PHYS 427 - Thermal and Statistical Physics - Discussion 12 Solutions

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Today we will discuss the phenomenological Landau theory of phase transitions. A phenomenological theory attempts to describe a set of physical phenomena (in this case phase transitions), but does not claim to be derived directly from first principles (aka fundamental laws). As such, Landau theory is **not** developed by starting from a microscopic description, i.e. a partition function, and then making a series of controlled approximations. Instead, it starts by appraising the broad features of phase transitions and making some assertions about which should be elevated to the status of assumptions.

This problem set guides you through the development of Landau theory for a specific system (the Ising ferromagnet) and uses it to reproduce some results we already know, namely the critical exponents for mean-field theory. But the real benefit of the Landau approach is that it provides a unified framework for phase transitions based on general considerations of symmetry and analyticity. Roughly speaking, phase transitions with the same type of symmetry have the same critical behavior (at least in mean field), even if the physical systems look quite different at first glance. This is the idea of universality, and it's made evident by the Landau theory.

Here are four basic **assumptions** of Landau theory. We will refer back to them later in the context of a specific system, so you can just skim them for now.

- A. There exists an order parameter ξ , which vanishes ($\xi = 0$) in the "disordered" phase $T > T_c$, and which is nonzero ($\xi \neq 0$) in the "ordered" phase $T < T_c$. We also assume that the order parameter is small when T is close to T_c in the ordered phase.
- B. There is a function $F_L(\xi, T)$, called the Landau free energy, depending on the order parameter ξ and temperature T. The state of the system is assumed to be specified by the global minimum of F_L . In other words, at a given T, the equilibrium value of the order parameter ξ is determined by solving

$$\left(\frac{\partial F_L}{\partial \xi}\right)_T = 0$$
 and $\left(\frac{\partial^2 F_L}{\partial \xi^2}\right)_T > 0.$ (1)

When there is more than one solution of (1), we take the one for which F_L is smallest.

C. We assume that, when T is close to T_c , it is possible to expand

$$F_L = g_0 + g_1 \xi + \frac{1}{2} g_2 \xi^2 + \frac{1}{3} g_3 \xi^3 + \frac{1}{4} g_4 \xi^4 + \dots,$$
 (2)

where $g_i = g_i(T)$ can themselves be expanded as Taylor series around $T = T_c$. In mathematical language, (2) means F_L is analytic at $\xi = 0$, $T = T_c$.

D. F_L must be invariant under all symmetries of the system.

1. Ising ferromagnet: Recall that the Ising model of a ferromagnet consists of a bunch of classical "spins" on a lattice. At each site i of the lattice, the spin can either point up $(s_i = +1)$ or down $(s_i = -1)$. Spins on neighboring sites can interact. If two neighboring spins are the same, their interaction energy is -J (spins like to be aligned). If two neighboring spins are opposite, their interaction energy is J > 0 (spins don't like to be unaligned). More precisely, the energy of a spin configuration $\{s_i\}$ is

$$E(\lbrace s_i \rbrace) = -J \sum_{\langle i,j \rangle} s_i s_j, \tag{3}$$

where the sum is over nearest neighbor pairs (i, j). This is the Ising model.

The macrostate can be characterized by the magnetization

$$M \propto \left\langle \sum_{i} s_{i} \right\rangle.$$
 (4)

- (a) Roughly sketch the graph of M as a function of T that you obtained in lecture from the Weiss mean-field theory. Label the critical temperature T_c on your sketch.
- (b) Why is $T < T_c$ called the "ordered" phase, i.e. what is "ordered" about it? Identify an order parameter for the Ising ferromagnet. Does your order parameter meet the requirements of Assumption A?
- (c) What symmetry does the Ising model (3) have? How do the spins transform under this symmetry? How does the order parameter transform? What is the physical interpretation of this symmetry?
- (d) According to Assumption C, we have

$$F_L = g_0 + g_1 M + \frac{1}{2} g_2 M^2 + \frac{1}{3} g_3 M^3 + \frac{1}{4} g_4 M^4 + \cdots,$$
 (5)

where $g_i = g_i(T)$. Use the symmetry from (c) together with Assumption D to argue that $g_1 = g_3 = g_5 = \cdots = 0$.

