Physics 7653: Statistical Physics
http://www.physics.cornell.edu/sethna/teaching/653/
In Class Exercises
Last correction at August 30, 2018, 11:55 am

9.5 **Landau theory for the Ising model.** (Condensed matter)③

This chapter has focused on the topological order parameter, which labels the different ground states of the system when there is a spontaneously broken symmetry. To study the defect cores, interfaces, and high temperatures near phase transitions, one would like an order parameter which can vary in magnitude as well as direction.

In Section 6.7, we explicitly computed a free energy for the ideal gas as a function of the density. Can we use symmetry and gradient expansions to derive free energy densities for more realistic systems—even systems that we do not understand microscopically? Lev Landau used the approach we discuss here to develop theories of magnets, superconductors, and superfluids—before the latter two were understood in microscopic terms.[1] In this exercise, you will develop a Landau[2] theory for the Ising model.[3]

Here we outline the general recipe, and ask you to implement the details for the Ising model. Along the way, we will point out places where the assumptions made in Landau theory can break down—often precisely in the cases where the theory is most useful. There are five steps.

[1] *Pick an order parameter field.*

Remember that the Ising model had a high-temperature paramagnetic phase with zero magnetization per spin m, and a low-temperature ferromagnetic phase with a net magnetization per spin $\pm m(T)$ that went to one at $T = 0$. The Ising model picks one of the two equilibrium states (up or down); we say it spontaneously breaks the up–down symmetry of the Hamiltonian

Hence the natural[4] order parameter is the scalar $m(\mathbf{x})$, the local magnetization averaged over some volume ΔV. This can be done by averaging the magnetization per spin in small boxes, as in Section 6.7.

[1] Physicists call this Landau theory. Rather similar formalisms have been developed in various other fields of physics and engineering, from liquid crystals to 'rational mechanics' treatments of martensites (see Exercises 11.7 and 11.8). The vocabulary is often different (Frank, Ericksen, and Leslie instead of Landau, constitutive relations rather than free energies, and internal state variables rather than order parameters) but the basic approach is similar.

[2] More properly, a Ginzburg–Landau theory, because we include gradient terms in the free energy density, which Landau first did in collaboration with Ginzburg.

[3] See also Exercise 12.5 for a more traditional mean-field theory approach.

[4] Landau has a more systematic approach for defining the order parameter, based on group representation theory, which can be quite useful in more complex systems.

(a) *What value will $m(\mathbf{x})$ take at temperatures high compared to the interaction J in the Ising model? What values will it take at temperatures very low compared to J?*

[2] *Write a general local*[5] *free energy density, for long wavelengths and translational symmetry.*

A local free energy is one which depends on the order parameter field and its gradients:

$$\mathcal{F}^{\text{Ising}}\{m, T\} = \mathcal{F}(\mathbf{x}, m, \partial_j m, \partial_j \partial_k m, \dots). \tag{1}$$

As in Section 9.3, we Taylor expand in gradients.[6] Keeping terms with up to two gradients of m (and, for simplicity, no gradients of temperature), we find

$$\begin{aligned}\mathcal{F}^{\text{Ising}}\{m, T\} =& A(m, T) + V_i(m, T)\partial_i m \\ &+ B_{ij}(m, T)\partial_i \partial_j m \\ &+ C_{ij}(m, T)(\partial_i m)(\partial_j m).\end{aligned} \tag{2}$$

(b) *What symmetry tells us that the unknown functions A, B, C, and V do not explicitly depend on position $\mathbf{x}$?* If a is the natural microscopic length of the problem (the size of the molecules, or lattice, or perhaps the correlation length), we expect all the terms in the expansion to be of the same order. *If the magnetization varies on a large length scale $D \gg a$, how much smaller would a term involving three derivatives be than the terms B and C that we have kept?*

[3] *Impose the other symmetries of the problem.*

The Ising model has an up–down symmetry[7] so the free energy density $\mathcal{F}^{\text{Ising}}\{m\} = \mathcal{F}\{-m\}$. Hence the coefficients A and C are functions of m^2, and the functions $V_i(m, T) = m v_i(m^2, T)$ and $B_{ij}(m) = m\, b_{ij}(m^2, T)$.

