

Chapter 5: The Berezinskii-Kosterlitz-Thouless transition

So far, we have assumed that the ϕ^4 theory used in the previous chapter has a discrete Z_2 symmetry, i.e., $H[-\phi(x)] = H[\phi(x)]$. On the other hand, if the order parameter is complex, the associated symmetry is actually a continuous $U(1)$ symmetry since the Ginzburg-Landau-Wilson Hamiltonian

$$H = \int dx v_2 |\nabla \phi(x)|^2 + u_2 |\phi(x)|^2 + u_4 |\phi(x)|^4 \quad (1)$$

is invariant under the transformation $\phi(x) \rightarrow \exp(i\theta)\phi(x)$.

One important consequence is that there are new excitations in the symmetry broken phase of a $U(1)$ phase. Since travelling along the θ direction in the symmetry broken phase does not cost any energy, these excitations are massless and their counterparts in quantum field theory are known as Goldstone bosons. On the other hand, the excitation along the radial direction of the order parameter field still costs energy, so these are massive excitations.

I. THE XY MODEL

One particularly important model that exhibits this $U(1)$ symmetry is the XY model, a spin model that is a slight extension of the Ising model. Its Hamiltonian is given by

$$H = -J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j = -J \sum_{\langle ij \rangle} (S_i^x S_j^x + S_i^y S_j^y), \quad (2)$$

with the spins \mathbf{S}_i being subject to the constraint that their length is unity. This allows to parametrize the spin vector by a single angle θ_i as

$$\mathbf{S}_i = \begin{pmatrix} \cos \theta_i \\ \sin \theta_i \end{pmatrix}, \quad (3)$$

leading to the Hamiltonian

$$H = -J \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j). \quad (4)$$

Clearly, the Hamiltonian is invariant under the transformation $\theta_i \rightarrow \theta_i + \alpha$, which is a manifestation of the $U(1)$ symmetry of the model.

To get a better feeling for the XY model, we first perform a mean-field analysis as in Chapter 2. As before, we also introduce an external field h along the x direction, which will lead us to the mean-field Hamiltonian

$$H_{MF} = -J \sum_{\langle ij \rangle} \left[\langle \cos \theta_j \rangle \cos \theta_i + \langle \sin \theta_j \rangle \sin \theta_i - \frac{1}{2} (\langle \cos \theta_i \rangle \langle \cos \theta_j \rangle + \langle \sin \theta_i \rangle \langle \sin \theta_j \rangle) \right] - h \sum_i \cos \theta_i. \quad (5)$$

We now introduce the complex order parameter $\langle \exp(i\theta_i) \rangle = m \exp(i\theta_0)$. Since the interaction does not depend of the global phase factor θ_0 , the mean-field energy is minimized by aligning θ_0 with the external field, i.e., $\theta_0 = 0$. Then, we obtain

$$H_{MF} = \sum_i -(zJm + h) \cos \theta_i - \frac{zJm^2}{2}. \quad (6)$$

Calculating the mean-field partition function leads us to

$$Z_{MF} = \left[\int d\theta_i \exp(\beta(zJm + h) \cos \theta_i) \exp\left(\frac{\beta zJm^2}{2}\right) \right]^N \quad (7)$$

$$= \left[2\pi I_0(\beta[h + zJm]) \exp\left(\frac{\beta zJm^2}{2}\right) \right]^N, \quad (8)$$

where I_o denotes the modified Bessel function. As for the Ising model, we can compute the mean-field equation of state according to $m = (\beta N)^{-1} \partial/\partial h \log Z$, which yields to

$$m = \frac{I_1(\beta(2zmJ + h))}{I_0(\beta(2zmJ + h))}. \quad (9)$$

Expanding for small m , we obtain in the limit of a vanishing field

$$m = \beta zJm - \frac{(\beta zJm)^3}{2} + O(m^5). \quad (10)$$

This expression has the same form as the mean-field equation of state for the Ising model. Therefore, the set of (mean-field) critical exponents is identical.

