

Elements of Phase Transitions and Critical Phenomena

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CHAPTER

7 Kosterlitz-Thouless transition ⓘ

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Abstract

As the spatial dimensionality d decreases, fluctuations become larger and the stability of the low-temperature ordered state deteriorates. The dimensionality where long-range order disappears is known as lower critical dimension. For instance, the Ising model in one dimension does not display long-range order at finite temperatures, however in two dimensions Peierls argument explains why the same model has an ordered phase below a certain critical temperature. If the basic variables and symmetries are continuous as in the XY and Heisenberg models, the (long-range) ordered state at any finite temperature disappears already in two dimensions. This is the result of Mermin-Wagner's theorem. The XY model nevertheless undergoes an unusual phase transition without an onset of long-range order in two dimensions, which is known as the Kosterlitz-Thouless transition. Gauge or local symmetries cannot spontaneously be broken as elucidated by Elitzur's theorem when applied to lattice gauge theories.

Keywords: Peierls argument, lower critical dimension, Elitzur theorem, lattice gauge theory

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As the spatial dimensionality d decreases, fluctuations become larger and the stability of the low-temperature ordered state deteriorates. Consequently, for instance, the Ising model in one dimension does not display long-range order at finite temperatures, i.e. does not have an ordered phase. If the basic variables and symmetries are continuous as in the XY and Heisenberg models, the (long-range) ordered state at any finite temperature disappears already in two dimensions. The XY model, nevertheless, undergoes an unusual phase transition without an onset of long-range order in two dimensions, which is known as the Kosterlitz-Thouless transition. We describe the theory of such interesting behavior in this chapter. Also elucidated is Elitzur's theorem for the absence of spontaneous symmetry breaking in lattice gauge theories.

7.1 Peierls argument

Mean-field theory correctly describes conventional critical phenomena above four dimensions (the upper critical dimension). As the spatial dimensionality d decreases, the effects of interactions between a spin and its neighbors become weaker due mainly to the decrease in the number of neighbors, and eventually long-range order disappears at finite temperatures below a certain dimension. This borderline dimensionality is the lower critical dimension d_{lc} . Systems with discrete degrees of freedom such as the Ising model have $d_{lc}=1$ and systems with continuous symmetries have typically $d_{lc}=2$. In the present section we introduce an argument that makes clear the difference, as far as long-range order at finite temperatures is concerned, between the one- and two-dimensional ferromagnetic Ising models. The argument can generically be applied to other systems such as the antiferromagnetic Ising and Potts models. Indeed, it constitutes a very useful tool to argue for the existence of long-range order at finite temperature in cases where no exact solution is available. The following sections will discuss the conditions for the existence and absence of long-range order in the XY model.

The first example is the one-dimensional Ising model, for which we develop a physical picture for the absence of long-range order not by solving the model explicitly (see Section 9.1) but by comparing the energy and entropy contributions to the free energy. Let us fix the left-most spin in the up (or $+$) state in the Ising model on a chain with length L . The right-most spin remains free. The ground state to be realized at $T=0$ has all spins up because of our particular boundary condition. As the temperature increases from zero, excited states appear, in which some spins have the opposite direction (down or $-$) as in the left panel of Fig. 7.1. A parallel pair of \downarrow

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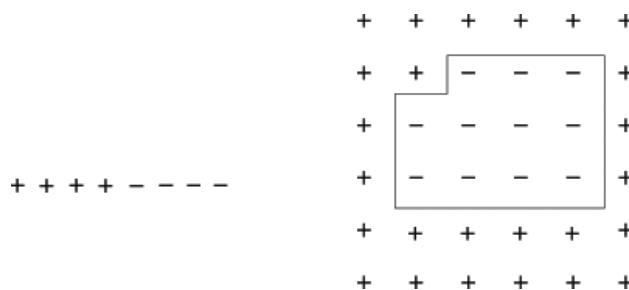


Fig. 7.1 Spin configurations where some spins are reversed from the ferromagnetic (all +) ground state in one dimension (left), and two dimensions (right).

spins (++ or - -) have energy $-J$ and antiparallel pairs (+- or -+) have energy J , with $J > 0$. Thus, the energy to reverse the state of a pair from the lower (parallel) to higher (antiparallel) energy configuration is $+2J$. The number of locations where such a reversal may happen is $L - 1 \approx L$, for large L , which implies an entropy of $\log L$. It follows that the free-energy increase due to the spin reversal is

$$\Delta F = 2J - T \log L. \quad (7.1)$$

This formula shows that, for a fixed value of J , the free energy decreases $\Delta F \propto 0$ by the reversal of spin pairs for a sufficiently large system ($L \gg 1$) and arbitrary finite temperature ($T > 0$). The perfectly (long-range) ordered state with all spins up is therefore easily destroyed by any small but finite temperature. Thus, a simple argument consisting of a comparison between the energy and entropy contributions to the free energy in the Ising model reveals the absence of long-range order in one dimension at finite temperatures.

A two-dimensional version of this argument proceeds as follows. Consider a configuration of spins such as the one shown in the right panel of Fig. 7.1. Suppose that an island of down ($-$) spins with perimeter Γ emerged in

the Ising model of N sites with a boundary condition consisting of all spins up (+), as in the right panel of Fig. 7.1. This boundary condition, which destroys the up/down symmetry of the model, i.e. \mathbb{Z}_2 , favors a particular ground state (the one with all +), and mimics an infinitesimal magnetic field. The continuous line separating the + spins from the - spins in the island is called a *domain wall*. In general, the latter is not a closed polygon and it can be open, but the chosen boundary condition forces the domain walls to be closed polygons.

The energy to generate such an island is $2J\Gamma$. The corresponding entropy is evaluated by counting the number of different ways to generate an island with perimeter Γ . This is the number of paths that return to the original position after Γ steps (the lattice spacing is the unit of length) with the constraint to pass through a single bond only once. On the square lattice, a single step to go from a site to the next has three possibilities because three bonds out of four are allowed to be chosen to avoid going back onto the same bond as in the preceding step. We therefore have roughly 3^Γ possibilities for Γ steps. The factor N results from the fact that there are at most N sites to start from.¹ Then, the entropy is $\log(3^\Gamma N)$, and the free energy cost to generate an island of reversed spins is

$$\Delta F = 2J\Gamma - T\Gamma \log 3 = \Gamma(2J - T \log 3), \quad (7.2)$$

if we choose an island such that $3^\Gamma \gg N$. For temperatures lower than $T_c \equiv 2J/\log 3 = 1.8J$, the island of reversed (-) spins costs a positive free energy ($\Delta F > 0$) and consequently is unlikely to happen, implying the stability of ferromagnetic long-range order. At high temperatures $T > T_c$, on the other hand, many islands can exist and the long-range order is destroyed. We therefore conclude that the two-dimensional Ising model undergoes a phase transition around $T_c = 1.8J$, which is fairly close to the exact solution $2.2J$. These ideas constitute the *Peierls argument* to show the existence of a phase transition in the two-dimensional Ising model. The Peierls argument is not a rigorous proof for the existence of long-range order. It, nevertheless, gives us a lucid physical picture that the existence of long-range order is determined by the balance between energy and entropy. A more formal mathematical proof of the existence of long-range order (ferromagnetic phase at finite temperature) can be developed based on the Peierls argument, see Appendix A.12.

The above argument applies to models with short-range interactions. If the system has long-range interactions, such as $J_{ij} = J/|i - j|^{1+\sigma}$, which decays in a power of the relative distance between two sites, a one-dimensional model can have a phase transition at a finite temperature.² We, nevertheless, concentrate ourselves on short-range interactions throughout this book unless otherwise stated explicitly (as in the infinite-range model of Section 2.5) because they represent typical situations.

7.2 Lower critical dimension of the XY model

Long-range order of systems with continuous degrees of freedom and symmetries, such as the XY model ($n=2$) and Heisenberg model ($n=3$), is vulnerable to instabilities due to thermal fluctuations and is actually absent at finite temperatures in two dimensions. Order is fragile in these systems and can be destroyed more easily than in systems with discrete degrees of freedom. Let us study in some detail how the lower critical dimension becomes two.

