

Landau Mean Field Theory

1. INTRODUCTION

In our course, when we calculated the thermodynamic properties of a system, we determined the microscopic states of the system. The machinery of the partition function,

$$(1) \quad Z = \sum_{\mu} e^{\frac{-H_{\mu}}{k_B T}}$$

where the sum is over all microstates of the system, is so useful because we can derive from it thermodynamic properties with simple calculus and algebra. However, as systems increase in complexity, the explicit calculation of the partition function from its microstates becomes increasingly difficult.

Landau's insight was that, near a phase transition, an approximate form of the free energy can be written without calculating the microstates of the system. The free energy contains information about the microstates through its relation to the partition function,

$$(2) \quad F = -k_B T \ln Z,$$

where F is the free energy, and through it we get an approximate thermodynamics.

2. NON-ANALYTIC FREE ENERGIES

Since at a phase transition a system undergoes a qualitative change in some thermodynamic quantity, call it X , the system does not vary smoothly as a function of the constraint that induces that change, call it Y . This gives us a non-analytic function $X(Y)$. From real analysis, we have that if a function f is real analytic on some open set U then there exists a convergent power series expansion,

$$(3) \quad f(x) = \sum_{n=0}^{\infty} a_n (x - x_0)^n$$

on some neighborhood of $x_0 \in U$ where $a_n \in \mathbb{R}$. But then any derivative of an analytic function must be analytic where the derivative is the piecewise derivative of the power series expansion. Accordingly the free energy F cannot be an analytic function with respect to Y . The reader may be familiar with the properties of complex analytic (holomorphic) functions, so I note more rigorously that by analytic continuation there exists a map extending each analytic function g on U to a complex analytic function g^* on $G \subset \mathbb{C}$ where $U \subset G$. So we can write the complex power series expansion, take derivatives, and then map $g^{*'} \rightarrow g'$. By Cauchy's Theorem the functions $g^{*'}$ are certainly analytic, so we have analytic restrictions to \mathbb{R} .

We now have the condition that a phase transition correspond to a nonanalytic free energy. The set of phase transitions becomes the set of points (in Y space) where there are singularities in the free energy. We call a phase transition first order when it is associated with a singularity in a first derivative of the free energy, and we call a phase transition second order when it is associated with a singularity in the second and higher derivatives of the free energy.

3. APPROXIMATING THE FREE ENERGY

Before we study singularities in the free energy, we must approximate it. First, we must choose the variable that we write the free energy with respect to. Second order phase transitions are characterized by a state of reduced symmetry developing from a disordered phase. We want our free energies to reflect this change in symmetry through some parameter so that we capture the qualitative behavior of the system through the transition. We choose the quantity that changes qualitatively as a function of our constraint and call this the order parameter of the phase transition. For example, in a ferromagnet we observe magnetic spins undergo a transition from a disordered

phase with no net magnetization to a phase with non-zero magnetization as temperature changes. We choose magnetization as our order parameter in this case.

Second, we choose to decompose our free energy in the following way:

$$(4) \quad F = F_0(Y) + F_L(Y, \phi)$$

where Y is our constraint and ϕ is the order parameter. F_0 is an analytic function of temperature and F_L is a nonanalytic function containing the dependence on the order parameter.

This amounts to a nontrivial assumption. Recall the discussion about coarse-graining in class. If we want to know the order parameter, say the mean magnetization, we can take a sampling of many microstates and a large sample will converge on the real value. We assume that all of the information about the microstates is contained in F_L . We can then convert our degree of freedom from μ to ϕ .

$$(5) \quad F = -k_B T \ln Z \implies e^{\frac{-F}{k_B T}} = \sum_{\mu} e^{\frac{-H_{\mu}}{k_B T}} = \sum_{\mu} \int D\phi \delta[\phi - \langle \mu \rangle] e^{\frac{-H_{\mu}}{k_B T}}$$

where $\int D\phi$ is a functional integral over all degrees of freedom associated with ϕ . By definition a functional integral is a limit of discrete integrals. For a 1D Hamiltonian we have,

$$\int D\phi(x) z[\phi(x), \partial\phi, \dots] = \lim_{a \rightarrow 0, N \rightarrow \infty} \int \prod_{i=1}^N d\phi_i z[\phi_i, (\phi_{i+1} - \phi_i)/a, \dots]$$