The two-dimensional Ising model on a square lattice is symmetric under 90° rotations. This tells us that $v_i = 0$ because no vector is invariant under 90° rotations. Similarly, b and C must commute with these rotations, and so must be multiples of the identity

[5] Not all free energies are local! Long-range Coulomb, gravitational, or elastic fields can be added to the order parameters. For a complete description the order parameter should incorporate long-range fields, conserved quantities, and all broken symmetries.

Also, in part (d) we notice that systems fluctuate on all length scales near continuous phase transitions (Chapter 12), and hence have non-local free energies.

[6] A gradient expansion will not be valid at sharp interfaces and in defect cores where the order parameter varies on microscopic length scales. Landau theory is often used anyhow, as a solvable if uncontrolled approximation to the real behavior.

[7] The equilibrium state may not have up–down symmetry, but the model—and hence the free energy density—certainly does.

matrix.[8] Hence we have

$$\mathcal{F}^{\text{Ising}}\{m,T\} = A(m^2,T) + m\,b(m^2,T)\nabla^2 m + C(m^2,T)(\nabla m)^2. \tag{3}$$

Many systems are isotropic: the free energy density is invariant under all rotations. For isotropic systems, the material properties (like the functions A, B_{ij}, and C_{ij} in eqn 2) must be invariant under rotations. All terms in a local free energy for an isotropic system must be writable in terms of dot and cross products of the gradients of the order parameter field.

(c) *Would the free energy density of eqn 3 change for a magnet that had a continuous rotational symmetry?*

[4] *Simplify using total divergence terms.*

Free energy densities are intrinsically somewhat arbitrary. If one adds to $\mathcal{F}$ a gradient of any smooth vector function $\nabla \cdot \boldsymbol{\xi}(m)$, the integral will differ only by a surface term $\int \nabla \cdot \boldsymbol{\xi}(m)\,\mathrm{d}V = \int \boldsymbol{\xi}(m) \cdot \mathrm{d}S$.

In many circumstances, surface terms may be ignored. (i) If the system has periodic boundary conditions, then the integral $\int \boldsymbol{\xi}(m) \cdot \mathrm{d}S = 0$ because the opposite sides of the box will cancel. (ii) Large systems will have surface areas which are small compared to their volumes, so the surface terms can often be ignored, $\int \nabla \cdot \boldsymbol{\xi}(m)\,\mathrm{d}V = \int \boldsymbol{\xi}(m) \cdot \mathrm{d}S \sim L^2 \ll \int \mathcal{F}\,\mathrm{d}V \sim L^3$. (iii) Total divergence terms can be interchanged for changes in the surface free energy, which depends upon the orientation of the order parameter with respect to the boundary of the sample.[9]

This allows us to integrate terms in the free energy by parts; by subtracting a total divergence $\nabla(uv)$ from the free energy we can exchange a term $u\,\nabla v$ for a term $-v\,\nabla u$.

[8] Under a 90° rotation $R = \left(\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right)$, a vector $\mathbf{v}$ goes to $R \cdot \mathbf{v}$. For it to be invariant, $(v_1\, v_2) = (v_1\, v_2)\left(\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right) = (-v_2, v_1)$, so $v_1 = -v_2 = -v_1 = 0$. An invariant symmetric matrix C rotates to $RCR^{-1} = \left(\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right)\left(\begin{smallmatrix} C_{11} & C_{12} \\ C_{12} & C_{22} \end{smallmatrix}\right)\left(\begin{smallmatrix} 0 & -1 \\ 1 & 0 \end{smallmatrix}\right) = \left(\begin{smallmatrix} C_{22} & -C_{12} \\ -C_{12} & C_{11} \end{smallmatrix}\right)$ so $C_{11} = C_{22}$ and $C_{12} = 0$, and hence C is a multiple of the identity.

