Appendix B

*Berezinskii-Kosterlitz-Thouless Transition

The Berezinskii-Kosterlitz-Thouless phase transition is unusual since it is driven by the condensation of topological defects. Although arguments for the existence of a transition were presented in chapter 5, a quantitative theory was absent. In this appendix we develop a renormalisation group procedure to verify the existence of a transition and study the critical phenomena. Out starting point will be a model in which the topological defects are separated from harmonic phase fluctuations of the field.

B.1 Effective Hamiltonian

Taking our notation from chapter 5, the distortion field, $\mathbf{u} \equiv \nabla\theta$, in the presence of a collection of vortices is similar to the velocity of a fluid. In the absence of vorticity, the flow is *potential*, i.e. $\mathbf{u} = \mathbf{u}_0 = \nabla\phi$, and $\nabla \times \mathbf{u}_0 = 0$. The topological charge can be related to $\nabla \times \mathbf{u}$ by noting that for any closed path

$$\oint \mathbf{u} \cdot d\mathbf{s} = \int (d^2\mathbf{x}\ \hat{z}) \cdot \nabla \times \mathbf{u},$$

where the second integral is over the area enclosed by the path. Since the left hand side is an integer multiple of 2π, we can set

$$\nabla \times \mathbf{u} = 2\pi\hat{z} \sum_i n_i \delta^2(\mathbf{x} - \mathbf{x}_i),$$

describing a collection of vortices of charge $\{n_i\}$ at locations $\{\mathbf{x}_i\}$. The solution to this equation can be obtained by setting $\mathbf{u} = \mathbf{u}_0 - \nabla \times (\hat{z}\psi)$, leading to

$$\nabla \times \mathbf{u} = \hat{z}\nabla^2\psi \Longrightarrow \nabla^2\psi = 2\pi \sum_i n_i \delta^2(\mathbf{x} - \mathbf{x}_i).$$

Thus ψ behaves like the potential due to a set of charges $\{2\pi n_i\}$. The solution

$$\psi(\mathbf{x}) = \sum_i n_i \ln(|\mathbf{x} - \mathbf{x}_i|),$$

is simply a superposition of the potentials. Any two-dimensional distortion can thus be written

$$\mathbf{u} = \mathbf{u}_0 + \mathbf{u}_1 = \nabla\phi - \nabla \times (\hat{z}\psi),$$

and the corresponding "kinetic energy", $\beta H = K \int d^2\mathbf{x}|\mathbf{u}|^2/2$, decomposed as

$$\beta H = \int d^2\mathbf{x} \left[(\nabla\phi)^2 - 2\nabla\phi \cdot \nabla \times (\hat{z}\psi) + (\nabla \times \hat{z}\psi)^2\right].$$

An integration by parts shows the second term to vanish ($\nabla \cdot \nabla \times \mathbf{u} = 0$), while the third term can be simplified by noting that $\nabla\psi$ and $\nabla \times (\hat{z}\psi)$ are orthogonal vectors of equal length. Hence

$$\beta H_1 \equiv \frac{K}{2} \int d^2\mathbf{x}(\nabla \times \hat{z}\psi)^2 = \frac{K}{2} \int d^2\mathbf{x}(\nabla\psi)^2 = -\frac{K}{2} \int d^2\mathbf{x}\psi\nabla^2\psi.$$

Finally, using Eqs. (B.1) and (B.1) we obtain

$$\begin{aligned} \beta H_1 &= -\frac{K}{2} \int d^2\mathbf{x} \left(\sum_i n_i \ln(|\mathbf{x} - \mathbf{x}_i|)\right) \left(2\pi \sum_i n_i \delta^2(\mathbf{x} - \mathbf{x}_i)\right) \\ &= -2\pi^2 K \sum_{ij} n_i n_j C(\mathbf{x}_i - \mathbf{x}_j), \end{aligned}$$

where $C(\mathbf{x}) = \ln|\mathbf{x}|/2\pi$ is the two-dimensional Coulomb potential. The breakdown of the continuum approximation results in an unphysical divergence for $i = j$ and should be replaced with the core energy βE_n^0.

$$\beta H_1 = \sum_i \beta E_{n_i}^0 - 4\pi^2 K \sum_{i<j} n_i n_j C(\mathbf{x}_i - \mathbf{x}_j), \tag{B.1}$$