The following XY model on a hypercubic lattice as introduced in Section 1.5 will be discussed as a concrete example,

This model has been used to study the critical behavior of the superfluid to normal phase transition in liquid ^4He and displays a global $U(1)$ symmetry, which amounts to a change $\phi_i \rightarrow \phi_i + \alpha$ on every site, with α a real number. Suppose that the temperature is very low and neighboring spins are aligned almost parallel to each other. Then, the ↴

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argument $\phi_i - \phi_j$ of the cosine is very small compared to π , and it would be a good approximation to expand the cosine to second order. Since we are interested in the behavior of the system over a large spatial scale, we are allowed to ignore discreteness of the spatial coordinates of the lattice. We therefore construct an effective Hamiltonian, valid at low temperatures, by using a Fourier representation as

$$H \approx -J \sum_{\langle ij \rangle} \left(1 - \frac{1}{2} (\phi_i - \phi_j)^2 \right) \approx \frac{J}{2} \int d\mathbf{r} (\nabla \phi)^2 = \frac{J}{2} \int \frac{dq}{(2\pi)^d} q^2 \tilde{\phi}(q) \tilde{\phi}(-q), \quad (7.4)$$

where we have dropped an additive constant that does not play a role, and considered the gradient along the spatial directions of the lattice $\phi_i - \phi_j \rightarrow (\mathbf{r}_i - \mathbf{r}_j) \cdot \nabla \phi((\mathbf{r}_i + \mathbf{r}_j)/2)$ with $\phi(\mathbf{r})$ a continuous function. This is the *spin-wave approximation* around an assumed ordered state, a quadratic Hamiltonian, which is expected to be valid at low temperatures. In this approximation no phase transition may occur, as seen in the Gaussian model with $t = 0$ in eqn (2.80). In general, effective Hamiltonians such as the one of eqn (7.4) with an analytic expansion, in terms of gradients of a slowly varying hydrodynamic (i.e. phenomenological) variable, characterize *generalized elasticity* problems. In the case of magnetic systems the parameter of *rigidity* J is known as the *spin-wave stiffness or the helicity modulus*, and it is proportional to the *superfluid density* in the case of superfluids, the latter being discussed in Section 7.4.

To understand what type of spin configurations are stable under the spin-wave approximation, we adopt the variational principle with respect to a local angle variable (or a scalar field) $\phi(\mathbf{r})$, $\delta H/\delta\phi(\mathbf{r})=0$, to find the following Laplace equation,³

$$\nabla^2 \phi = 0. \quad (7.5)$$

We solve this Laplace equation under the boundary condition that the left boundary ($x=0$) has $\phi=0$ and the right ($x=L$) has $\phi=\phi_0$, along the chosen x -direction. The solution is the uniformly rotated state, $\phi=x\phi_0/L$, as depicted in Fig. 7.2. Then, the energy of this configuration has the value

$$E = \frac{J}{2} L^{d-2} \phi_0^2, \quad (7.6)$$

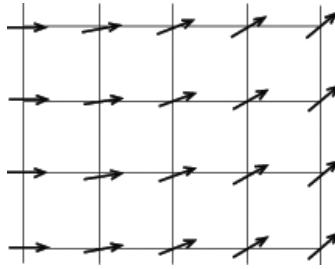


Fig. 7.2 The stable spin configuration with the left and right boundaries fixed.

p. 157 as can be verified by inserting $\nabla\phi=(\phi_0/L, 0, 0, \dots)$ to the intermediate expression of eqn (7.4), assuming that the volume of the system is L^d . This result shows that energy increases indefinitely as $L \rightarrow \infty$ for $d > 2$. A very large energy is needed to twist both sides of the system by a finite angle, suggesting that the system is robust against the change of boundary conditions. The information on the specific state that one end has propagates through the system to the other end. The system is thus considered to have rigid long-range order. If $d < 2$, the twist energy (7.6) does not increase with system size and the effects of the boundaries do not propagate deep into the system. Hence no long-range order exists. This simple argument therefore illustrates that the stability of the long-range order in the XY model changes when the dimension of the system is $d = 2$. The case $d = 2$ is marginal and needs more careful scrutiny.

So far, the theory was just developed for the susceptibility of the energy against a change of boundary conditions and did not include the effects of temperature. We therefore must evaluate the behavior of the system at finite temperatures to confirm the validity of the conclusion that $d = 2$ is the borderline dimensionality, i.e. the lower critical dimension. The goal is to calculate the fluctuation of the relative orientation of two spins as a function of their distance. The fluctuation of the relative orientation is written as, using the Fourier representation,

$$\langle(\phi(r) - \phi(0))^2\rangle = \int \frac{dq_1 dq_2}{(2\pi)^{2d}} (e^{-iq_1 \cdot r} - 1)(e^{-iq_2 \cdot r} - 1) \langle\tilde{\phi}(q_1)\tilde{\phi}(q_2)\rangle. \quad (7.7)$$

The expectation value of Fourier-transformed angle variables in the integrand is to be calculated from the Hamiltonian (7.4). Since eqn (7.4) is a quadratic form of $\phi(q)$, i.e. a Gaussian theory, it is straightforward to apply the computations of Section 2.9 with $t=0$ and $b=J/2$ to find

$$\langle\tilde{\phi}(q_1)\tilde{\phi}(q_2)\rangle = \frac{(2\pi)^d T}{J q_1^2} \delta(q_1 + q_2). \quad (7.8)$$

We then have

$$\langle(\phi(r) - \phi(0))^2\rangle = \frac{T}{J} \int \frac{dq}{(2\pi)^d} \frac{|e^{-iq \cdot r} - 1|^2}{q^2} \propto \frac{T}{J} \int_{r^{-1}}^{a^{-1}} dq q^{d-3}, \quad (7.9)$$

where the upper limit of the integral, the largest allowed wave number, has been replaced by the largest absolute value of the wave number, which is proportional to the inverse of the lattice constant a^{-1} . The lower

limit of the integral is chosen to be the inverse of the distance, r^{-1} , because the integrand in the middle expression is very small for $q \ll r^{-1}$, i.e. $e^{-i\mathbf{q} \cdot \mathbf{r}} \approx 1$.⁴ For $d \geq 2$, the last integral of eqn (7.9) is

$$\frac{T}{J(d-2)} (a^{2-d} - r^{2-d}). \quad (7.10)$$

- p. 158 Since $2 - d < 0$, this expression converges to a finite value for large r . This suggests that fluctuations of the angle difference stay finite and long-range order is not destroyed because two spins far apart share essentially the same angle. If the dimensionality is exactly two, the integral (7.9) yields a logarithmic term, $\log r$, which diverges as r tends to infinity. Fluctuations grow indefinitely as the distance increases. Therefore, the two angle variables $\phi(\mathbf{r})$ and $\phi(0)$ become uncorrelated in the limit $r \rightarrow \infty$ as long as the temperature is finite. We conclude that long-range order does not exist at finite temperatures in the two-dimensional XY model. The same is true for $d < 2$.

We have used several approximate estimates in the above discussion. It is possible to derive the same result rigorously by using Schwarz inequalities, as will be shown in the next section.

7.3 Mermin-Wagner theorem: Absence of spontaneous magnetization

The Mermin-Wagner theorem states that two-dimensional short-range interacting systems with continuous degrees of freedom and symmetries do not have spontaneous magnetization at finite temperatures. More generally, it is a statement relating the dimensionality of a system with continuous symmetry with the existence of the phenomenon of spontaneous symmetry breaking. We have made use of the spin-wave approximation in the previous section, and the same conclusion is derived rigorously in the present section. The original theorem was given in the context of quantum spin systems, but we explain here a classical version since it is slightly simpler and does not need the introduction of quantum spin operators. A common physical mechanism, related to symmetry and fluctuations, lies behind the formal proofs both for quantum and classical systems. The quantum version of the theorem is proved in Appendix A.13. Although illuminating, the reader who is not interested in the details of the proof can skip this section.