[9] See Exercise 9.3 and [1]. One must also be wary of total divergence terms for systems with topological defects, which count as internal surfaces; see [3].

For example, we can subtract a term $-\nabla \cdot (m\, b(m^2,T)\nabla m)$ from the free energy 3:

$$\begin{aligned}
&\mathcal{F}^{\text{Ising}}\{m,T\} \\
&\quad = A(m^2,T) + m\, b(m^2,T)\nabla^2 m \\
&\qquad + C(m^2,T)(\nabla m)^2 \\
&\qquad - \nabla \left(m\, b(m^2,T)\cdot \nabla m\right) \\
&\quad = A(m^2,T) + C(m^2,T)(\nabla m)^2 \\
&\qquad - \nabla \left(m\, b(m^2,T)\right)\cdot \nabla m \\
&\quad = A(m^2,T) + C(m^2,T)(\nabla m)^2 \\
&\qquad - \left(b(m^2,T) + 2m^2 b'(m^2,T)\right)(\nabla m)^2 \\
&\quad = A(m^2,T) \\
&\qquad + \big(C(m^2,T) - b(m^2,T) \\
&\qquad\qquad - 2m^2 b'(m^2,T)\big)(\nabla m)^2,
\end{aligned} \tag{4}$$

replacing $(m\, b(m^2,T))\,(\nabla^2 m)$ with the equivalent term $-(\nabla m)(\nabla(m\, b(m^2,T)\nabla m)\cdot \nabla m)$. Thus we may absorb the b term proportional to $\nabla^2 m$ into an altered $c = C(m^2,T) - b(m^2,T) - 2m^2 b'(m^2,T)$ term times $(\nabla m)^2$:

$$\mathcal{F}^{\text{Ising}}\{m,T\} = A(m^2,T) + c(m^2,T)(\nabla m)^2. \tag{5}$$

[5] *(Perhaps) assume the order parameter is small.*[10]

If we assume m is small, we may Taylor expand A and c in powers of m^2, yielding $A(m^2,T) = f_0 + (\mu(T)/2)m^2 + (g/4!)m^4$ and $c(m^2,T) = \frac{1}{2}K$, leading to the traditional Landau free energy for the Ising model:

$$\mathcal{F}^{\text{Ising}} = \tfrac{1}{2}K(\nabla m)^2 + f_0 + (\mu(T)/2)m^2 + (g/4!)m^4, \tag{6}$$

where f_0, g, and K can also depend upon T. (The factors of 1/2 and 1/4! are traditional.)

The free energy density of eqn 6 is one of the most extensively studied models in physics. The field theorists use ϕ instead of m for the order parameter, and call it the ϕ^4 model. Ken Wilson added fluctuations to this model in developing the renormalization group (Chapter 12).

[10] Notice that this approximation is not valid for abrupt phase transitions, where the order parameter is large until the transition and zero afterward. Landau theories are often used anyhow for abrupt transitions (see Fig. 11.2(a)), and are illuminating if not controlled.

We shall see in Chapter 12 that Landau theory *also* fails when the order parameter is small near a continuous phase transition. For example, just below T_c in the Ising model, the average M is small but simulations show large, scale-invariant fluctuations in the magnetization (Exercise 8.1). These lead to power law singularities $\mathcal{F}^{\text{Ising}}\{m,T\} = M^{1+\delta}(a + bM/(T_c - T)^{\beta} + \dots)$ where in 3D $\delta = 4.7898\dots$ and $\beta = 0.326\dots$.

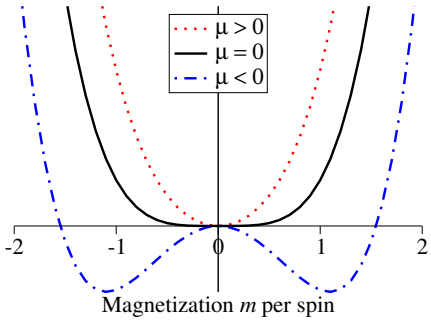

Fig. 1 Landau free energy density for the Ising model 6, at positive, zero, and negative values of the quadratic term μ.