The configuration space of the XY-model close to zero temperature can thus be partitioned into different topological components: One set arises from the degrees of freedom associated with the charges, $\{n_i\}$, while the other reflects the elementary spin-wave excitations of the field $\phi(\mathbf{x})$. The partition function of the model is then approximately given by

$$\mathcal{Z} = \prod_i \int_0^{2\pi} \frac{d\theta_i}{2\pi} \exp\left[K \sum_{\langle ij\rangle} \cos(\theta_i - \theta_j)\right] \propto \mathcal{Z}_{\text{s.w.}} \mathcal{Z}_{\text{Q}},$$

$$\mathcal{Z}_{\text{s.w.}} = \int D\phi \exp\left[-\frac{K}{2} \int d^2\mathbf{x}\ (\nabla\phi)^2\right], \qquad \mathcal{Z}_{\text{Q}} = \sum_{\{n_i\}} \int d^2\mathbf{x}_i e^{-\beta H_1},$$

$\mathcal{Z}_{\text{Q}}$ describes a grand canonical gas of charged particles interacting via the two-dimensional Coulomb interaction. In obtaining Eq. (B.1) we performed an integration by parts. The surface integral that was ignored in the process in fact grows with system size as $(\sum_i n_i)\ln L$. Thus only configurations that are overall neutral are included in $\mathcal{Z}_Q$.

The problem is further simplified by considering only the elementary excitations with $n_i = \pm 1$, which are energetically most favoured at low temperatures. If we define the fugacity of the vortices as $y_0 \equiv \exp[-\beta E^0_{\pm 1}]$,

$$\mathcal{Z}_Q = \sum_{N=0}^{\infty} y_0^N \int \prod_{i=1}^{N} d^2\mathbf{x}_i \exp\left[4\pi^2 K \sum_{i<j} q_i q_j C(\mathbf{x}_i - \mathbf{x}_j)\right], \tag{B.2}$$

where $q_i = \pm 1$, and $\sum_i q_i = 0$.

B.1.1 Screening of Vortices

Since $\mathcal{Z}_{\text{s.w.}}$ and $\mathcal{Z}_{\text{Q}}$ are independent they can be treated separately. As the Gaussian partition function is analytic, any phase transition of the XY-model must originate from the Coulomb gas. As briefly discussed earlier, in the low temperature phase the charges appear only in the small density of tightly bound dipole pairs. The dipoles dissociate in the high temperature phase forming a plasma. The two phases can be distinguished by examining the interaction between two *external* test charges at a large separation X. In the absence of *internal* charges (for $y_0 = 0$) in the medium, the two particles interact by the *bare* Coulomb interaction $C(X)$. A finite density of internal charges for small y_0 partially screens the external charges, and reduces the interaction between the test charges to $C(X)/\varepsilon$, where ε is an effective dielectric constant. There is an *insulator* to *metal* transition at sufficiently large y_0. In the metallic (plasma) phase, the external charges are completely screened and their effective interaction decays exponentially.

To quantify the above picture, we shall compute the effective interaction between two external charges at $\mathbf{x}$ and $\mathbf{x}'$ perturbatively in the fugacity y_0. To lowest order, we need to include configurations with two *internal* charges (at $\mathbf{y}$ and $\mathbf{y}'$). The effective interaction can be written

$$\begin{aligned} e^{-\beta V_{\text{eff.}}(\mathbf{x}-\mathbf{x}')} &\equiv \left\langle e^{-4\pi^2 K C(\mathbf{x}-\mathbf{x}')}\right\rangle_Q \equiv \overset{x}{\oplus} -- \overset{x'}{\ominus} \\ &= \overset{x}{\oplus}\cdots\overset{x'}{\ominus} + \frac{y_0^2 \int d^2\mathbf{y}d^2\mathbf{y}' \begin{matrix}\overset{y}{\oplus}\cdots\overset{y'}{\ominus}\\ \overset{x}{\oplus}\cdots\overset{x'}{\ominus}\end{matrix} + O(y_0^4)}{1 + y_0^2\int d^2\mathbf{y}d^2\mathbf{y}' \,\overset{y}{\oplus}\cdots\overset{y'}{\ominus} + O(y_0^4)}, \end{aligned}$$