The form of the functional integral respects the following symmetries of the coarse-grained Hamiltonian selected by Ginsberg and Landau. First, locality. The Hamiltonian should depend on the local behavior of the thermodynamic variable underlying our transition which we represent by gradient expansions,

$$(6) \quad \beta H = \int dx f[\phi(x), \phi, \dots].$$

Second, rotational symmetry. Outside of a magnetic field the Hamiltonian should be isotropic in space and invariant under rotations $\phi \rightarrow R_n \phi$,

$$(7) \quad \beta H[\phi] = \beta H[R_n \phi].$$

Third, translational and rotational symmetry in x . This leads to a Hamiltonian of the form,

$$(8) \quad \beta H = \int dx \left[\frac{t}{2} \phi^2 + u \phi^4 + \dots + \frac{K}{2} (\nabla \phi)^2 + \frac{L}{2} (\nabla^2 \phi)^2 + \frac{N}{2} \phi^2 (\nabla \phi)^2 + \dots - h \cdot \phi \right]$$

which is known as the Ginsberg-Landau Hamiltonian, and depends on the parameters t, u, K, \dots which are functions of microscopic interactions and external constraints (temperature and pressure for instance). Continuing from (5), we are left with

$$(9) \quad \approx \int D\phi g(\phi) e^{\frac{-H_{\phi}}{k_B T}} = \int D\phi e^{\frac{-(H_{\phi} - k_B T \ln g(\phi))}{k_B T}}$$

where $g(\phi)$ represents the degeneracy of ϕ . Note that the transition from $H_{\mu} \rightarrow H_{\phi}$ is extremely difficult in practice because ϕ and μ have a complicated relationship. We now employ the saddle point approximation method. The general idea is that since the negative exponential function $e^{-f(x)}$ is so rapidly vanishing as $f(x)$ increases, we only need to look at contributions where $f(x)$ is at its minimum. But then the integral will be like integrating over a spike and we can write,

$$(10) \quad F \approx \min_{\phi} [H_{\phi} - k_B T \ln g(\phi)]$$

by comparison of the arguments of the exponentials. If we recall that the thermodynamic free energy is given by $F = E - TS$, we get,

$$(11) \quad F \approx E_0 - E_* \phi^2 + \dots - T[S_0 - a \phi^2 + \dots] = F_0 + a \left(T - \frac{E_*}{a} \right) \phi^2$$

where the orders of the terms allowed in the expansion are chosen to protect translational and other symmetries, see (8) above. Physically, we interpret the $E_*\phi^2$ term as an attraction that induces order but this attraction increases as entropy decreases. These competing effects (one reduces F , one increases F) give rise to the phase transition. Notice that this method implies the connectedness between thermodynamic free energy $F(E) = E - TS(E)$ and statistical mechanics free energy $F = -k_B T \ln Z$. We will evaluate some real systems to see how this works out in practice.

4. WORKED EXAMPLE: ISING MAGNET

We will do the Ising Magnet two different ways. First we will start with the partition function and give a worked example of the derivation in the last section. Second we will start directly from the approximation of the free energy.

The partition function is the sum over all configurations,

$$(12) \quad Z = \sum_{\sigma_j = \pm 1} e^{-\beta E}.$$

To do the mean field averaging, we imagine that we can fix an overall magnetization per site, say the average magnetization in a region U is $M = \sum_j \frac{\sigma_j}{N}$ for N sites. Then we sum over all of these values of M in U ,

$$(13) \quad Z = \sum_M \sum_{\sigma_j = \pm 1 | \sum_j \sigma_j = MN} e^{-\beta E}$$

Then by choosing a proper function $f(M)$ with energy and volume dependence we can write

$$(14) \quad e^{-\beta V f(M)} = \sum_{\sigma_j = \pm 1 | \sum_j \sigma_j = MN} e^{-\beta E}.$$

and since for large N , M becomes essentially continuous via averaging, we can replace the sum with an integral,

$$(15) \quad Z = \int_{-1}^1 dM e^{-\beta V f(M)}$$

This is the result found in (9).

Now we start from the free energy. First we select our order parameter. In the Ising model we have spins that point either up or down. The ordering of the spins changes; at high temperatures the spins are disordered, and at low temperatures the spins choose whether to point up or down based on surrounding spins, call it "spontaneous choice". Let the order parameter be the mean value of the spins,

$$(16) \quad M = \langle S_i \rangle_{i+\Delta}$$

where we are averaging within an area around the spin Δ , which we will call the coarse graining length (must be much larger than the lattice spacing, etc). Our constraint variable will be T since the phase transition happens when T changes. We desire $F(M, T)$.

Second we identify our symmetries. Up and down are identical states corresponding to a rotation by π of the sample. That means that the free energy should be the same if we change all spin orientations, $M \rightarrow -M$.

Third we write the free energy that respects this symmetry. We need all powers of M to be even to respect $M \rightarrow -M$. Consider the free energy density $f_L = \frac{F_L}{V}$. Then

$$(17) \quad f_L = \frac{1}{2}a(T - T_c)M^2 + \frac{1}{4}cM^4 + \dots$$

where a, c are parameters. At the phase transition order parameters go to zero. This requires that the $(T - T_c)$ be included in (17) because since (we know from experiment) $f'_L = 0$ for second order phase transitions,

$$(18) \quad f'_L = 0 = a(T - T_c)M + cM^3$$

implies a nonzero solution for M if we don't include the $T - T_c$ term. We include orders only up to 4 because (it turns out) higher orders do not contribute qualitatively. Quantitative differences do not matter because we have already washed out that information and will add it back through the values of the parameters. From the derivative with respect to M we get minima of M at 0 for $T > T_c$ and $\pm \sqrt{\frac{a(T_c - T)}{c}}$ for $T < T_c$. This is a continuous phase transition since the magnetization grows smoothly from 0.

