$$

for  $\alpha_2 < 0$  (i.e.,  $T < T_c$ ) and  $\mathbf{M} = \mathbf{0}$  for  $T > T_c$ . In the former case, when  $|\mathbf{M}|^2 \neq 0$  we have spontaneous symmetry breaking, as the vector  $\mathbf{M}$  has to choose some direction to point in.

For definiteness, let us consider the case of  $n = 2$ , i.e., the XY-model. Here, the free energy as a function of  $\mathbf{M}$  has a mexican hat shape (see figure 5.2). The symmetry breaking is quite similar to that of the Ising model, except that in the XY-model there is now a continuum of directions that  $\mathbf{M}$  can choose to point in. Our objective here is to consider the effect of the Goldstone mode. In other words, we hope to consider the effects of fluctuations near the rim of the Mexican hat.

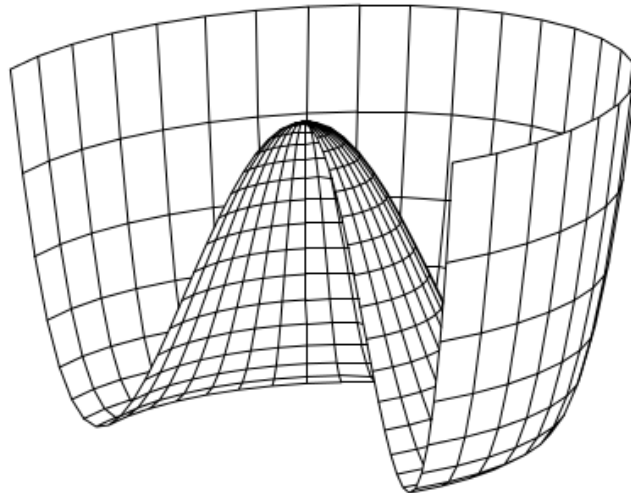


Figure 5.2: A mexican hat potential. Free energy is vertical versus the order parameter  $\mathbf{M}$  horizontally.

It is convenient to represent  $\mathbf{M}$  in complex notation  $M = Me^{i\theta}$  where  $M$  is real. The free energy can then be rewritten as

$$f = \alpha_0 + \alpha_2 M^2 + \alpha_4 M^4 + \dots \\ + \kappa |\nabla M|^2 + \kappa M^2 |\nabla \theta|^2 + \dots$$

Assuming that  $\alpha_2 < 0$ , and symmetry is spontaneously broken. We can define

$$M = M_0 + \delta M$$

where  $M_0^2 = \alpha_2/(2\alpha_4)$  is the value of  $M$  at the minimum of the mexican hat. In terms of this parameter, we can rewrite the free energy as

$$\begin{aligned} f &= f_M + f_\theta \\ f_M &= \tilde{\alpha}_0 - 2\alpha_2(\delta M)^2 + \kappa|\nabla(\delta M)|^2 + \dots \\ f_\theta &= \kappa M_0^2|\nabla\theta|^2 + \dots \end{aligned}$$

Note that the term  $-2\alpha_2$  is overall positive. We will drop all higher order terms represented here by  $\dots$

We can now write the partition function as a functional integral over the  $\delta M$  and the  $\theta$  degrees of freedom.

$$\begin{aligned} Z &= \int \mathcal{D}(\delta M(\mathbf{x})) \int \mathcal{D}\theta(\mathbf{x}) e^{-\beta \int \mathbf{d}\mathbf{x} f(\delta M(\mathbf{x}), \theta(\mathbf{x}))} \\ &= \int \mathcal{D}(\delta M(\mathbf{x})) e^{-\beta \int \mathbf{d}\mathbf{x} f_M(\delta M(\mathbf{x}))} \int \mathcal{D}\theta(\mathbf{x}) e^{-\beta M_0^2 \int \mathbf{d}\mathbf{x} |\nabla\theta(\mathbf{x})|^2} \end{aligned}$$