from which we obtain

$$\begin{aligned} & e^{-\beta V_{\text{eff.}}(\mathbf{x}-\mathbf{x}')+4\pi^2 K C(\mathbf{x}-\mathbf{x}')} \\ &= \frac{1 + y_0^2 \int d^2\mathbf{y}d^2\mathbf{y}' e^{-4\pi^2 K C(\mathbf{y}-\mathbf{y}')+4\pi^2 K[C(\mathbf{x}-\mathbf{y})-C(\mathbf{x}-\mathbf{y}')-C(\mathbf{x}'-\mathbf{y})+C(\mathbf{x}'-\mathbf{y}')]} + O(y_0^4)}{1 + y_0^2 \int d^2\mathbf{y}d^2\mathbf{y}' e^{-4\pi^2 K C(\mathbf{y}-\mathbf{y}')} + O(y_0^4)} \\ &= 1 + y_0^2 \int d^2\mathbf{y}d^2\mathbf{y}' e^{-4\pi^2 K C(\mathbf{y}-\mathbf{y}')}\left(e^{4\pi^2 K D(\mathbf{x},\mathbf{x}',\mathbf{y},\mathbf{y}')} - 1\right) + O(y_0^4), \end{aligned} \tag{B.3}$$

where $D(\mathbf{x}, \mathbf{x}', \mathbf{y}, \mathbf{y}')$ is the interaction *between* the internal and external dipoles. The direct interaction tends to keep the separation $\mathbf{r} = \mathbf{y}' - \mathbf{y}$ small. Using the centre of mass

$\mathbf{R} = (\mathbf{y} + \mathbf{y}')/2$, we can change variables to $\mathbf{y} = \mathbf{R} - \mathbf{r}/2$ and $\mathbf{y}' = \mathbf{R} + \mathbf{r}/2$, and expand the dipole-dipole interaction for small $\mathbf{r}$ as

$$\begin{aligned} D(\mathbf{x}, \mathbf{x}', \mathbf{y}, \mathbf{y}') &= C(\mathbf{x} - \mathbf{R} + \mathbf{r}/2) - C(\mathbf{x} - \mathbf{R} - \mathbf{r}/2) \\ &\qquad - C(\mathbf{x}' - \mathbf{R} + \mathbf{r}/2) + C(\mathbf{x}' - \mathbf{R} - \mathbf{r}/2) \\ &= -\mathbf{r} \cdot \nabla_{\mathbf{R}} C(\mathbf{x} - \mathbf{R}) + \mathbf{r} \cdot \nabla_{\mathbf{R}} C(\mathbf{x}' - \mathbf{R}) + O(r^3). \end{aligned}$$

To the same order

$$\begin{aligned} e^{4\pi^2 K D(\mathbf{x},\mathbf{x}',\mathbf{y},\mathbf{y}')} - 1 = -4\pi^2 K \mathbf{r} \cdot \nabla_{\mathbf{R}} (C(\mathbf{x} - \mathbf{R}) - C(\mathbf{x}' - \mathbf{R})) \\ +8\pi^4 K^2 \left[\mathbf{r} \cdot \nabla_{\mathbf{R}} (C(\mathbf{x} - \mathbf{R}) - C(\mathbf{x}' - \mathbf{R}))\right]^2 + O(r^3). \end{aligned}$$

Substituting this expression into Eq. (B.3), changing integration variables, we find that the term linear in $\mathbf{r}$ integrates to zero while the angular average of $(\mathbf{r} \cdot \nabla_{\mathbf{R}} C)^2$ is $r^2 |\nabla_{\mathbf{R}} C|^2/2$. Thus, to $O(r^4)$, we obtain

$$\begin{aligned} e^{-\beta V_{\text{eff}}(\mathbf{x}-\mathbf{x}')} &= e^{-4\pi^2 K C(\mathbf{x}-\mathbf{x}')} \\ \times &\left[1 + y_0^2 \int (2\pi r dr) e^{-4\pi^2 K C(r)} 8\pi K^2 \frac{r^2}{2} \int d^2\mathbf{R} \left(\nabla_{\mathbf{R}}(C(\mathbf{x} - \mathbf{R}) - C(\mathbf{x}' - \mathbf{R}))\right)^2\right]. \end{aligned}$$

