Chapter 11

Phase Transition and Low Temperature Physics

5. Landau Theory of Second Order Phase Transitions

Order Parameter

Second order phase transitions occur when a new state of reduced symmetry develops continuously from the disordered (high temperature) phase. The ordered phase has a lower symmetry than the Hamiltonian – the phenomenon of spontaneously broken symmetry. There will therefore be a number (sometimes infinite) of equivalent (e.g. equal free energy) symmetry related states. These are macroscopically different, and so thermal fluctuations will not connect one to another in the thermodynamic limit. To describe the ordered state we introduce a macroscopic order parameter that describes the character and strength of the broken symmetry.

Examples

1. Ising ferromagnet: the Hamiltonian is invariant under all $s_i \to -s_i$, whereas the low temperature phase has a spontaneous magnetization, and so is not. A convenient order parameter is the total average spin $S = \sum_i (s_i)$ or the magnetization $M = \mu S$. This reflects the

nature of the ordering (under the transformation $s_i \rightarrow -s_i$ we have $S \rightarrow -S$) and goes to zero continuously at T_c.

2. Ising antiferromagnet on a simple cubic lattice: the ordering is the staggered magnetization $N = \sum_n (-1)^n (\vec{s}_n)$ where alternate sites are labelled even or odd.

3. Heisenberg ferromagnet: now the Hamiltonian is invariant under any rotation of all the spins together. The ordering is characterized by a vector order parameter. A convenient choice is again the total spin $\vec{S} = \sum_i \langle \vec{s}_i \rangle$ or magnetization.

4. Heisenberg antiferromagnet on a simple cubic lattice: the staggered magnetization is now a vector $\vec{N} = \sum_n (-1)^n \langle \vec{s}_n \rangle$.

5. Superfluid: the broken symmetry is the invariance of the (quantum) Hamiltonian under a phase change of the wave function. Since for a charge system a gauge transformation also changes the quantum phase, this is also known as broken gauge symmetry. The order parameter can be thought of as the one particle wave function into which the particle Bose condense, multiplied by the number of condensed atoms. This picture is good for a non - or weakly interacting system. For a strongly interacting system a better definition is the "expectation value of the particle annihilation operator" $\langle \psi(\vec{r}) \rangle$.

6. Solid: has broken translational and rotational symmetry, and a convenient order parameter is the amplitude of the density wave. In three dimensions the liquid – solid transition is always first order, but in two dimensions may be second order.

7. Nematic liquid crystal: consists of long molecules which align parallel to one another at low temperatures, although the position of the molecules remains disorder as in a liquid. The liquid becomes anisoiropic and a second rank tensor characterizes the strength of the anisotropy and can be used as the order parameter.

Free energy expansion

Since the order parameter grows continuously from zero at the transition temperature. Landau suggested that an expansion of the free energy in a Taylor expansion in the order parameter would tell us about the behavior near the transition. The free energy must be invariant under all symmetry operations of the Hamiltonian, and the terms in the expansion are restricted by symmetry considerations.

The order parameter may eonceivably take on different values ("point in different directions") in different pads of the system (for example due to thermal fluctuations), and so we first write

$$F = \int d^3x f(\psi, T) \qquad \text{(i)}$$

introducing the free energy density f which is a function of the local order parameter $\psi(\vec{r})$ and temperature, and is then expanded in small ψ.

To be explicit, lets consider the Ising ferromagnet, and $\psi = m(\vec{r})$, with $m(\vec{r})$ the magnetization per unit volume or the magnetization per spin averaged over some reasonably macroscopic volume. Since the free energy is invariant under spin inversion, the Taylor expansion must contain only even powers of m. Hence

$$f(m,T) = f_0(T) + \alpha(T)m^2 + \frac{1}{2}\beta(T)m^4 + \gamma(T)\vec{\nabla}m \cdot \vec{\nabla}m \qquad \text{(ii)}$$

The last term in the expansion gives a free energy cost for a non-uniform $m(\vec{r})$, again using the idea of a Taylor expansion, now in spatial derivatives as well. A positive γ ensures that the spatially uniform state gives the lowest value of the free energy F. Sixth and higher order terms in m could be retained, but are not usually necessary for the important behavior near T_c. Note that we keep the fourth order term, because at T_c the coefficient of the second order term $\alpha(T)$ becomes zero. Only quadratic derivative terms are usually needed since $\gamma(T_c)$ remains nonzero.