The first functional integral is quite similar to one that we have evaluated previously (See section 4.2). We obtain

$$\langle \delta M(\mathbf{x}) \delta M(\mathbf{y}) \rangle \sim \int \mathbf{d}\mathbf{k} \frac{e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}}{-2\alpha_2 + |\mathbf{k}|^2 \kappa} \sim e^{-|\mathbf{x}-\mathbf{y}|/\xi}$$

where

$$\xi = \sqrt{\kappa/(-2\alpha_2)}$$

The functional integral over  $\theta$  is somewhat similar. Strictly speaking there is a complication from the fact that  $\theta$  is only defined modulo  $2\pi$ , so we cannot treat it as a simple scalar field. However, if we assume (for now) that the fluctuations in  $\theta$  are not too large (much less than  $2\pi$ ) then we can treat it as a simple scalar field — and the calculation becomes similar to other functional integrals we have done.

We thus first assume that  $\theta$  is globally ordered, and arbitrarily (for simplicity) assume that the average direction is  $\langle \theta \rangle = 0$ . We then use the same approach as above to calculate that<sup>5</sup>

$$\langle \theta(\mathbf{x}) \theta(0) \rangle \sim \int \mathbf{d}\mathbf{k} \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{|\mathbf{k}|^2} \quad (5.3)$$

The denominator here has only the  $|\mathbf{k}|^2$  term since the free energy  $f_\theta$  at quadratic order has no  $\theta^2$  term. Performing the integral exactly analogous to how we did it before in Eq. 4.5, we obtain

$$\langle \theta(\mathbf{x}) \theta(0) \rangle \sim \frac{1}{|\mathbf{x}|^{D-2}}$$

We see that there is a change in behavior between  $D > 2$  and  $D < 2$ . (For  $D = 2$  this is the marginal dimension and the correlation function is proportional to  $\log|\mathbf{x} - \mathbf{y}|$ ).

<sup>5</sup>For very small  $\mathbf{x}$  one has to keep track of the fact that this integral has a cutoff for large  $\mathbf{k}$  corresponding to the inverse of the microscopic lattice spacing. Thus, the given expression in Eq. 5.3 is not valid for very small  $\mathbf{x}$ .

For  $D > 2$  the correlations decay over increasing distance (the short distance behavior is controlled by the large  $\mathbf{k}$  cutoff rather than being divergent). This means that over long length scales the angle  $\theta$  always comes back to the same zero value. Deviations from this value are small and decay as a power-law back to the "mean" value.

However, for  $D < 2$ , the integral becomes divergent at large  $\mathbf{x}$ , which is not sensible. This is a real divergence and signals a breakdown in our calculation. Indeed, the problem is that for  $D < 2$  the fluctuations in phase are sufficiently severe that globally nonzero  $\langle \mathbf{M} \rangle$  cannot exist.

The lack of order is an example of the so-called "Mermin-Wagner Theorem" which states that there can be no spontaneous breaking of a continuous symmetry in  $D \leq 2$ . The marginal dimension  $D = 2$  is known as the "lower critical dimension" and it needs to be treated very carefully (which we will not do in this course).

## 5.4 Summary

A nice summary is given by the following diagram<sup>6</sup>

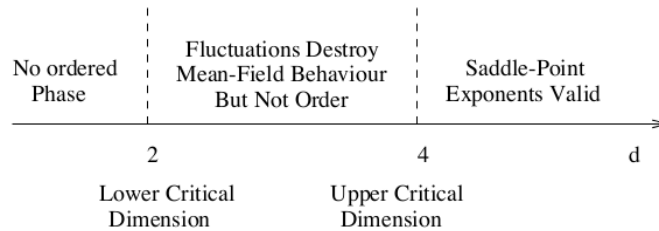


Figure 5.3: Upper and Lower Critical Dimensions for  $O(n)$  models. Above the upper critical dimension  $d > 4$ , mean field exponents (so called "saddle point exponents" are valid". In between the upper and lower critical dimensions, mean field is inaccurate, but there is order. Below the lower critical dimension (here  $d < 2$ ) order is destroyed by fluctuations.