Fourth we calculate the thermodynamics. When we plug these minima back into F we get, $F = F_0(T)$ when $T > T_c$ and $F = F_0(T) - V \frac{1}{2} \frac{a(T_c - T)^2}{c}$ when $T < T_c$. The derivative with respect to temperature therefore vanishes at the critical point. We find a discontinuity in the second derivative:

$$(19) \quad \left. \frac{\partial^2 F}{\partial T^2} \right|_{T_c^+} - \left. \frac{\partial^2 F}{\partial T^2} \right|_{T_c^-} = 0 - \left(-\frac{a}{c}V\right) = \frac{a}{c}V$$

Thus we have a second order phase transition and have characterized its relevant features. We can find the properties of other thermodynamic quantities by taking other derivatives of F and evaluating them about the phase transition.

Notice, vitally, that the coefficients of these thermodynamic quantities and of M depend on the on the details of the theory (couplings of T_c, a, c) but the exponents do not. This validates Landau's qualitative approach.

5. FLUCTUATIONS

Until now we have turned complicated interacting many-body systems into non-interacting ones by averaging over all interactions. This was the mean theory approximation. Here we will generalize Landau's theory to include fluctuations. Consider the Ising Model case taken before. This time, divide the system into a large number of subsystems with N_s spins each, giving a magnetization

$$(20) \quad M_s = \frac{1}{N_s} \sum_{j \in s} \sigma_j$$

Now our partition function becomes,

$$(21) \quad \sum_{\sigma_j = \pm 1} e^{-\beta E} = \sum_s \sum_{M_s} \sum_{\sigma_j \in s | \sum_{j \in s} \sigma_j = MN_s} e^{-\beta E}$$

where since the subsystems contain so many spins, the spins can be allowed to range from -1 to 1 . We can also label their subsystems by location through a single variable \bar{x} and take $M_s = M(\bar{x})$. Then as before we write

$$(22) \quad Z = \int DM(\bar{x}) e^{-\beta \int d^d x f(M(\bar{x}))}$$

another functional integral. If we put the model in a box of volume V with periodic boundary conditions, we get

$$(23) \quad M_{\bar{k}} = \sum_V d^d x M(\bar{x}) e^{i\bar{k} \cdot \bar{x}}$$

where k is quantized. So the partition function becomes,

$$(24) \quad \int DM(x) = \prod_{\bar{k}} \int_{-\infty}^{\infty} dM_{\bar{k}}$$

Now each integral is over a field $M(\bar{x})$ which demonstrates why the mean field theory works so well for phase transitions. When fluctuations are small it is possible to include them with dependence on their spatial derivatives. We assume that the theory in the long-distance limit is fully invariant under rotations (consider the symmetry depending on the underlying lattice and invariant interactions under some group of rotations). Then we find the free-energy density in the limit of small fluctuations,

$$(25) \quad f(M(x)) = a + \kappa \nabla M \cdot \nabla M - hM + bM^2 + cM^4$$

where the dot product is in real space and κ is the coupling. Note that it raises the free energy for spatial variations and favors a uniform M . This is stiffness. Consider a field $\phi(\bar{r})$. We consider it as an averaged difference between a fluctuating degree of freedom and its expectation value. This characterizes fluctuations. We rewrite the free energy density in terms of this ϕ . For $T > T_c$ and vanishing magnetic field the expectation value of the magnetization vanishes so we replace M with ϕ in f ,

$$(26) \quad \beta f(\phi(\bar{r})) = \kappa |\nabla \phi|^2 + b\phi^2 + c\phi^4 + \dots$$

for $T > T_c$. Then we take the partition sum over ϕ just like we did for M . For $T < T_c$ and $h=0$, the expectation of M is nonvanishing such that $M^2 = \frac{-b}{2c}$. So we choose the minimum of interest. We get,

$$(27) \quad \beta f(\phi) = \kappa |\nabla \phi|^2 - 2b\phi^2 + (\phi^3)$$

for $T < T_c$ for either minimum. The odd term in ϕ comes about because the potential is not symmetric around the minimum.

6. FAILURES

- (a) Landau's theory is an effective theory. It uses as its cornerstone the fact that different systems have quantitatively identical critical behavior, and neglects details of the system. By construction, it therefore can't give numbers of a particular T_c for a system without already having found it in an experiment and plugging in the parameters of that system.
- (b) Some phase transitions are described by multiple order parameters and sometimes different order parameters can vanish at the same point.
- (c) Topological order can not be described because topological character is non-local, while Landau's theory is a local mean field theory.