- (e) It will be sufficient to work to $\mathcal{O}(M^4)$ in (5), i.e. we drop the "···". (You'll justify this in the homework, but assume it for today.) Argue that we must have $g_4 > 0$ at all temperatures in order for F_L to possess a finite global minimum. Therefore, expanding $g_4 = g_4^0 + g_4^1 \cdot (T T_c) + \cdots$ near the critical temperature, we find $g_4^0 > 0$. It will be sufficient to set $g_4^1 = \cdots = 0$, because this choice will not affect the leading behavior of the phase transition near T_c .
- (f) Find the equilibria of F_L , i.e. find the solutions M of $(\partial F_L/\partial M)_T = 0$. For each equilibrium, find the conditions under which it is a global minimum of F_L . Answer: $M_0 = 0$ is always an equilibrium, and it is a global minimum when $g_2 > 0$. $M_{\pm} = \pm \sqrt{-g_2/g_4^0}$ are equilibria that appear when $g_2 < 0$, and they are global minima.

¹Recall that a symmetry is something you can do to the system which doesn't alter the *form* of the physical laws describing that system's behavior. For example, a system consisting of two gravitationally attracted objects has $translational\ symmetry$ —the dynamical equations describing the system take the same form if the two objects are picked up and moved together 20 km in some direction, because the dynamics only depends on the objects' relative positions. In equilibrium statistical mechanics, the behavior of the system is dictated entirely by the form of the energy function E, so you are looking for a transformation that leaves the energy function invariant.

- (g) Using your answer to (f), sketch the graph of $F_L(M)$ when $g_2 > 0$ and when $g_2 < 0$. Identify the equilibria M_0 and M_{\pm} in your graphs.
- (h) Argue that, if Landau theory is to correctly describe the known behavior of the Ising ferromagnet, then g_2 must be positive when $T > T_c$ and negative when $T < T_c$. Therefore, near the critical temperature, we must have $g_2 = g_2^1 \cdot (T T_c) + g_2^3 (T T_c)^3 + \cdots$, where $g_2^1 > 0$ is independent of T. It will be sufficient to set $g_2^3 = \cdots = 0$. Re-title your two plots from part (g)—which one is $T > T_c$ and which is $T < T_c$?

Note that when $T < T_c$, there are two minima M_{\pm} with the same value of F_L . How does the system decide which minimum to actually occupy? Roughly speaking, it comes down to the chance values of external fields. It is impossible to *entirely* shield the magnet from outside magnetic fields. The presence of a magnetic field, however small, will make one minimum lower than the other (you'll see this explicitly in part (k)), and the system will settle into that minimum rather than the other².

Note also that the equilibrium state of the system when $T < T_c$, being that it has nonzero M, does not respect the symmetry from part (c). Indeed, under the transformation $s_i \to -s_i$, the magnetization M flips sign, and we end up with an entirely different state—the north/south poles of the magnet have swapped! We say that the equilibrium state of the system "spontaneously breaks" the symmetry. More generally, spontaneous symmetry breaking is the term used whenever the state of a system does not obey the same symmetries as the dynamical laws describing that system.