<sup>6</sup>This diagram is stolen from Ben Simons — no relation, except that he is a friend of mine, and I am therefore assuming that neither he nor his publisher will not sue me for stealing his diagram.



## Chapter 6

# A Super Example: BEC and Bose Superfluids

Let us consider an interacting system of bosons. We will study such systems in some depth later in the term (C6 students are invited, but not required, to attend later).

Recall from last term when we have weakly interacting bosons, in the "superfluid" phase, we have

$$\langle c_{\mathbf{k}=\mathbf{0}} \rangle = \sqrt{N_0}$$

where here  $c_{\mathbf{k}=\mathbf{0}}$  is the annihilation operator for the zero momentum mode.

Several things to note here. First, we are working in a "grand" canonical ensemble where the wavefunction is a superposition of different particle numbers. Second, this operator takes a nonzero value below some critical condensation temperature — which signals the onset of superfluidity or bose condensation. Third, in the case of noninteracting bosons at  $T = 0$ , we have  $N_0$  being the total number of particles in the system. Finally, because the expectation of this operator is macroscopic with small fluctuations, it can often be treated as simply a complex number rather than an operator (this will be justified later in the term). Thus we have, for example,

$$\langle c_{\mathbf{k}=\mathbf{0}}^\dagger c_{\mathbf{k}=\mathbf{0}} \rangle = N_0$$

Note that

$$\langle c_{\mathbf{k}=\mathbf{0}} \rangle = e^{i\theta} \sqrt{N_0}$$

is also possible, and all values of  $\theta$  are physically equivalent to each other by redefinition of the phases of orbitals. No physical observable would be able to detect the globally defined value of  $\theta$  so long as no particles are added or removed from the system (so long as number is conserved).

Let us now make the usual fourier transform of operators

$$\hat{\psi}(\mathbf{x}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{p}} e^{i\mathbf{p}\cdot\mathbf{x}} c_{\mathbf{p}}$$

(occasionally written instead as  $c(\mathbf{x})$ ). Note that these operators obey canonical commutations

$$[\hat{\psi}(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{x}')] = \delta(\mathbf{x} - \mathbf{x}')$$

The expectation of these operators are then

$$\langle \hat{\psi}(\mathbf{x}) \rangle = e^{i\theta} \sqrt{N_0/V}$$

with  $N_0/V = n_0$  being the density of "condensed" bosons, and it is the full density for noninteracting bosons at  $T = 0$ .

Given this as input, it is quite reasonable to guess at the appropriate ginzburg-landau free energy functional for this bose system

$$f = \alpha_0 + \alpha_2 \psi^2 + \alpha_4 \psi^4 + \dots \\ + \kappa |\nabla \psi|^2 + \dots$$

where here now  $\psi(\mathbf{x})$  is a complex scalar representing  $\langle \hat{\psi}(\mathbf{x}) \rangle$ .

For bose systems this is known as the Gross-Pitaevskii free energy and it is equivalent to the  $O(2)$  or XY-model. (We will later actually derive this free energy in some detail).

As we discussed above, due to the Mermin-Wagner theorem, we should expect that this model does not order in  $D \leq 2$  and indeed there are no real superfluids at nonzero temperature in  $D \leq 2$ .

In fact, one can extend this idea to consider superconductors as well, which we should think of (at least for now) as charged superfluids. Here the only difference is that  $\nabla \psi$  should be replaced by the gauge covariant derivative

$$\nabla \psi \rightarrow (\nabla - q\mathbf{A}/\hbar)\psi$$

where  $q$  is the charge of the boson (for superconductors the boson is a cooper pair of charge  $2e$ ) and  $\mathbf{A}$  is the electromagnetic vector potential. We will not pursue this further at the moment (we will spend a lot of time later in the term discussing this in depth).