Using the fact that $\nabla^2 C(\mathbf{r}) = \delta^2(\mathbf{r})$, the remaining integral can be evaluated by parts

$$\int d^2\mathbf{R} \left[\nabla_{\mathbf{R}} (C(\mathbf{x} - \mathbf{R}) - C(\mathbf{x}' - \mathbf{R}))\right]^2 = 2 \left(C(\mathbf{x} - \mathbf{x}') - C(0)\right).$$

The short distance divergence can be absorbed into a proper cut-off with $C(x) \to \ln(x/a)/2\pi$, and

$$e^{-\beta V_{\text{eff}}(\mathbf{x}-\mathbf{x}')} = e^{-4\pi^2 K C(\mathbf{x}-\mathbf{x}')} \left[1 + 16\pi^5 K^2 y_0^2 C(\mathbf{x} - \mathbf{x}') \int dr r^3 e^{-2\pi K \ln r} + O(y_0^4)\right].$$

Exponentiating the second term we obtain the effective interaction

$$\beta V_{\text{eff}}(\mathbf{x} - \mathbf{x}') \equiv 4\pi^2 K_{\text{eff}} C(\mathbf{x} - \mathbf{x}'), \tag{B.4}$$

where

$$K_{\text{eff}} = K - 4\pi^3 K^2 y_0^2 \int dr r^{3-2\pi K} + O(y_0^4), \tag{B.5}$$

This completes the derivation of the dielectric constant of the medium $\varepsilon = K/K_{\text{eff}}$ to $O(y_0^2)$. However, as long as the integral converges at large r, the perturbative correction is small. The breakdown of the perturbation theory for $K < K_c = 2/\pi$ occurs precisely at the point where the free energy of an isolated vortex changes sign. This breakdown of the perturbation theory is reminiscent of that encountered in the Landau-Ginzburg model for $d < 4$. We will follow the approach used there and reorganise the perturbation series into a renormalisation group for the parameters K and y_0.

B.1.2 Renormalisation Group

The difficulty associated with the divergence at small K can be overcome by employing a renormalisation procedure first used by José et al. (Phys. Rev. B **16**, 1217 (1977)). By breaking the integral in Eq. (B.5) into two parts, $\int_a^\infty \to \int_a^{ba} + \int_{ba}^\infty$, the non-singular short-distance part of the integral can be evaluated an incorporated into K. This procedure can be carried out order by order in y_0 even though the coefficient of y^2 is formally divergent. This leads to a new equation

$$K_{\text{eff}}^{-1} = \widetilde{K}^{-1} + 4\pi^3 y_0^2 \int_{ba}^{\infty} dr r^{3-2\pi K} + O(y_0^4),$$

where

$$\widetilde{K}^{-1} = K^{-1} + 4\pi^3 y_0^2 \int_{a}^{ba} dr r^{3-2\pi K} + O(y_0^4).$$

Finally, the cut-off in the remaining integral can be rescaled ($ba \to a$) to yield an equation for K_{eff}^{-1} equivalent to Eq. (B.5) but with the shifted and rescaled parameters K and y_0:

$$K_{\text{eff}}^{-1} = \widetilde{K}^{-1} + 4\pi^3 \widetilde{y}_0^2 \int_{a}^{\infty} dr r^{3-2\pi \widetilde{K}} + O(y_0^4),$$

where $\widetilde{y}_0 = b^{2-\pi K} y$. By choosing an infinitesimal $b = e^\ell \approx 1 + \ell$, we obtain the recursion relations are

$$\begin{cases} \frac{dK^{-1}}{d\ell} = 4\pi^3 a^4 y_0^2 + O(y_0^4), \\ \frac{dy_0}{d\ell} = (2 - \pi K) y_0 + O(y_0^3). \end{cases} \tag{B.6}$$

While $dK^{-1}/d\ell \geq 0$, the recursion relation for y_0 changes sign at $K_c^{-1} = \pi/2$. At high temperatures, when the value of K^{-1} is small, y_0 is relevant, while at lower temperatures it is irrelevant. The RG flows, shown in fig. B.1.2a, separate the parameter space into two regions. At low temperatures and small y_0, flows terminate on a *fixed line* at $y_0 = 0$ and $K_{\text{eff}} \geq 2/\pi$. This is the insulating phase in which only dipoles of finite size occur. (Hence the vanishing of y_0 under coarse-graining.) The strength of the effective interaction is given by the point on the fixed line that the flows terminate on. Flows not terminating on the fixed line asymptote to larger values of K^{-1} and y_0 where perturbation theory breaks down. This is the signal of the high temperature phase where vortices proliferate.