- (i) The critical exponent β is defined by $M \sim (T_c T)^{\beta}$ when $T < T_c$. Using the results of (f) and (h), show that $\beta = 1/2$. Plot M as a function of T near T_c .
- (j) So far the magnetic field B = 0. If $B \neq 0$, describe how (3) would be modified, and convince yourself that the transformation from part (c) is no longer a symmetry of the modified (3). Now the argument from (d) no longer applies, so we are allowed to have $g_1 \neq 0$. Indeed, argue that $g_1 = -B$. (We could also put in a nonzero g_3 , but this would turn out not to affect the leading behavior near the critical point.)
- (k) Sketch four graphs of F_L vs. M: one where B > 0 and $T > T_c$, one B > 0 and $T < T_c$, one B < 0 and $T > T_c$, one B < 0 and $T > T_c$. Identify the equilibria in your graphs. How do the equilibria change as $B \to 0$ at fixed T? Is this all physically compatible with the conclusions of the Weiss model?
- (l) The critical exponent δ is defined by $M \sim B^{1/\delta}$ when $T = T_c$. Show that $\delta = 3$. Plot M as a function of B at $T = T_c$.
- (m) Now consider $T > T_c$. Write out the equation $0 = (\partial F_L/\partial M)_T$ and differentiate both sides with respect to B at fixed T. In the resulting equation, you will encounter the isothermal magnetic susceptibility $(\partial M/\partial B)_T \equiv \chi_T$. Solve for χ_T .

The critical exponent γ is defined by $\chi_T \sim (T - T_c)^{-\gamma}$ when B = 0. Using your above expression for χ_T , show that $\gamma = 1$.

²Another example: if you balance a pencil perfectly on its tip, which direction will it fall over? It's just a poorly posed question. It's not possible to balance a pencil perfectly on its tip. You will always accidentally tilt it a fraction of a degree away from the vertical, or the wind will be blowing a tiny bit east, etc.

SOLUTIONS:

(a)

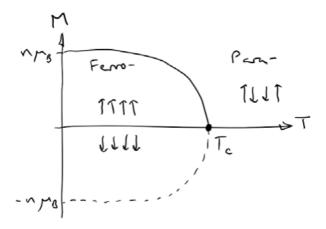


Figure 1

(b) As seen in Fig. 1, when $T < T_c$ the system spontaneously acquires a net magnetization. That means that, on average, more spins are pointing in one direction than the other. That is, the spins are *ordered*. This is in contrast to the phase $T > T_c$, in which the spins are jumbled up and on average the total spin is zero. That's disordered.

The magnetization M is an order parameter for this transition. That is, in the context of the Ising ferromagnet, the thing we abstractly called ξ in Assumption A can be identified with the magnetization M. In other systems (like a fluid undergoing a liquid/gas transition) the order parameter ξ would be identified with something else.

The magnetization is an order parameter because it's something that vanishes when $T > T_c$ and it's nonzero in the phase $T < T_c$. In other words, it's an indicator of whether the system is ordered or not.

(c) If you flip all of the spins simultaneously, then the total interaction energy doens't change. That's because any pair of spins which was aligned will still be aligned after flipping all the spins (albeit aligned in the other direction). Similarly, any pair of spins which was anti-aligned will still be anti-aligned. MOre formally, if you simultaneously flip $s_i \to -s_i$ for all sites i, then (3) doesn't change (because $s_i s_j \to (-1)^2 s_i s_j$.

From (4) we see that $M \to -M$ under this symmetry.

(d) Assumption D, more precisely, says that Landau theory must treat on equal footing any two order parameter values which differ by a symmetry transformation. In light of part (c), this means for the Ising ferromagnet that the Landau free energy must have the same value for M as it has for -M, otherwise the theory would be unfairly prejudiced. That is, F_L must be an even function of M, so its Taylor expansion cannot contain any odd-order terms in M. Hence $g_2 = g_3 = g_5 = \cdots = 0$, and we have

$$F_L = g_0 + \frac{1}{2}g_2M^2 + \frac{1}{4}g_4M^4. (6)$$

Notice that we're *theory builders* now. We are making decisions about what is relevant in our description of Nature. The first thing a theorist always goes to when deciding what's relevant is symmetry.