Notice that the Landau free energy density has a qualitative change at $\mu = 0$. For positive μ it has a single minimum at $m = 0$; for negative μ it has two minima at $m = \pm\sqrt{-6\mu/g}$. Is this related to the transition in the Ising model from the paramagnetic phase ($m = 0$) to the ferromagnetic phase at T_c?

The free energy density already incorporates (by our assumptions) fluctuations in m on length scales small compared to the coarse-graining length W. *If we ignored fluctuations on scales larger than* W then the free energy of the whole system[11] would be given by the volume times the free energy density, and the magnetization at a temperature T would be given by minimizing the free energy density. The quadratic term $\mu(T)$ would vanish at T_c, and if we expand $\mu(T) \sim a(T - T_c) + \ldots$ we find $m = \pm\sqrt{6a/g}\sqrt{T_c - T}$ near the critical temperature.

[11] The total free energy is convex (Fig. 11.2(a)). The free energy density $\mathcal{F}$ in Fig. 1 can have a barrier if a boundary between the phases is thicker than the coarse-graining length. The total free energy also has singularities at phase transitions. $\mathcal{F}$ can be analytic because it is the free energy of a finite region; thermal phase transitions do not occur in finite systems.

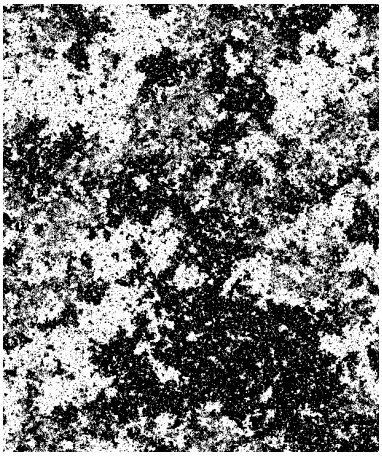

Fig. 2 Fluctuations on all scales. A snapshot of the Ising model at T_c. Notice that there are fluctuations on all length scales.

This is qualitatively correct, but quantitatively wrong. The magnetization does vanish at T_c with a power law $m \sim (T_c - T)^\beta$, but the exponent β is not generally 1/2; in two dimensions it is $\beta_{\rm 2D} = 1/8$ and in three dimensions it is $\beta_{\rm 3D} \approx 0.32641\ldots$. These exponents (particularly the presumably irrational one in 3D) cannot be fixed by keeping more or different terms in the analytic Landau expansion.

(d) *Show that the power-law $\beta_{\rm Landau} = 1/2$ is not changed in the limit $T \to T_c$ even when one adds another term $(h/6!)\, m^6$ into eqn 6. (That is, show that $m(T)/(T - T_c)^\beta$ goes to a constant as $T \to T_c$.)* (Hint: You should get a quadratic equation for m^2. Keep the root that vanishes at $T = T_c$, and expand in powers of h.) *Explore also the alternative phase transition where $g \equiv 0$ but $h > 0$; what is β for that transition?*

As we see in Fig. 2 there is no length W above which the Ising model near T_c looks smooth and uniform. The Landau free energy density gets corrections on all length scales; for the infinite system the free energy has a singularity at T_c (making our power-series expansion for $\mathcal{F}^{\rm Ising}$ inadequate). The Landau free energy density is only a starting-point for studying continuous phase transitions;[12] we must use the renormalization-group methods of Chapter 12 to explain and predict these singularities.

12.17 **Random walks and critical exponents.** ⓘ

Figure 2.2 shows that a random walk appears statistically self-similar. Random walks naturally have self-similarity and power laws: they are said to exhibit *generic scale invariance.*

[12] An important exception to this is superconductivity, where the Cooper pairs are large compared to their separation. Because they overlap so many neighbors, the fluctuations in the order parameter field are suppressed, and Landau theory is valid even very close to the phase transition.