The critical trajectory that separates the two regions of the phase diagram flows to a fixed point at ($K_c^{-1} = \pi/2$, $y_0 = 0$). To find the critical behaviour at the transition, we must expand the recursion relations in the vicinity of this point by setting $x = K^{-1} - \pi/2$ and $y = y_0 a^2$. To lowest order Eqs. (B.6) simplify to

$$\begin{cases} \frac{dx}{d\ell} = 4\pi^3 y^2 + O(xy^2, y^4), \\ \frac{dy}{d\ell} = \frac{4}{\pi} xy + O(x^2 y, y^3). \end{cases}$$

The recursion relations are inherently *non-linear* in the vicinity of the fixed point (see fig. B.1.2b). This is quite different from the linear recursion relations that we encountered previously and the resulting critical behaviour is likely to be non-standard.

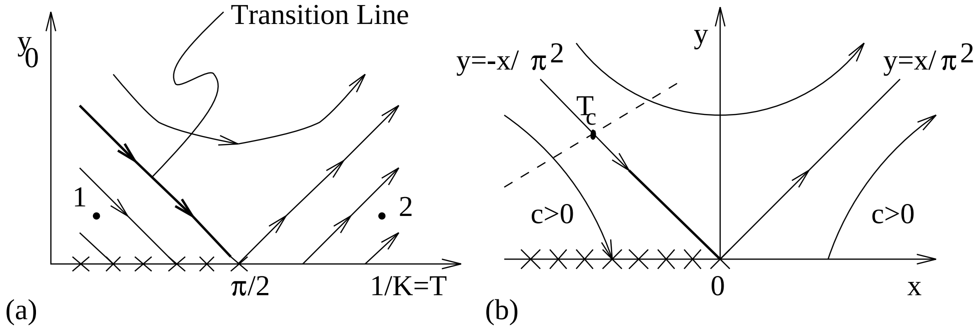

Figure B.1: RG flow for the XY-model, (a) schematic, and (b) in the vicinity if the critical point.

Firstly, we note that

$$\frac{dx^2}{d\ell} = 8\pi^3 y^2 x = \pi^2 \frac{dy^2}{d\ell}, \quad \Rightarrow \quad \frac{d}{d\ell}(x^2 - \pi^4 y^2) = 0 \quad \Longrightarrow \quad x^2 - \pi^4 y^2 = c.$$

The RG flows thus proceed along hyperbolae characterised by different values of c. For $c > 0$, the focus of the hyperbola is along the y-axis, and the flows proceed to $(x, y) \to \infty$. The hyperbolae with $c < 0$ have foci along the x-axis, and have two branches in the half-plane, $y \geq 0$: the branches for $x < 0$ flow to the fixed line, while those in the $x > 0$ quadrant flow to infinity. The critical trajectory separating flows to zero and infinite y corresponds to $c = 0$, i.e. $x_c = -\pi^2 y_c$. Therefore, a small but finite fugacity y_0 reduces the critical temperature to $K_c^{-1} = \pi/2 - \pi^2 y_0 a^4 + O(y_0^2)$.

In terms of the original XY-model, the low temperature phase is characterised by a line of fixed points with $K_{\text{eff}} = \lim_{\ell\to\infty} K(\ell) \geq 2/\pi$. There is no correlation length at a fixed point, and indeed the correlations in this phase decay as a power law,

$$\langle \cos(\theta(\mathbf{r}) - \theta(0)) \rangle \sim \frac{1}{r^\eta},$$

with $\eta = 1/2\pi K_{\text{eff}} \leq 1/4$. Since the parameter c is negative in the low temperature phase, and vanishes at the critical point, we can set it to $c = -b^2(T_c - T)$ close to the transition. In other words, the trajectory of initial points tracks a line $(x_0(T), y_0(T))$. The resulting $c = x_0^2 - \pi^4 y_0^2 \propto (T_c - T)$ is a linear measure of the proximity of the phase transition. Under renormalisation, such trajectories flow to a fixed point at $y = 0$, and $x = -b\sqrt{T_c - T}$. Thus in the vicinity of the transition, the effective interaction parameter

$$K_{\text{eff}} = \frac{2}{\pi} - \frac{4}{\pi^2} \lim_{\ell\to\infty} x(\ell) = \frac{2}{\pi} + \frac{4b}{\pi^2}\sqrt{T_c - T},$$

has a square root singularity.