(e) If $g_4 < 0$, then the graph of F_L would to go - as $M \to \pm \infty$. Hence, according to Assupption B, the state of the system would always be an infinitely magnetized state! That's obviously nonsense, so we can't permit it in our theory. In the common terminology, if $g_4 < 0$ our theory would be thermodynamically unstable, and that's unacceptable.

By Assumption C, we can expand

$$g_4(T) = g_4^0 + g_4^1 \cdot (T - T_c) + g_4^2 (T - T_c)^2 + \cdots,$$
(7)

where g_4^i are constant coefficients. Since we have decided $g_4 > 0$ for all temperatures near T_c (it must be thermodynamically stable at all temperatures, and we're only attempting to describe the physics near T_c), in particular we need $g_4 > 0$ when $T = T_c$, and this implies $g_4^0 > 0$. The other coefficients in (7) are arbitrary, but it turns out that omitting them will not alter the critical behavior predicted by our theory. You can check that, e.g. by leaving in the term proportional to g_4^1 and seeing what happens. So we will set $g_4 = g_4^0 > 0$ in what follows.

(f) To recap, we have

$$F_L = g_0 + \frac{1}{2}g_2M^2 + \frac{1}{4}g_4^0M^4.$$
 (8)

Therefore

$$\left(\frac{\partial F_L}{\partial M}\right)_T = g_2 M + g_4^0 M^3 \tag{9}$$

and

$$\left(\frac{\partial^2 F_L}{\partial M^2}\right)_T = g_2 + 3g_4^0 M^2.$$
(10)

Setting (9) to zero we find three solutions:

$$M_0 = 0$$
 $M_{\pm} = \pm \sqrt{-g_2/g_4^0}$. (11)

Inserting M=0 into (10), we find that M_0 is a local minimum if $g_2>0$, else it is a local maximum. Similarly, we note that M_{\pm} only exist (are real) when $g_2<0$, and from (10) we find that $(\partial^2 F_L/\partial M^2)=-2g_2$. Hence M_{\pm} are local minima whenever they exist.

Combining the above observations with the fact that $F_L \to \infty$ when $M \to \infty$, we can say the following. If $g_2 > 0$, then there is only one equilibrium, at $M = M_0$, and it is a global minimum. If $g_2 < 0$, then there are two degenerate minima at $M = M_{\pm}$ separated by a local maximum at M = 0.

- (g) The graph when $g_2 > 0$ is shown in the second row, first column of Fig. 2. The graph when $g_2 < 0$ is shown in the second row, third column of Fig. 2.
- (h) In the $g_2 > 0$ graph, we see that the state of the system (as determined by Assumption C) is M = 0, i.e. zero magnetization. From experiments (and Weiss mean field theory), this is what we know happens when $T > T_c$. Conversely, in the $g_2 < 0$ graph, we see that there are two degenerate states of the system, both of which have $M \neq 0$. This is what we know happens when $T < T_c$.

Hence we must have that $g_2 > 0$ whenever $T > T_c$ and $g_2 < 0$ whenever $T < T_c$, and in particular $g_2 = 0$ when $T = T_c$. But we can expand

$$g_2(T) = g_2^0 + g_2^1 \cdot (T - T_c) + \cdots$$
 (12)

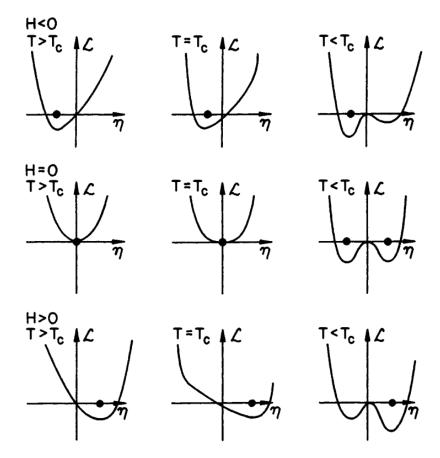


Figure 2: Notation: η is our M, \mathcal{L} is our F_L , and H is our B. Taken from the magnificent book Lectures on Phase Transitions and the Renormalization Group by Nigel Goldenfeld.