(a) *Argue that the fractal dimension of the random walk is two, independent of dimension (see note 6, p. 27.)* (Hint: How does the mass of the ink T needed to draw the walk scale with the distance d between endpoints?)

DNA has a *persistence length* of 50nm; one can model it roughly as a random walk with a step size of the persistence length. The diameter of a DNA molecule is 2nm, and will not overlap with itself during the random walk. Will the thickness change the power law $d \sim T^{\nu}$ relating distance d versus length T, and hence the fractal dimension $1/\nu$? More generally, are *self-avoiding* random walks a different universality class?

(b) *Show that $d_f = \nu = 1$ for a one-dimensional self-avoiding random walk.* (Hint: The are only two allowed walks.)

We can think about self-avoidance in general dimensions by asking whether a typical random walk will intersect itself. In the spirit of the renormalization group, let us divide a long polymer of N persistence lengths into M segments, with $1 \ll M \ll N$, each of which forms a fuzzy blob of dimension d_f. Suppose two of the blobs from distant parts of the polymer overlap. Each may have lots of empty space between the polymer segments, so they may or may not intersect even if they overlap. If they typically intersect, intersections would happen on all scales, and the critical exponents would likely change. If overlapping blobs rarely intersect, one would reasonably expect that the polymer would act like an ordinary random walk on long length scales.

(c) *What is the likely dimension of the intersection of two D-dimensional smooth surfaces in the same vicinity of $\mathbb{R}^d$?* (Hint: We can define a smooth D dimensional set in d dimensions as the solution of $d - D$ constraint equations. Check your answer for two curves on the plane (which typically intersect in isolated points), and two curves in three dimensions (which typically will miss one another).) *Argue by analogy that* self-avoiding *random walks in dimensions two and three will likely have a different fractal dimension than ordinary random walks (see note 9, p. 29 and Exercise 2.10), but in dimensions above four they could be in the same universality class.*

Indeed, it turns out that self-avoiding random walks have $\nu_{2D} = 3/4$ and $d_f = 4/3$ in two dimensions, $\nu_{3D} \approx 0.588$ and $d_f = 1/\nu_{3D}$ in three dimensions, and logarithmic corrections in four dimensions; above four dimensions (the 'upper critical dimension') they obey the 'mean-field' behavior of ordinary random walks at long length scales.

This pattern (varying critical exponents shifting to mean-field above an upper critical dimension) is common to most statistical mechanical models. Also, we should note that the self-avoiding random walk can be viewed as the limit of an n-component spin model as $n \to 0$; the Ising model ($n = 1$) also obeys mean-field theory above four dimensions.

12.4 **Bifurcation theory.** (Dynamical systems)ⓘ

Dynamical systems theory is the study of the time evolution given by systems of differential equations. Let $\mathbf{x}(t)$ be a vector of variables evolving in time t, let $\boldsymbol{\lambda}$ be a vector

of parameters governing the differential equation, and let $\mathbf{F}_\lambda(\mathbf{x})$ be the differential equations

$$\dot{\mathbf{x}} \equiv \frac{\partial \mathbf{x}}{\partial t} = \mathbf{F}_\lambda(\mathbf{x}). \tag{7}$$

The typical focus of the theory is not to solve the differential equations for general initial conditions, but to study the qualitative behavior. In general, they focus on *bifurcations*—special values of the parameters $\boldsymbol{\lambda}$ where the behavior of the system changes qualitatively.

(a) *Consider the differential equation in one variable $x(t)$ with one parameter μ:*

$$\dot{x} = \mu x - x^3. \tag{8}$$

Show that there is a bifurcation at $\mu_c = 0$, by showing that an initial condition with small, non-zero $x(0)$ will evolve qualitatively differently at late times for $\mu > 0$ versus for $\mu < 0$. Hint: Although you can solve this differential equation explicitly, we recommend instead that you argue this qualitatively from the bifurcation diagram in Fig. 3; a few words should suffice.