The Hamiltonian of the XY model in the presence of a finite external field h is

$$H = -J \sum_{\langle ij \rangle} \cos (\phi_i - \phi_j) - h \sum_i \cos \phi_i. \quad (7.11)$$

The sum in the first term on the right-hand side runs over nearest-neighbor pairs on the square lattice. The starting point of the proof is the following Schwarz inequality that holds under very general conditions,

$$\langle AA^* \rangle \geq \frac{|\langle AB^* \rangle|^2}{\langle BB^* \rangle}, \quad (7.12)$$

where A and B are functions of angle variables (ϕ_i, ϕ_j) and $\langle \dots \rangle$ denotes the thermal average with respect to the canonical ensemble Boltzmann weight $e^{-\beta H}$ with $\beta = 1/T$.

The crux of the proof is to choose A and B as follows,

$$A = \frac{1}{N} \sum_j e^{-iq \cdot r_j} \sin \phi_j, \quad B = \frac{1}{N} \sum_l e^{-iq \cdot r_l} \frac{\partial H}{\partial \phi_l}. \quad (7.13)$$

p. 159 Here, \mathbf{q} is a wave vector and \mathbf{r}_j and \mathbf{r}_l are position vectors. We insert these definitions into the Schwarz inequality (7.12) and sum both sides over \mathbf{q} for a finite-size system with periodic boundary conditions. The left-hand side is bounded as

$$\sum_{\mathbf{q}} \langle AA^* \rangle = \frac{1}{N^2} \sum_{i,j} \sum_{\mathbf{q}} e^{-i\mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j)} \langle \sin \phi_i \sin \phi_j \rangle = \frac{1}{N} \sum_i \langle \sin^2 \phi_i \rangle \leq 1. \quad (7.14)$$

The numerator of the right-hand side of eqn (7.12) is

$$\langle AB^* \rangle = \frac{Tm}{N}, \quad (7.15)$$

where m is the magnetization per spin. To derive this identity we first note that

$$\langle AB^* \rangle = \frac{1}{N^2} \sum_{j,l} e^{-i\mathbf{q} \cdot (\mathbf{r}_j - \mathbf{r}_l)} \left\langle \sin \phi_j \frac{\partial H}{\partial \phi_l} \right\rangle, \quad (7.16)$$

whose last expectation value is rewritten, after integration by parts, as

$$\frac{1}{Z} \int_0^{2\pi} \prod_i d\phi_i e^{-\beta H} \sin \phi_j \frac{\partial H}{\partial \phi_l} = \frac{T}{Z} \int_0^{2\pi} \prod_i d\phi_i e^{-\beta H} \cos \phi_j \delta_{lj}, \quad (7.17)$$

where we used $e^{-\beta H} \partial H / \partial \phi_l = -\beta^{-1} \partial e^{-\beta H} / \partial \phi_l$. It then follows

$$\langle AB^* \rangle = \frac{T}{N^2} \sum_j \langle \cos \phi_j \rangle = \frac{Tm}{N}. \quad (7.18)$$

The denominator of the right-hand side of eqn (7.12) is upper-bounded as ($q=|\mathbf{q}|$)

$$\langle BB^* \rangle \leq T \left(\frac{Jq^2 + h}{N} \right). \quad (7.19)$$

To understand this inequality it is useful first to insert the definition of eqn (7.13),

$$\langle BB^* \rangle = \frac{1}{N^2} \sum_{l,j} e^{-i\mathbf{q} \cdot (\mathbf{r}_l - \mathbf{r}_j)} \left\langle \frac{\partial H}{\partial \phi_l} \frac{\partial H}{\partial \phi_j} \right\rangle. \quad (7.20)$$

We next use $e^{-\beta H} \partial H / \partial \phi_l = -\beta^{-1} \partial e^{-\beta H} / \partial \phi_l$ to rewrite the expectation value on the right-hand side, after integration by parts, as

$$\frac{1}{Z} \int_0^{2\pi} \prod_i d\phi_i e^{-\beta H} \frac{\partial H}{\partial \phi_l} \frac{\partial H}{\partial \phi_j} = \frac{T}{Z} \int_0^{2\pi} \prod_i d\phi_i e^{-\beta H} \frac{\partial^2 H}{\partial \phi_l \partial \phi_j}. \quad (7.21)$$

The second order derivative appearing here is evaluated according to the combination of indices.

- For $l=j$.

$$\frac{\partial^2 H}{\partial \phi_l \partial \phi_j} = \frac{\partial^2 H}{\partial \phi_l^2} = J \sum_{\delta} \cos(\phi_l - \phi_{l+\delta}) + h \cos \phi_l. \quad (7.22)$$

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↳ Here, δ is the vector to the nearest-neighbor site on the square lattice. There are four of them.

- For neighboring l and j .

$$\frac{\partial^2 H}{\partial \phi_l \partial \phi_j} = \frac{\partial}{\partial \phi_l} \left(J \sum_{\delta} \sin(\phi_j - \phi_{j+\delta}) + h \sin \phi_j \right) = -J \cos(\phi_j - \phi_l). \quad (7.23)$$

- Otherwise, it is 0.

Combining these three cases, we have

$$\begin{aligned} & \beta \langle BB^* \rangle \\ &= \frac{1}{N^2} \sum_l \left(J \sum_{\delta} \langle \cos(\phi_l - \phi_{l+\delta}) \rangle + h \langle \cos \phi_l \rangle \right) - \frac{J}{N^2} \sum_{l,\delta} e^{-i\mathbf{q} \cdot \delta} \langle \cos(\phi_l - \phi_{l+\delta}) \rangle \\ &= \frac{J}{N^2} \sum_l (4 - \sum_{\delta} e^{-i\mathbf{q} \cdot \delta}) \langle \cos(\phi_l - \phi_{l+\delta}) \rangle + \frac{h}{N^2} \sum_l \langle \cos \phi_l \rangle, \end{aligned} \quad (7.24)$$

where $\langle \cos(\phi_l - \phi_{l+\delta}) \rangle$ respects the symmetry of the square lattice in the sense that it is independent of δ . Now, note that the sum over vectors to neighboring sites gives⁵

$$\sum_{\delta} e^{-i\mathbf{q} \cdot \delta} = 2 \cos q_x + 2 \cos q_y. \quad (7.25)$$

Using the trivial inequality $1 - \cos q \leq q^2/2$, which can be verified by graphical means, and another trivial relation $\langle \cos(\dots) \rangle \leq 1$, we can rewrite the final expression of eqn (7.24) as

$$\begin{aligned}\beta \langle BB^* \rangle &= \frac{J}{N^2} \sum_l (4 - 2 \cos q_x - 2 \cos q_y) \langle \cos (\phi_l - \phi_{l+\delta}) \rangle + \frac{h}{N} m \\ &\leq \frac{J}{N} (q_x^2 + q_y^2) + \frac{h}{N} = \left(\frac{Jq^2 + h}{N} \right).\end{aligned}\tag{7.26}$$

This is eqn (7.19).