Minimum Free Energy

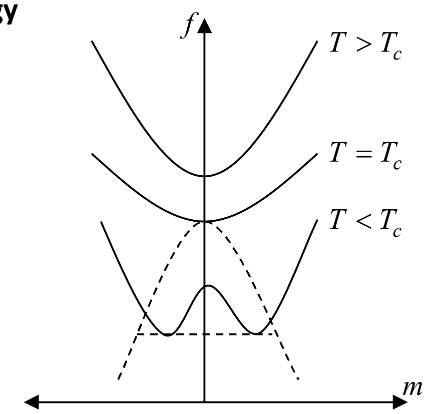

Figure: Free energy density f as a function of (uniform) m. Below T_c new minima at nonzero $\pm\bar{m}$ develop (the dashed curve denote $\bar{m}(T)$. If the magnetization of the system is varied (rather than the field) the dotted line is the tie line giving the variation of the free energy as a function of the total magnetization density $m = M/V$.

We expect the state that minimizes the free energy to be the physically realized state. This is true so long as the fluctuations around this most probably value are small compared to this value. We will find that this is not always the ease, and Landau's theory then corresponds to a mean field theory that ignores these fluctuations.

For the Ising ferromagnet the minimum of A is given by a uniform $m(\vec{r})=\bar{m}$ satisfying

$$\alpha\bar{m}+\beta\bar{m}^3=0 \tag{3}$$

The solutions corresponding to a minimum are

$$\bar{m}=\pm\sqrt{-\alpha/\beta} \text{ for } \alpha<0 \tag{4a}$$

$$=0 \text{ for } \alpha>0 \tag{4b}$$

We identify $\alpha=0$ as where the temperature passes through T_c and expand near here

$$\alpha(T)\approx a(T-T_c)+... \tag{5a}$$

$$\beta(T)\approx b+.... \tag{5b}$$

$$\gamma(T)\approx\gamma+.... \tag{5c}$$

so that

$$f\approx f_0(T)+a(T-T_c)m^2+\frac{1}{2}bm^4+\gamma\left(\vec{\nabla}m\right)^2 \tag{6}$$

and $$\bar{m}\approx\left(\frac{a}{b}\right)^{1/2}(T_c-T)^{1/2} \text{ for } T<T_c \tag{7}$$

Evaluating f at $\bar{m}$ gives

$$\bar{f}=f_0-\frac{a^2(T-T_c)^2}{2b} \tag{8}$$

showing the lowering of the free energy by the ordering. Note that $\bar{f}(T)$ deviates from f_0 quadratically, as we found for the mean field theory of the Ising ferromagnet. This will yield a jump discontinuity in the specific heat

$$c=\begin{cases} c_0 & T\geq T_c \\ c_0+\dfrac{a}{b}T & T<T_c \end{cases} \tag{9}$$

with c_0 the smooth contribution coming from $f_0(T)$.

We can gain useful insight into the transition by plotting $f(m)$ for a uniform m for various temperatures, as in figure. For $T>T_c$ the free energy has a single minimum at $m=0$. Below T_c

two new minima at $\pm\bar{m}$ develop. Right at T_c the curve is very flat at the minimum (varying as m): we might expect fluctuations to be particularly important here.

It is easy to add the coupling to a magnetic field

$$f(m,T,B) = f_0(T) + a(T - T_c)m^2 + \frac{1}{2}bm^4 + \gamma(\vec{\nabla}m)^2 - mB \qquad (10)$$

The magnetic field couples directly to the order parameter and is a symmetry breaking field: with the magnetic field the full Hamiltonian is not invariant under spin inversion. Now the free energy is minimized by a non zero m. Minimizing f again with respect to m, we find the above T_c the diverging susceptibility

$$\chi = \left.\frac{\bar{m}}{B}\right|_{B=0} = \frac{1}{2a}(T - T_c)^{-1} \qquad (11)$$

and at $T = T_c$ for small B

$$m = \left(\frac{1}{2b}\right)^{1/3} B^{1/3} \qquad (12)$$

Note that the exponents (power laws) are the same as we found in the direct mean field theory calculations.