The *stiffness*, K_{eff} can be measured in experiments on superfluid fluids. In the superfluid phase the order parameter is the condensate wavefunction $\Psi(\mathbf{x}) = \Psi e^{i\theta}$. Variations in the phase θ lead to a superfluid kinetic energy

$$H = \int d^d\mathbf{x} \psi^* \left(-\frac{\hbar^2 \Psi^2}{2m}\right) \psi = \frac{\hbar^2 \nabla^2}{2m} \int d^d\mathbf{x} (\nabla\theta)^2,$$

where m is the particle (He^4) mass. The corresponding XY-model has a stiffness $K = \hbar^2\rho_s/2mk_BT$, where $\rho_s = \Psi^2$ is the superfluid density. The density ρ_s is measured by examining the changes in the inertia of a torsional oscillator; the superfluid fraction, $\rho_s m$ experiences no friction and does not oscillate. Bishop and Reppy (Phys. Rev. Lett. **40**, 1727 (1978)) examined ρ_s for a variety of superfluid films (of different thickness, He^3 concentration, etc.) wrapped around a torsional cylinder. They constructed the effective stiffness K as a function of temperature, and found that for all films it undergoes a universal jump of $2/\pi$ at the transition. The behaviour of K for $T < T_c$ was consistent with a square root singularity.

B.1.3 Correlation Length

Correlations decay exponentially in the high temperature phase. How does the correlation length ξ diverge at T_c? The parameter $c = x^2 - \pi^4 y^2 = b^2(T - T_c)$ is now positive all along the hyperbolic trajectory. The recursion relation

$$\frac{dx}{d\ell} = 4\pi^3 y^2 = \frac{4}{\pi}(x^2 + b^2(T - T_c)),$$

can be integrated to give

$$\frac{4}{\pi}\ell = \frac{1}{b\sqrt{T - T_c}} \arctan\left(\frac{x}{b\sqrt{T - T_c}}\right).$$

The contribution of the initial point to the left hand side of this equation can be left out if $x_0 \propto (T - T_c) \ll 1$. The integration must be terminated when $x(\ell) \sim y(\ell) \sim 1$ since beyond there the perturbative calculation is invalid. This occurs for a value

$$\ell^* \approx \frac{\pi}{4b\sqrt{T - T_c}} \frac{\pi}{2},$$

where we have used $\arctan(1/b\sqrt{T - T_c}) \approx \arctan(\infty) = \pi/2$. The resulting correlation length is

$$\xi \approx a e^{l^*} \approx a \exp\left(\frac{\pi^2}{8b\sqrt{T - T_c}}\right). \tag{B.7}$$

Unlike any of the transitions encountered so far, the divergence of the correlation length is not through a power law. This is a consequence of the non-linear nature of the recursion relations in the vicinity of the fixed point.

Vortices occur in bound pairs for distances smaller than ξ while there can be an excess of vortices of one sign or the other at larger separations. The interactions between vortices at large distances can be obtained from Debye-Hückel theory of polyelectrolytes. According to this theory, the free charges screen each other leading to a screened Coulomb interaction $\exp(-r/\xi)C(r)$. On approaching the transition from the high temperature side the singular part of the free energy

$$f_{\text{sing.}} \propto \xi^{-2} \propto \exp\left(-\frac{\pi^2}{4b\sqrt{T - T_c}}\right), \tag{B.8}$$

has only an essential singularity. All derivatives of this function are finite at T_c. Thus the predicted heat capacity is quite smooth at the transition. Numerical results based on the RG equations (Berker and Nelson) indicate a smooth maximum in the heat capacity at a temperature higher than T_c corresponding to the point at which the majority of dipoles unbind.

The Kosterlitz-Thouless picture of vortex unbinding has found numerous applications in two-dimensional systems such as superconducting and superfluid films, thin liquid crystals, Josephson junction arrays, electrons on the surface of helium films, two-dimensional melting, etc.