Dynamical systems theory has much in common with equilibrium statistical mechanics of phases and phase transitions. The liquid–gas transition is characterized by external parameters $\boldsymbol{\lambda} = (P, T, N)$, and has a current state described by $\mathbf{x} = (V, E, \mu)$. Equilibrium phases correspond to fixed-points ($x^*(\mu)$ with $\dot{x}^* = 0$) in the dynamics, and phase transitions correspond to bifurcations.[13] For example, the power laws we find near continuous phase transitions have simpler analogues in the dynamical systems.

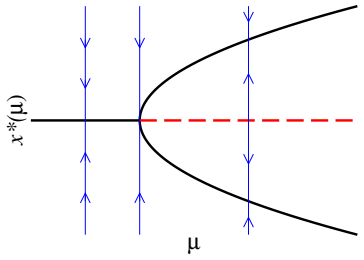

Fig. 3 Pitchfork bifurcation diagram. The flow diagram for the pitchfork bifurcation (eqn 8). The dashed line represents unstable fixed-points, and the solid thick lines represent stable fixed-points. The thin lines and arrows represent the dynamical evolution directions. It is called a pitchfork because of the three tines on the right emerging from the handle on the left.

(b) *Find the critical exponent β for the pitchfork bifurcation, defined by $x^*(\mu) \propto (\mu - \mu_c)^\beta$ as $\mu \to \mu_c$.*

[13] In Section 8.3, we noted that inside a phase all properties are analytic in the parameters. Similarly, bifurcations are values of λ where non-analyticities in the long-time dynamics are observed.

Bifurcation theory also predicts universal behavior; all pitchfork bifurcations have the same scaling behavior near the transition.

(c) *At what value λ_c does the differential equation*

$$\dot{m} = \tanh(\lambda m) - m \tag{9}$$

have a bifurcation? Does the fixed-point value $m^*(\lambda)$ behave as a power law $m^* \sim |\lambda - \lambda_c|^\beta$ near λ_c (up to corrections with higher powers of $\lambda - \lambda_c$)? Does the value of β agree with that of the pitchfork bifurcation in eqn 8?

Just as there are different universality classes for continuous phase transitions with different renormalization-group fixed points, there are different classes of bifurcations each with its own *normal form*. Some of the other important normal forms include the saddle-node bifurcation,

$$\dot{x} = \mu - x^2, \tag{10}$$

transcritical exchange of stability,

$$\dot{x} = \mu x - x^2, \tag{11}$$

and the Hopf bifurcation,

$$\begin{aligned} \dot{x} &= (\mu - (x^2 + y^2))x - y, \\ \dot{y} &= (\mu - (x^2 + y^2))y + x. \end{aligned} \tag{12}$$

Thus normal form theory describes universality classes for continuous transitions in low-dimensional dynamical systems. It also describes continuous transitions in mean-field theory (Exercise 12.5). Finally, the renormalization group transforms coarse-graining of statistical mechanical systems into an ordinary differential equation in system space – the domain of dynamical systems theory. Normal form theory [2] explains why one can linearize this flow (by changing variables) if the fixed point is suitably hyperbolic, and the normal forms for those cases that cannot be linearized can be used to group the exceptions into universality *families*.

References

[1] Langer, S. A. and Sethna, J. P. (1986). Textures in a chiral smectic liquid crystal film. *Physical Review A*, **34**, 5305.

[2] Raju, A., Clement, C. B., Hayden, L. X., Kent-Dobias, J. P., Liarte, D. B., Rocklin, D. Z., and Sethna, J. P. (2017). Renormalization group and normal form theory. *(submitted)*.

[3] Sethna, J. P. (1985). Frustration, curvature, and defect lines in metallic glasses and cholesteric blue phases. *Physical Review B*, **31**, 6278.