Replacement of the relations (7.14), (7.15) and (7.19) into the corresponding expressions in the Schwarz inequality (7.12) gives

$$1 \geq \frac{T}{N} m^2 \sum_q \frac{1}{Jq^2 + h}.\tag{7.27}$$

In the thermodynamic limit $N \rightarrow \infty$ the sum becomes an integral,

$$1 \geq T m^2 \int \frac{d\mathbf{q}}{(2\pi)^2} \frac{1}{Jq^2 + h}.\tag{7.28}$$

- p. 161 In two dimensions, for any $T > 0$, this integral diverges as $h \rightarrow 0$ due to the singularity at the origin (*infrared divergence*). The inequality is satisfied only if $m \rightarrow 0$ as $h \rightarrow 0$, i.e. no spontaneous symmetry breaking can occur. This ends the proof that there is no spontaneous magnetization in the XY model at finite temperatures in two dimensions.⁶

The square of the wave number q^2 in the denominator of eqn (7.28) represents essentially the same long-range processes as in the evaluation of the energy of a spin wave in eqn (7.4). In the spin-wave approximation this q^2 leads to the power of $d - 3$ in eqn (7.9) for the fluctuation of relative angles, and as a result, the integral diverges in two dimensions. The same mechanism is seen to work to give a diverging integral as $h \rightarrow 0$ in eqn (7.28). We would like to mention that the general Mermin-Wagner theorem of this section and Appendix A.13 can be applied to other classical or quantum models with short-range interactions. Indeed, the original formulation was applied to the classical Heisenberg model to prove that ferromagnetism (or antiferromagnetism) cannot be present in $d \leq 2$. When applied to other models, the starting point is always the inequality of eqn (7.12) with appropriately chosen functions A and B depending on the model. Notice that the theorem does not exclude the possibility to have spontaneous symmetry breaking at $T=0$. Indeed, at exactly $T=0$ the two-dimensional classical XY model has long-range order.

EXERCISE 7.1 Generalize the proof of this section to an arbitrary dimension d and show that there is no spontaneous magnetization for $d < 2$ and that it is impossible to show the same result for $d > 2$.

7.4 Kosterlitz-Thouless transition

We have seen that the two-dimensional XY model has no spontaneous magnetization (long-range order) at finite temperatures and consequently has no ordinary (Landau-type) phase transition. This system is, nevertheless, known to have a special type of phase transition without long-range order. The low-temperature phase does not display long-range order but has clearly different correlation properties from the high-temperature paramagnetic phase. While correlation functions decay exponentially in the paramagnetic phase, they slowly decrease as a power law in the low-temperature phase (except at exactly $T = 0$ where there is long-range order). This power-law correlation is reminiscent of what happens at the critical point. An important difference from the usual critical point, though, is that this power-law behavior extends over a finite temperature range. Sometimes this phase is referred to as a low-temperature *critical phase*. Systems with power-law decay of (potential) order parameter correlation functions are said to have *quasi-long-range order*. The XY model is at the lower critical dimension in two dimensions, and this fact causes such singular behavior. This special transition from quasi-long-range order to disorder is ↴ known as the Kosterlitz-Thouless (KT) transition, and the critical phase is called the Kosterlitz-Thouless (KT) phase.⁷

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Let us calculate the correlation function using the spin-wave approximation, which is valid at low temperatures, to verify its power-law behavior. The correlation function of the XY model is expressed as

$$\langle \cos(\phi(\mathbf{r}) - \phi(0)) \rangle = \langle e^{i(\phi(\mathbf{r}) - \phi(0))} \rangle. \quad (7.29)$$

Note that the imaginary part of the right-hand side vanishes due to the symmetry of global reversal of angle variables, $\phi(\mathbf{r}) \rightarrow -\phi(\mathbf{r}) \forall \mathbf{r}$, under which the Hamiltonian remains invariant. The goal is to evaluate the expectation value on the right-hand side using the spin-wave Hamiltonian (7.4). Since this Hamiltonian is quadratic in the angle variables, the corresponding Gibbs-Boltzmann distribution is Gaussian. We therefore use the fact that the cumulants of order higher than the second order vanish for the Gaussian distribution (see Appendix A.4) to find

$$\langle \cos(\phi(\mathbf{r}) - \phi(0)) \rangle = \langle e^{i(\phi(\mathbf{r}) - \phi(0))} \rangle = e^{-\frac{1}{2}\langle (\phi(\mathbf{r}) - \phi(0))^2 \rangle}. \quad (7.30)$$

The expression in the exponent can be evaluated as in the integral (7.9) for the case $d = 2$,

$$\langle (\phi(\mathbf{r}) - \phi(0))^2 \rangle \approx \frac{T}{J(2\pi)^2} \int_0^{2\pi} d\theta \int_{r^{-1}}^{a^{-1}} \frac{dq}{q} = \frac{T}{\pi J} \log \left(\frac{r}{a} \right). \quad (7.31)$$

Inserting this result into eqn (7.30), we have ($r = |\mathbf{r}|$)

$$\langle \cos(\phi(\mathbf{r}) - \phi(0)) \rangle = r^{-T/2\pi J}. \quad (7.32)$$

Usually, correlation functions do not decay with distance if long-range order exists and decay exponentially in the paramagnetic phase. Equation (7.32) shows a slow, power-law decay in between, which is characteristic of systems exactly at the critical point. However, the exponent $\eta = T/2\pi J$ is not universal since it explicitly depends

on T and J . Remarkably, this result holds for any temperature as long as the spin-wave approximation is a justified assumption. We conclude that the system is critical for a finite temperature range. This may also be understood as if there exists a fixed line, i.e. a set of fixed points, under the renormalization group. Thus, this behavior is called quasi-long-range order. The relative angle of the spin variables does not have (long-range) order but changes slowly.

EXERCISE 7.2 Calculate the correlation function (7.29) for general $d(\neq 2)$ and confirm that $d = 2$ is the borderline dimension of stability, the lower critical dimension.

The spin-wave quadratic model is critical and it displays no phase transition. However, at sufficiently high temperatures we would expect the XY model to be in a paramagnetic phase with exponentially decaying
p. 163 relative angle correlations. ↴

As the temperature increases from the low-temperature limit, it must happen that the angle variables change more drastically than those expressed in the spin-wave approximation. The Laplace equation $\nabla^2 \phi = 0$ admits, besides the uniform solutions $\phi = \text{const.}$ studied above, non-uniform singular solutions. Topological vortex solutions (see Section 5.8) are inhomogeneous states that cannot be described by a continuous function such as the smoothly varying spin waves. In particular, vortex configurations, not taken into account in the spin-wave approximation of the XY model, gradually affect the state of the system, eventually destroying the quasi-long-range order.

To express configurations with vortices, we write the angle field variable $\phi(\mathbf{r})$ as a function of the angle θ measured from the x-axis as $\phi(\mathbf{r}) = n\theta + c$, with n an integer known as the winding number (a topological invariant) and c a constant, Fig. 7.3. Then, the derivative of the angle variable $\nabla\phi$ appearing in the spin-wave Hamiltonian (7.4) has as radial and azimuthal components as

$$(\nabla\phi)_r = \frac{\partial\phi}{\partial r} = 0, \quad (\nabla\phi)_\theta = \frac{1}{r} \frac{\partial\phi}{\partial\theta} = \frac{n}{r}. \quad (7.33)$$

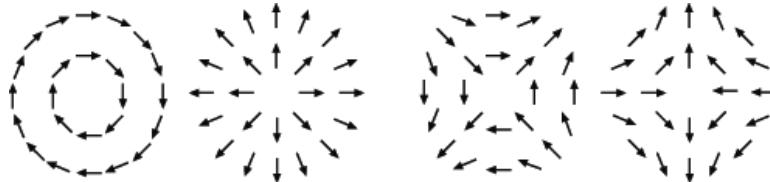


Fig. 7.3 Vortices with $n=1, 1, -1, -1$ and $c = -\pi/2, 0, \pi/2, \pi$ from left to right, respectively, where n and c are defined by $\phi(\mathbf{r}) = n\theta + c$.