Putting $T = T_c$, we find $g_2^0 = 0$. Then the remarks of the previous paragraph imply $g_2^1 > 0$. As with g_4 , it will not be necessary to keep any higher order terms in $T - T_c$ (omitting these terms will not affect predictions of e.g. critical exponents.) So from now on we put $g_2 = g_2^1 \cdot (T - T_c)$ with $g_2^1 > 0$.

(i) When $T < T_c$, the state of the system is either M_+ or M_- . Inserting $g_2 = g_2^1(T - T_c)$, we have

$$M_{\pm} = \pm \sqrt{-g_2^1 (T - T_c)/g_4^0} \propto (T_c - T)^{1/2}.$$
 (13)

The plot of M vs T near T_c precisely reproduces Figure.

(j) The new Ising model is

$$E = -J\sum_{\langle i,j\rangle} s_i s_j - B\sum_i s_i, \tag{14}$$

where the B-dependent term is the usual interaction between a spin and a magnetic field. Well, there should be a factor of the Bohr magneton in there, but we can absorb those into our definition of B. After all, we are looking for form right now, not precise accounting of numerical values.

Now if we try to transform $s_i \to -s_i$ in (14), the *B*-dependent term will change signs, i.e. E will not be invariant. The addition of a nonzero magnetic field *explicitly* breaks the spin-flip symmetry (in contrast to the notion of spontaneous symmetry breaking discussed above). Now we should no longer demand that $F_L(M) = F_L(-M)$, so we must restore the g_1 and g_3 terms.

Since F_L is supposed to represent some kind of free energy, similar (but not identical) to the thermodynamic Gibbs free energy, we should consider the term g_1M in F_L as corresponding to the spin-alignment interaction -BM between the system and an external magnetic field, i.e. we put $g_1 = -B$. In principle we should deal with g_3 as well, but (sing it with me this time) omitting it will not affect the predicted behavior near the critical point.

(k) See Fig. 2. This is all compatible with the conclusions of the Weiss model near the critical point. It's good to think this through and make sure you can explain the general features of Fig. 3 using Fig. 2.

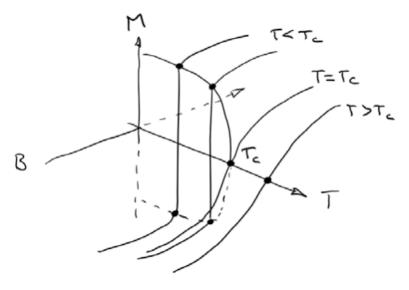


Figure 3

(1) We now have

$$F_L = g_0 - BM + \frac{1}{2}g_2^1 \cdot (T - T_c)M^2 + \frac{1}{4}g_4^0 M^4, \tag{15}$$

SO

$$\left(\frac{\partial F_L}{\partial M}\right)_T = -B + g_2^1 (T - T_c) M + g_4^0 M^3.$$
(16)

When we put $T = T_c$ and set (16) to zero, we find $M \propto B^{1/3}$.

(m) Now take a look at (16) with $T > T_c$. Setting it to zero, we could solve for M(T, B), although it wouldn't be so pretty. But assume we have done this and imagine we have replaced M with this M(T, B) in (16). Now (16) is just a function of T and T and T and T are this function of T and T with respect to T and T are the function of T and T are the f

$$-1 + g_2^1(T - T_c)\chi_T + 3g_4^0 M^2 \chi_T \qquad \Longrightarrow \qquad \chi_T = \frac{1}{g_2^1(T - T_c) + 3g_4^0[M(T, B)]^2}. \tag{17}$$

Now if we put B = 0, we know that at $T > T_c$ we will find M = 0. So we insert M = 0 into (17) to get

$$\chi_T \propto (T - T_c)^{-1}$$
 when $B = 0$. (18)