II. THE MERMIN-WAGNER THEOREM

From our RG analysis, we know that the mean-field picture is only correct above four spatial dimensions. However, this does not tell us much about what happens below the upper critical dimension. Even performing an ϵ expansion might be tricky, as for the physical

dimensions two and three, the expansion series is formally divergent. Of course, this is especially true in two dimensions, where fluctuations are even stronger.

To understand the implications of fluctuations in two dimensions, it is instructive to look at the continuum field theory of the XY model. Here, we will only look at phase fluctuations, i.e., the massless Goldstone modes. Starting from the Hamiltonian in the form

$$H = -J \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j), \quad (11)$$

we can expand the Hamiltonian for weak phase fluctuations according to

$$H = -J \sum_{\langle ij \rangle} (\theta_i - \theta_j)^2 + \text{const.} \quad (12)$$

In the continuum limit, these terms simply reduce to the quadratic fluctuations of the θ fields,

$$H = \int dx v_2 [\nabla \theta(x)]^2. \quad (13)$$

Note that this field theory is a Gaussian theory in the absence of a mass term proportional to $\theta(x)^2$. Hence, the correlation function of the field is given by [cf. Eq. (3.21)]

$$G_\theta(x) = \langle \theta(x) \theta(0) \rangle = \int \frac{dq}{(2\pi)^d} \frac{\exp(iqx)}{\beta v_2 q^2}. \quad (14)$$

Since the correlation function satisfies

$$\beta v_2 \nabla^2 \theta(x, 0) = \delta(x), \quad (15)$$

we may make use of Gauss' theorem to carry out the Fourier transform. In particular, we have

$$1 = \beta v_2 \int dx \nabla^2 \theta(x, 0) = \beta v_2 \oint dS \nabla G_\theta(x). \quad (16)$$

The surface integral can be evaluated for the angular variables in hyperspherical coordinates [1], leading to

$$1 = \beta v_2 S_d x^{d-1} \frac{dG_\theta(x)}{dx}. \quad (17)$$

The resulting differential equation can be readily solved, yielding

$$G_\theta(x) = \frac{x^{2-d}}{(2-d) S_d \beta v_2} + \theta_0, \quad (18)$$

where θ_0 is a integration constant that only affects the short distance behavior of the correlation function. In contrast, the long distance behavior strongly depends on the spatial dimensions, i.e.,

$$\lim_{x \rightarrow \infty} G_\theta(x) \sim \begin{cases} \theta_0 & d > 2 \\ x^{2-d} & d < 2 \\ \ln(x) & d = 2. \end{cases} \quad (19)$$

Crucially, the correlation function diverges for dimension two and lower. Since the phase $\theta(x)$ gets wrapped around at 2π , this implies that the phases of the order parameter field $\phi(x)$ are completely random at large distances. In this case the correlation function $\langle \phi(x)\phi^*(0) \rangle$ also vanishes [1], i.e., there cannot be a spontaneous symmetry breaking in two dimensions or lower, a statement known as the Mermin-Wagner theorem. Note that our analysis applies to any model that has a continuous symmetry leading to a Goldstone mode, provided that the interaction is sufficiently short-ranged [2].

III. VORTICES IN TWO DIMENSIONS

Let us take a more detailed look at the two-dimensional case. The angular correlation function can be written as,

$$G_\theta(x) = \frac{1}{\pi K} \log(x/x_0), \quad (20)$$

where we have introduced $K = \beta v_2/2$ and the short distance cutoff x_0 , which is equivalent to the integration θ_0 . For Gaussian variables, the correlation function of the order parameter field ϕ may be calculated as [1]

$$\langle \phi(x)\phi^*(0) \rangle = \langle e^{i[\theta(x)-\theta(0)]} \rangle = \exp \left[-\frac{1}{2} G_\theta(x) \right] = \left(\frac{x_0}{x} \right)^{\frac{1}{2\pi K}}. \quad (21)$$

Remarkably, this correlation function describes an algebraic power law decay, like what one normally would expect to find in a system close to a critical point. We also note that this behavior is at odds with the behavior of the correlation function expected for a high temperature phase, which follows an exponential decay according to

$$\langle \phi(x)\phi^*(0) \rangle \sim e^{-x/\xi}. \quad (22)$$

This implies that the algebraic correlation function of Eq. (21) is only valid for low temperatures. Since it is not possible to analytically connect the power law behavior to the

exponential case, there must be a phase transition between these two regimes. Since Eq. (21) describes an algebraic behavior for all temperatures, it is evident that we are missing something here.