An excitation with a positive winding number is a vortex and one with a negative value of n is also known as an antivortex. Then, the energy needed to create such a vortex configuration is, according to eqn (7.4),

$$E = \frac{J}{2} \int \frac{n^2}{r^2} r dr d\theta = n^2 \pi J \log \frac{R}{r_0} + E_C. \quad (7.34)$$

Here, R is the linear size (radius) of the system, r_0 is the radius of the vortex core (the lower bound of the integral and the short-distance cutoff), and E_C is the vortex core energy. We have assumed that the upper bound of the integral is R , the lower bound r_0 , and the contribution below the lower bound $r < r_0$ gives a finite

energy E_C . Thus, the total energy of a vortex has two contributions, the first term in eqn (7.34) represents the elastic energy while the energy E_C is a microscopic contribution associated with the destruction of the uniform order at the core of the vortex. The entropy of a single vortex S is given by the logarithm of the number of ways to place the center of the vortex in the region having a radius between r_0 and R . This number of ways is expected to be proportional to the relevant area of the region. We thus have

$$S = \log \left\{ \left(\frac{R}{r_0} \right)^2 \cdot \text{const} \right\}. \quad (7.35)$$

- p. 164 The combination of these estimates of energy and entropy leads to the following free energy needed to create a vortex with winding number $n = 1$,

$$\Delta F = (\pi J - 2T) \log R + \text{const.} \quad (7.36)$$

For the temperature range $T > T_{KT} = \pi J/2$, the creation of vortices causes a free-energy decrease. We therefore conclude that a phase transition takes place at $T_c = T_{KT}$, above which a large number of vortices proliferate and the spin-wave approximation breaks down. For $T > T_{KT}$, the angle variable around a vortex changes very quickly invalidating the spin-wave approximation, and the relative angle between spins far apart are correlated only very weakly. Then, the quasi-long-range order is destroyed and the system becomes paramagnetic. This is the Kosterlitz-Thouless (KT) transition. The low-temperature region below T_{KT} with quasi long-range order is the KT phase.

In the KT phase the creation of a vortex increases the free energy, and a single vortex is not stable. Nevertheless, a pair of vortices with different signs of their winding number n may be stable if the distance between them is not too large. To show this result we assume that several vortices exist around the origin. Then, the angle field far from the origin is written as, instead of eqn (7.33),

$$(\nabla\phi)_r = \frac{\partial\phi}{\partial r} = 0, \quad (\nabla\phi)_\theta = \frac{1}{r} \frac{\partial\phi}{\partial\theta} = \frac{\sum_i n_i}{r}. \quad (7.37)$$

The energy corresponding to eqn (7.34) is

$$E = \left(\sum_i n_i \right)^2 \pi J \log \frac{R}{r_0} + E_C, \quad (7.38)$$

where E_C is the total vortex core energy. We may therefore conclude that several vortices may exist even in the low-temperature KT phase as long as the condition of neutrality $\sum_i n_i = 0$ is satisfied. In particular, a pair of vortices having the same absolute value but opposite signs of their winding numbers, $\pm n$, are allowed to exist.

Since at low temperatures vortices can be bound in pairs, the Kosterlitz-Thouless transition is physically associated with the unbinding of vortices. The simple and heuristic energy-entropy argument developed in this section neglects interactions between vortices that will be studied in the next section. A more sophisticated renormalization group analysis, to be developed in a later section, shows that this qualitative picture is the correct description of the transition.

EXERCISE 7.3 Draw vortex configurations with $n = 2$ and $n = -2$ similarly to Fig. 7.3.

EXERCISE 7.4 Derive the condition for the term $\sum_i \cos(p\phi_i)$ with p a natural number to be relevant in the sense of renormalization group for the XY model. It will be useful first to estimate the scaling dimension x_p from the calculation of the corresponding correlation function $\langle \cos(p\phi(r) - p\phi(0)) \rangle$ generalizing the discussions ↴ in the first half of the present section. The result will reveal the condition for the exponent y_p to be positive. In particular, show that the term $\sum_i \cos(p\phi_i)$ is relevant if p is larger than a threshold p_0 and the temperature is lower than some T_p . This implies that this term is irrelevant in the temperature range $T_p < T < T_{KT}$ where the KT phase is realized. On the other hand, this term is relevant for $T < T_p$ and the system has the same properties as the *clock model* in which the angles assume only discrete values $\phi_i = 2\pi k/p$ ($k = 0, 1, 2, \dots, p - 1$).

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A few words are in order on the superfluid transition of liquid helium. The kinetic energy of a thin film of superfluid helium is written as

$$E = \frac{\rho_s}{2} \int v_s^2 dx dy = \frac{\rho_s}{2} \left(\frac{\hbar}{m}\right)^2 \int (\nabla \psi)^2 dx dy, \quad (7.39)$$

where ρ_s is the superfluid density per area and v_s is the superfluid velocity and we have used the Landau-Ginzburg relation $v_s = (\hbar/m)\partial\psi$. Comparison with eqn (7.4) or eqn (7.48) in the next section reveals the relation $J = \rho_s \hbar^2/m^2$. It follows that the ratio of ρ_s to T at the transition point $T_c = T_{KT}$ ($= \pi J/2$) assumes a universal value independent of experimental details,

$$\frac{\rho_s}{T_{KT}} = \frac{2m^2}{\pi\hbar^2}. \quad (7.40)$$

Since $\rho_s = 0$ above the transition due to the absence of superfluidity, ρ_s/T jumps from the above finite value to zero at the transition. This is called the *universal jump* of the superfluid density (stiffness) and has been confirmed experimentally. Also, the problem of a roughening transition of equilibrium crystal surfaces displays a universal jump in the smoothness parameter and has also been confirmed experimentally.

Equation (7.40) represents a quantity proportional to the ratio of J and T . This turns out to lead to the fact that the critical exponent η assumes a specific number $\eta(T_{KT}) = 1/4$ at the transition point. The reason is that eqn (7.32) implies that $\eta = T/2\pi J$, proportional to the ratio between T and J , has the value $1/4$ at the transition point because $T_{KT} = \pi J/2$. The relation $\eta(T_{KT}) = 1/4$ is often used to check if a transition belongs to the same universality class as the KT transition.

7.5 Interaction energy of vortex pairs

We have learned that a vortex pair can exist in a stable manner around the origin if the neutrality condition is satisfied. The physical properties of vortices are better understood when we study the energy of vortices in their general configurations. In the following we will establish a connection between the XY model and a neutral Coulomb gas in two dimensions with charges n_i , such that $\sum_i n_i = 0$.

The angle variable or field for a single vortex with winding number $n = 1$ located at the origin is written as

$$(\nabla\phi)_r = 0, \quad (\nabla\phi)_\theta = \frac{1}{r}. \quad (7.41)$$

p. 166 Let us integrate the field $v \equiv \nabla\phi$ around the vortex, along a closed circuit,

$$\oint v \cdot dr = \int_0^{2\pi} \frac{1}{r} r d\theta = 2\pi. \quad (7.42)$$

Then, the Stokes theorem implies that $(\text{curl } v)_z = 2\pi\delta(r)$, where the z -direction is perpendicular to the two-dimensional xy plane. For a more general configuration with many vortices, we have

$$(\text{curl } v)_z = 2\pi \sum_i n_i \delta(r - r_i) \equiv 2\pi N(r), \quad (7.43)$$

where r_i is the position of the vortex i , i.e. the location of its core.

Now, the Cartesian components of the vector field $v = \nabla\phi$ for a single vortex with $n = 1$ are, according to eqn (7.41),

$$v_x = \frac{\partial\phi}{\partial x} = -\frac{y}{r^2}, \quad v_y = \frac{\partial\phi}{\partial y} = \frac{x}{r^2}. \quad (7.44)$$

If we introduce a new scalar field $\psi = -\log(r/r_0)$, the above components are expressed as

$$v_x = \frac{\partial\psi}{\partial y}, \quad v_y = -\frac{\partial\psi}{\partial x}. \quad (7.45)$$

In a superfluid the real physical vortices can be described by these variables, in which case v is called the superfluid velocity, ϕ the velocity potential, and ψ the stream function. For a generic case with many vortices, we generalize $\psi = -\log(r/r_0)$ to

$$\psi(r) = - \sum_i n_i \log \frac{|r-r_i|}{r_0}. \quad (7.46)$$

It is instructive to verify the validity of this generalization. From eqns (7.45) and (7.46), we find

$$(\text{curl } v)_z = \frac{\partial v_y}{\partial x} - \frac{\partial v_x}{\partial y} = -\frac{\partial^2 \psi}{\partial x^2} - \frac{\partial^2 \psi}{\partial y^2} = -\nabla^2 \psi = 2\pi N(r), \quad (7.47)$$

which is consistent with eqn (7.43).

The total energy of a (neutral) system with many vortices is therefore

$$\begin{aligned} E &= \frac{J}{2} \int (v_x^2 + v_y^2) dx dy = \frac{J}{2} \int (\nabla \psi)^2 dx dy \\ &= -\frac{J}{2} \int (\psi \nabla^2 \psi) dx dy \\ &= -\pi J \sum_{i \neq j} n_i n_j \log \frac{|r_i - r_j|}{r_0} + E_C. \end{aligned} \quad (7.48)$$

This equation can be interpreted as the total energy of a set of charged vortices (with charge n_i) interacting via p. 167 a two-dimensional Coulomb potential having a logarithmic dependence on the relative distance. Notice that the energy of a pair of vortices with opposite charges, $n_i n_j < 0$, is minimized when they are close to each other, i.e. tightly bound. At low temperatures two vortices with different signs (such as $n = \pm 1$) are bound together, creating a gas of vortex-antivortex pairs or *molecules*, and the system may be regarded as a dielectric. Above the KT transition point those pairs are destroyed (melted) by thermal fluctuations and single vortices freely move around, forming a plasma-like state. Unbound vortices correspond to free or mobile charges. In this sense, the physics of the KT transition is equivalent to the statistical mechanics of a two-dimensional Coulomb gas. Equation (7.48) suggests that the coupling constant J is related to the dielectric constant ϵ by $\pi J = 1/\epsilon$. The effective interaction energy between vortices (7.48) will be rederived in Section 10.3.4 without the *ad hoc* introduction of vortex degrees of freedom.

7.6 Renormalization group analysis

An analysis of the KT transition by the renormalization group method is a prominent example in which the real-space renormalization works very successfully.

7.6.1 Renormalization group equation to describe the KT transition

Let us first identify the variables that determine the critical behavior of the present system. Physical intuition is useful to find the relevant variables, and we eventually write renormalization group equations for these variables. The temperature is clearly the most important variable. The corresponding scaling field x is chosen as $x = 2 - \pi K (= 2 - \pi J/T)$ such that it vanishes at the fixed point.⁸ The variable x is actually not relevant but marginal. In conventional critical phenomena, the temperature variable is relevant and renormalizes toward zero if the initial value is below the critical point, as illustrated in Fig. 1.5. However, in the KT transition, there is no isolated fixed point and all temperatures below the critical point are attracted to corresponding points on a fixed line, which represents a set of fixed points. The KT transition point does not correspond to an unstable fixed point characteristic of a relevant scaling field. Nevertheless, the temperature is not irrelevant but is marginal.

Another important variable to take into consideration is the number of vortices. If there are few vortices, the spin-wave approximation describes the system qualitatively faithfully and the system is in the KT phase. As the number of vortices increases, the slow and smooth change of angles, as assumed in the spin-wave approximation, is not respected and the angles vary quickly near vortices, eventually leading to the KT transition into the paramagnetic phase. It is therefore reasonable to introduce as a relevant variable the chemical potential μ of vortices, which controls the number of vortices, or equivalently the fugacity obtained by exponentiating the chemical potential, $y_0 = e^{-\beta\mu}$. For small y_0 (large chemical potential) the number of

p. 168 vortices \downarrow is small and the system is in the KT phase, whereas the paramagnetic phase has a large y_0 with very many vortices. This means that we have to see whether the fugacity increases or decreases under a renormalization group transformation.

A more quantitative analysis is facilitated by the energy

$$E(r_1, r_2) = 2\pi J \log \frac{|r_1 - r_2|}{r_0} + E_C, \quad (7.49)$$

which describes a pair of vortices with opposite winding numbers $n = \pm 1$, located at r_1 and r_2 . This equation is derived from eqn (7.48) when we set $n_1 = -n_2 = 1$ or $n_1 = -n_2 = -1$ with all other n_i 's vanishing. The chemical potential for two vortices is 2μ , and the corresponding fugacity is y_0^2 . Then, the probability for the above configuration of a pair of vortices to appear should be proportional to the following expression

$$y_0^2 e^{-\beta E(r_1, r_2)} = y_0^2 e^{-\beta E_C} \left| \frac{r_1 - r_2}{r_0} \right|^{-2\pi K}. \quad (7.50)$$

The correlation function of vortex variables $\langle |n(r_1)n(r_2)| \rangle$ is calculated from contributions of non-vanishing values of $|n(r_1)|$ and $|n(r_2)|$ and hence is proportional to the probability of eqn (7.50) when there are only a small number of vortices ($|n(r_1)|, |n(r_2)| = 0$ or 1). This observation leads to two interesting facts. First, the distance-independent part of the above equation, $y_0^2 e^{-\beta E_C}$, implies that the fugacity y_0 always appears as a product with $e^{-\beta E_C/2}$. We may thus adopt $y = y_0 e^{-\beta E_C/2}$ as a basic scaling field instead of y_0 . Secondly, the scaling dimension of a vortex is $v_x = \pi K$.⁹

We are now ready to write the renormalization group equation for y , which controls the number of vortices, using the relation between the scaling dimension v_x and the renormalization group exponent v_y , $v_y = d - v_x$.

The relation $y' = b^{v_y}y$ with the scaling factor b reduces in the limit of an infinitesimal scaling factor $b = 1 + dl$ to

$$\frac{dy}{dl} = v_y \cdot y = (2 - v_x)y = (2 - \pi K)y = xy, \quad (7.51)$$

if we notice that $b^{v_y} \approx 1 + v_y dl$. This is the differential renormalization group equation for y .

To derive the renormalization group equation for the scaling field x , we assume that the system is close to the KT transition point ($|x| \ll 1$). Moreover, we are interested in whether or not the number of vortices increases by a renormalization group transformation. These aspects justify keeping only the lowest-order term in the Taylor expansion of the right-hand side of the renormalization group equation (beta function) in powers of x and y . Since vortices show up as pairs in the KT phase, the \downarrow second-order term is the lowest-order one in the variable y . As will be shown later, the renormalization group equation for x is readily written only in terms of this effect,¹⁰

$$\frac{dx}{dl} = a^2 y^2. \quad (7.52)$$

Since the presence of vortices disorders the system, x should increase by the effects of y , and the coefficient on the right-hand side is chosen to be positive, a^2 . Let us confirm that no other additive terms including a constant and a low-order term in x appear. It is first clear that a constant term does not exist because $x^* = y^* = 0$ is a fixed point. A term proportional to x represents an instability of the fixed point $x^* = 0$ since a temperature lower than the critical one renormalizes to still lower temperatures, see Fig. 4.4, which is in conflict with the physical picture that the KT phase corresponds to a fixed line, not an isolated fixed point. Similarly, x^2 increases the temperature with $x < 0$ toward $x = 0$, and the KT transition point $x = 0$ becomes a stable, isolated fixed point, again incompatible with our physical intuition. Similar considerations exclude all terms written as functions of x on the right-hand side of eqn (7.52). We therefore conclude that eqns (7.52) and (7.51) are the right renormalization group equations to describe the KT transition. They are called the *Kosterlitz equations*.