It might be tempting to think that the higher order corrections to the Gaussian theory might be responsible for the phase transition, i.e., quartic terms of the form $[\nabla\theta(x)]^4$. The RG treatment of the Goldstone modes is quite involved in order to respect their symmetry properties. The details are found in [1], with the final RG flow for the temperature T being given in the lowest order by

$$\frac{dT}{dl} = -(d-2)T + (n-2)\frac{S_d}{(2\pi)^d}\Lambda^{d-2}T^2, \quad (23)$$

where n is the number of components in the spin vector (i.e., $n = 2$ for the XY model). The RG flow vanishes for $d = 2$ and $n = 2$, such perturbations are commonly referred to as being “marginal”. Crucially, this is actually true for all orders in T [3], leading to a serious challenge to our whole Ginzburg-Landau-Wilson machinery.

The reason for this problem is our assumption of a slowly varying field $\theta(x)$. Going to polar coordinates, consider the parameter field $\theta(r, \phi)$ given by

$$\theta(r, \varphi) = \varphi + \theta_0. \quad (24)$$

Note that the gradient term $\nabla\theta = 1/r$ diverges at the origin, which can be cured by letting the order parameter field $\varphi(x)$ vanish there such that the phase $\theta(0)$ is not defined [4]. Such a configuration is called a vortex. Vortices are characterized by their winding number n , which is given by the condition $\phi(\theta) = \phi(\theta + 2n\pi)$, i.e., the periodicity of the order parameter field with respect to the angular part. One can compute the winding number by considering a closed curve at constant r that is parameterized according to $\theta(r, \varphi(t))$. Then, the winding number is given by

$$n = \frac{\theta(t_f) - \theta(t_i)}{2\pi}. \quad (25)$$

Importantly, vortices are topological defects as they cannot be removed by continuously deforming the order parameter field. This also has implications for the stability of vortex excitations of a system. Although vortex excitations have a large energy associated with them ($\sim J \ln L$), the energy barrier for removing them scales even stronger with system size ($\sim JL$) [4]. Therefore, it is very important to consider vortex excitations when dealing with a two-dimensional XY model.

In a sufficiently large system, we can expect configurations containing more than one vortex. If we have two vortices with opposite winding numbers, we are able to continuously deform the system to a perfectly aligned state, as long as we look at the spins far away from the vortex pair.

IV. VORTEX ENERGIES

The energy stored in a vortex consists of two parts. The first part is the core energy E_c describing the energy cost of setting the order parameter field to zero at the center of the vortex to avoid any singular behavior. The exact value of E_c depends on the microscopic details and is usually quite involved to calculate [4]. Here, we capture the core energy in terms of a chemical potential to create vortices with winding number $n = \pm 1$, which we can cast into a fugacity of the form

$$y_0 = \exp(-\beta E_c^{\pm 1}). \quad (26)$$

The second part comes from the interaction between the vortices. Consider a system of vortices with winding number n_i at positions x_i . For any closed loop enclosing a vortex, we have the relation $\oint(\nabla\theta)dS = 2n_i\pi$. Note that this expression is nothing but the integral form of Gauss' law in two dimensions. Hence, the interaction energy between two vortices is the same as the interaction energy between two (topological) charges. Note, however, that in two dimensions, the solution to the Laplace equation

$$\nabla^2\psi = 2\pi \sum_i n_i \delta(x - x_i) \quad (27)$$

is no longer the usual Coulomb energy scaling like $1/|x_i|$, but instead we obtain

$$\psi(x) = \sum_i n_i \ln(|x - x_i|). \quad (28)$$

Therefore, the Ginzburg-Landau-Wilson Hamiltonian of a system of interacting vortices is given by

$$\beta H = \sum_i \beta E_c^{\pm 1} - 4\pi^2 K \sum_{i < j} n_i n_j \ln |x_i - x_j|. \quad (29)$$