7.6.2 Solving the Kosterlitz equations

To solve the Kosterlitz equations, it is useful to note that the scale variable l can be eliminated by taking the ratio between both sides of eqns (7.52) and (7.51),

$$\frac{dx^2}{dy^2} = a^2. \quad (7.53)$$

The result is an equation for x and y , and its analytic solution is a hyperbola

$$x^2 - a^2 y^2 = \text{const.} \quad (7.54)$$

Since the KT transition point is at $x = y = 0$, the solution corresponding to the transition point has a vanishing constant on the right-hand side of eqn (7.54). This means that the line $y = \pm x/a$ should go through the transition point on the xy plane. The renormalization group flow is drawn in Fig. 7.4. Within the KT phase, the spin-wave

approximation captures the essence of the relevant physics and vortices do not play an essential role, irrelevant in the renormalization group sense, and hence y is renormalized to 0. This is the situation to the left of the line $y = -x/a$ in Fig. 7.4. In the paramagnetic phase y renormalizes to larger and larger values, as in the region to the right of the line $y = -x/a$. These considerations lead to the renormalization group flow illustrated in Fig. 7.4. On the low-temperature side, the KT phase, y is renormalized to 0 and x is to a finite value that corresponds to the initial (bare) value, and the system is attracted to the fixed line $y^* = 0, x < 0$. On the high-temperature side, the paramagnetic phase, y increases indefinitely and more and more vortices are created as the renormalization group process goes on. The line $y = -x/a$ separates these two phases and is known as a *separatrix*. ↴

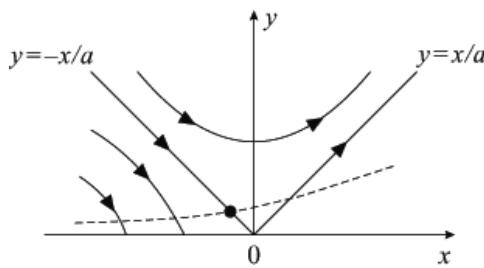


Fig. 7.4 Renormalization group flow of the Kosterlitz equations. The dashed line represents the bare XY model before renormalization. The small black dot on this line is the KT transition point written in terms of the bare coupling.

We have seen that the scaling field y is related to the fugacity y_0 and the chemical potential μ for vortices by the relation $y = y_0 e^{-\beta E_c/2} = e^{-\beta \mu - \beta E_c/2}$. These quantities, fugacity and chemical potential, have been introduced artificially to study the situation with a small number of vortices and do not exist in the original XY model. The original problem corresponds to $\mu = 0$ or $y_0 = 1$, and hence the bare couplings lie on the curve $y = e^{-\beta E_c/2}$ drawn as a dashed line in Fig. 7.4. This figure shows that the value of x increases toward a slightly larger value on the line $y = 0, x < 0$ after renormalization even within the KT phase (to the left of the line $y = -x/a$). Correspondingly the temperature is also renormalized to a larger value. The fixed line is reached after many steps of the renormalization group transformation, and the dashed line of the original system itself is not invariant under renormalization. It should also be noticed that the fixed-point condition $x^* = 0$ ($T = T_{KT} = \pi J/2$) representing the KT transition point is to be described by the renormalized temperature. The transition temperature in terms of the original variable is at the crossing point of the line $y = -x/a$ and the dashed curve, the small black dot in Fig. 7.4. Since this crossing point has $x < 0$, the KT transition temperature in terms of the original variable is smaller than $\pi J/2$.

We next study the singularities of physical quantities near the transition point using the solution of the Kosterlitz equations. Since $x^2 - a^2 y^2 = 0$ at the transition point, we will have $x^2 - a^2 y^2 = -ct$ ($t = (T - T_{KT})/T_{KT}, c > 0$) slightly above the transition point. Then, the solution to the Kosterlitz equation

$$\frac{dx}{dt} = a^2 y^2 = x^2 + ct \quad (7.55)$$

is

$$l = l_0 + \frac{1}{\sqrt{ct}} \arctan \frac{x}{\sqrt{ct}}. \quad (7.56)$$

Equation (7.55) indicates that x increases with l ($x \neq 0$) independent of its sign, meaning that the renormalization flows to the right in Fig. 7.4.

EXERCISE 7.5 Confirm that the Kosterlitz equation near the transition point (7.55) has the solution (7.56).

- p. 171 Now, suppose that l (essentially the same as the scale b of renormalization) has reached the size of the system after many renormalization steps. If we write l_f for this l and set the value of arctan on the right-hand side of eqn (7.56) to its largest possible value $\pi/2$, we have

$$l_f = l_0 + \frac{k}{\sqrt{t}} \quad \left(k = \frac{\pi}{2\sqrt{c}} \right). \quad (7.57)$$

We will later use the fact that vortices cease to exist in pairs when l reaches l_f since almost all degrees of freedom have been traced out. In order to connect this l_f with the correlation length, we notice that the correlation length ξ^* measured from the standard of the renormalized system of scale b is related to the correlation length ξ in the original scale as $\xi^* = \xi/b$. Then, the renormalization group equation for the infinitesimal scaling $b = 1 + dl$ is

$$\frac{d\xi}{dl} = -\xi. \quad (7.58)$$

This equation is solved as $\xi \propto e^{-l}$. The value of ξ obtained by integration of eqn (7.58) is the correlation length measured in the standard after renormalization. If this value is A , the correlation length measured in the unit of the unrenormalized system is $\xi = Ae^{-l}$. We therefore conclude that the limit length for a vortex pair to exist, measured in the original scale (standard of length) is, from eqn (7.57),

$$\xi \approx \xi_0 e^{l_f} \approx \exp \left(\frac{k}{\sqrt{t}} \right). \quad (7.59)$$

The correlation length diverges exponentially, with a non-universal coefficient k , as the temperature approaches the transition point from above. An exponential divergence is very strong. For example, when $t = 10^{-2}$, eqn (7.59) gives $\xi \approx 2 \times 10^5$ if k is unity. It is therefore necessary to take sufficient care in numerical studies of the KT transition.

In order to check the singularity of the free energy, we note that the scaling law $f(t) = b^{-d} f(b^{-y} t)$ can be rewritten as $f = b^{-d} g(b/\xi)$ because we have $f(b^{-y} t) = f((b/t)^{-y} t^y) = g(b/\xi)$ from $\xi = t^{-y} = t^{-1/y}$. This expression $f = b^{-d} g(b/\xi)$ for the scaling function is valid even when the correlation length diverges exponentially, not polynomially, because the argument is written as the ratio of b and ξ without reference to a power of t explicitly. Let us set $b = \xi$ in $f = b^{-d} g(b/\xi)$ and apply eqn (7.59) to find

$$f = \xi^{-d} g(1) \approx \exp \left(-\frac{2k}{\sqrt{t}} \right), \quad (7.60)$$

which expresses the essential singularity of the free energy. This equation shows that the free energy has a very weak singularity that is differentiable arbitrarily many times. Consequently, the same is true for the specific heat. The essential singularity in the specific heat at T_{KT} is very weak and unobservable experimentally and in numerical simulations. Indeed the specific heat has a broad non-universal peak slightly above the transition point and has no sign of singularity.

Those peculiar exponential singularities in the correlation function and specific heat reflect the lower critical dimension (two) of the XY model. As seen in \downarrow Section 3.6.3, similar exponential singularities are shared by the Ising model at its lower critical dimension $d = 1$ near the transition point $T = 0$.

7.7 Lattice gauge theory and Elitzur's theorem

In this section we digress from the main topic of KT transition and discuss the absence of spontaneous symmetry breaking in systems with local (gauge) symmetry. The theorem of Mermin and Wagner claims that continuous global symmetries do not break down spontaneously in two or lower dimensions. The same is true for discrete global symmetries in one dimension. We show in the present section that there exist no spontaneous symmetry breaking in any dimensions for local symmetries. This result contrasts the difference between global and local symmetries.

For this purpose we analyze the *lattice gauge theory*, which has been introduced to understand the mechanism of confinement of quarks. Although the physical motivation is different, some models in the lattice gauge theory show phase transitions, whose properties are controlled by the symmetry and dimensionality of the system, similarly to conventional spin systems.

7.7.1 Lattice gauge theory

Symmetries of a physical system can be classified into global or local (gauge) depending on the character of the transformation realizing the mathematical mapping.¹¹ For example, in the conventional Ising model, one needs to change the sign of *all* spins ($S_i \rightarrow -S_i, \forall i$) to realize the global \mathbb{Z}_2 discrete symmetry of the model. The same happens in the XY model, where *all* angle variables need to be transformed by the same amount ($\phi_i \rightarrow \phi_i + \alpha, \forall i$) to realize the global U(1) continuous symmetry¹² On the other hand, there are models where transforming only *some* degrees of freedom is enough to achieve invariance. A *gauge theory* is defined by a Hamiltonian or action, classical or quantum, that is invariant under a local or gauge transformation. It can be defined on a lattice or in the continuum, e.g. as a field theory. According to the *gauge principle* adopted widely in field theory, all fundamental physical interactions in nature arise from actions or Hamiltonians that are invariant under local transformations. The primary motivation to study lattice gauge theories is to provide a non-perturbative approach for the standard theory of strong interactions in high-energy physics, also known as quantum chromodynamics, and thus to attempt to explain the phenomenon of quark confinement. This is well beyond the scope of this book, and we will only concentrate on some of the aspects of critical phenomena in classical models of the lattice gauge theory.