V. RG ANALYSIS OF THE TWO-DIMENSIONAL COULOMB GAS

The RG analysis is quite complicated [1], so we only discuss the final result. We have two coupling constants, the inverse temperature K and the fugacity y_0 . Within a perturbative treatment of the fugacity, the flow equations are given by

$$\frac{dK^{-1}}{dl} = 4\pi^3 a^4 y_0^2 \quad (30)$$

$$\frac{dy_0}{dl} = (2 - \pi K)y_0. \quad (31)$$

Interestingly, the relation for y_0 changes sign at $K_c^{-1} = \pi/2$. For large K (i.e., low temperatures) and small y_0 , the RG flows terminate on the line $y_0 = 0$. This describes the phase where vortices are bound together and appear only rarely in the system. In this phase, the correlations decay algebraically, according to (cf. 21)

$$\langle \exp(i[\theta(x) - \theta(0)]) \rangle = \left(\frac{x_0}{x}\right)^{\frac{1}{2\pi K_\infty}}, \quad (32)$$

with $K_\infty = \lim_{l \rightarrow \infty} K(l)$ [1]. For larger temperatures or y_0 , the flows diverge towards larger values, where the perturbative treatment of y_0 eventually breaks down. This is the disordered

high-temperature phase, in which vortices are no longer bound together (i.e., a plasma of vortices of opposite charge) and correlations decay exponentially.

Close to the critical point at $K_c^{-1} = \pi/2$ and $y_0 = 0$, the flow equations are given by

$$\frac{dx}{dl} = 4\pi^3 y^3 \quad (33)$$

$$\frac{dy}{dl} = \frac{4}{\pi} xy, \quad (34)$$

where we have introduced the variables $x = 1/K - \pi/2$ and $y = y_0 a^2$. Crucially, even in lowest order, the flow equations are nonlinear, in contrast to the cases that we studied previously. This nonlinearity has important consequences.

Eqs. (33–34) can be rewritten as

$$\frac{d}{dl}(x^2 - \pi^4 y^2) = 0, \quad (35)$$

which has the solution

$$x^2 - \pi^4 y^2 = c. \quad (36)$$

Since the critical point is characterized by $x = 0$ and $y = 0$, the constant c has to vanish there. Therefore, c controls the distance to the critical point, which we can capture in terms of the temperature T , according to.

$$c = b^2(T - T_c), \quad (37)$$

where b is an unimportant prefactor. We can now use this expression to evaluate several important quantities. For instance, K_∞ is then given by

$$K_\infty = \frac{2}{\pi} - \frac{4}{\pi^2} \lim_{x \rightarrow \infty} x(l) = \frac{2}{\pi} + \frac{4b}{\pi^2} \sqrt{T_c - T}, \quad (38)$$

which now itself is non-analytic at the phase transition. Furthermore, we can evaluate the decay of correlation function in the high temperature phase. Using (33), we can write

$$\frac{dx}{dl} = 4\pi^3 y^2 = \frac{4}{\pi} [x^2 + b^2(T - T_c)], \quad (39)$$

which has a solution of the form

$$\arctan\left(\frac{x}{b\sqrt{T - T_c}}\right) = \frac{4b\sqrt{T - T_c}}{\pi} l. \quad (40)$$

Importantly, the integration has to be stopped when the $x(l) \sim 1$, as then our perturbative treatment breaks down [1]. Crucially, this happens at a scale

$$l^* \approx \frac{\pi^2}{8b\sqrt{T - T_c}}, \quad (41)$$

which can be cast into the correlation length

$$\xi = a \exp(l^*) = a \exp\left(\frac{\pi^2}{8b\sqrt{T - T_c}}\right). \quad (42)$$

Note that the correlation length is no longer a power law even close to the transition! For the singular part of the free energy,

$$f_{sing} \sim \xi^{-2} = a \exp\left(-\frac{\pi^2}{4b\sqrt{T - T_c}}\right). \quad (43)$$

This is an essential singularity, i.e., the function is non-analytic but differentiable up to infinite orders.

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