An example of a classical model that displays discrete gauge symmetries is the \mathbb{Z}_2 lattice gauge theory, also known as the Z_2 *gauge theory* or the *Ising lattice gauge theory*. Consider Ising spins $S_i = \pm 1$ that reside on the bonds i ,¹³ and not on the vertices (sites), of a three-dimensional cubic lattice. Then, the Hamiltonian of the Z_2

p. 173 gauge theory is defined as

\downarrow

$$H = -J \sum_{\square} B_{\square}, \quad (7.61)$$

where the sum spans all possible square plaquettes \square on the lattice each containing four spins and, as we will see, is invariant under the $\mathfrak{S} = \mathbb{Z}_2$ gauge group. The interaction term comprises the product of these four spins, as depicted in Fig. 7.5,

$$B_{\square} = \prod_{i \in \square} S_i. \quad (7.62)$$

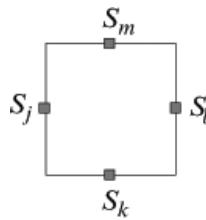


Fig. 7.5 The product of four spins on bonds around a plaquette constitutes the basic interaction B_{\square} in the Z_2 gauge theory.

In addition to the global \mathbb{Z}_2 symmetry, $S_i \rightarrow -S_i$ ($\forall i$), this Hamiltonian has a \mathbb{Z}_2 gauge symmetry which consists of the following transformation (see Fig. 7.6): Select any vertex \mathcal{J} of the lattice shared by six bonds (four bonds for $d = 2$ as in Fig. 7.6), flip the sign of the spins on these six (four) bonds, $S_i \rightarrow -S_i$, if i emanates from \mathcal{J} . Since each plaquette connected with vertex \mathcal{J} has two spins flipped, their product B_{\square} , and thus the overall Hamiltonian, remains invariant.

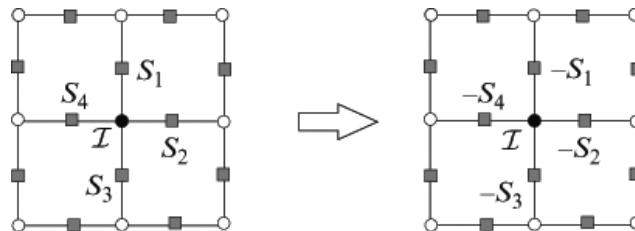


Fig. 7.6 The signs of spin variables on bonds emanating from a site \mathcal{J} are changed. This is a local, gauge transformation and keeps the Hamiltonian invariant.

Notice that, while the lowest-energy state in the usual Ising model is two-fold degenerate, the ground-state degeneracy is much more enormous in the Z_2 gauge theory. For example, if the configuration on the left panel p. 174 of Fig. 7.6 is a ground state, the one on the right panel is also a ground state. This gauge transformation that generates another state with the same energy is applicable to any vertex. Consequently there exist a large number of degenerate states (exponential in the system size).

Another example of a classical model of gauge theory is the $U(1)$ gauge theory ($U(1)$ lattice gauge theory) with a continuous local symmetry

$$H = -J \sum_{\square} A_{\square}, \quad (7.63)$$

where the plaquette interaction A_{\square} is defined in terms of elements of the group $U(1)$, i.e. complex fields $\phi_j = e^{iA_j}$ with gauge variables $-\pi < A_j \leq \pi$ defined on the bonds j , as

$$A_{\square} = \frac{1}{2} (\phi_j \phi_k \phi_l \phi_m^* + \phi_j^* \phi_k^* \phi_l \phi_m) = \cos(A_j + A_k - A_l - A_m), \quad (7.64)$$

with j, k, l, m bonds belonging to the plaquette \square as in Fig. 7.7. We assume that those plaquette interaction terms are defined on a general hypercubic lattice.

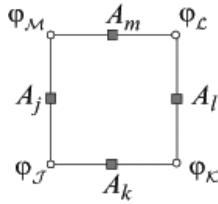


Fig. 7.7 Allocation of variables on a plaquette to generate a gauge transformation in the $U(1)$ gauge theory.

The following $U(1)$ gauge transformation is a symmetry of the Hamiltonian of eqn (7.63),

$$A_j \rightarrow A_j + \phi_{\mathcal{J}} - \phi_{\mathcal{M}} \quad (7.65)$$

$$A_k \rightarrow A_k + \phi_{\mathcal{K}} - \phi_{\mathcal{J}} \quad (7.66)$$

$$A_l \rightarrow A_l + \phi_{\mathcal{L}} - \phi_{\mathcal{K}} \quad (7.67)$$

$$A_m \rightarrow A_m + \phi_{\mathcal{L}} - \phi_{\mathcal{M}}, \quad (7.68)$$

with arbitrary c -number functions $\phi_{\mathfrak{I}}$ defined on the vertices \mathfrak{I} of the lattice as indicated in Fig. 7.7. It is straightforward to check that eqns (7.65) to (7.68) keep eqn (7.64) invariant. This transformation is *Abelian* because the group $U(1)$ is Abelian; two successive changes of angles are equivalent to the changes in the other order and are thus commutable. There are several non-Abelian generalizations of these models.

7.7.2 Elitzur's theorem

The presence of local (gauge) invariance has important physical consequences. One of those consequences is *Elitzur's theorem*, which states that non-gauge-invariant (or gauge-variant) local physical quantities cannot exhibit spontaneous breaking of gauge ↴

symmetries, discrete or continuous, in any dimensions. This does not imply that a phase transition, signaled as a singularity in the free energy, cannot occur, as we will see in the example of the three-dimensional Z_2 gauge theory below. Therefore, the expectation value of a gauge-variant quantity cannot be used as a Landau-type local order parameter to describe such a phase transition. Since symmetry breaking of local quantities is precluded, differences in the behavior of correlation functions in different phases have to manifest themselves in non-local quantities written in terms of the original local degrees of freedom.

We now prove Elitzur's theorem. The essence of the proof is as follows. Consider the absolute value of the average of any local quantity $f(\phi_i)$ (involving only a finite number of fields or variables $\{\phi_i\}$ like S_i), which is bounded and non-invariant under a gauge symmetry group \mathfrak{S} of a Hamiltonian H (such as \mathbb{Z}_2 in the Z_2 gauge theory). This $|f(\phi_i)|$ is shown to be bounded from above by the absolute mean value of the same quantity computed for a zero-dimensional Hamiltonian H (i.e. it involves a finite number of degrees of freedom) which is globally invariant under \mathfrak{S} and preserves the range of the interactions. This upper bound is shown to vanish in the zero-field limit after the thermodynamic limit due to the local character of the symmetry.

More explicitly, to determine if spontaneous symmetry breaking occurs, we evaluate

$$\langle f(\phi_i) \rangle = \lim_{h \rightarrow 0} \lim_{N \rightarrow \infty} \langle f(\phi_i) \rangle_{h,N}, \quad (7.69)$$

where $\langle f(\phi_i) \rangle_{h,N}$ is the average value of $f(\phi_i)$ calculated on a finite lattice of N sites and in the presence of a symmetry breaking field h . Simple examples of $f(\phi_i)$ are S_i for the Z_2 gauge theory and $e^{i\phi_i}$ for the $U(1)$ gauge theory. Since the lattice Λ is formed out of the union of smaller finite sublattices, $\Lambda = \cup_l C_l$, the bond i belongs at least to one subset (see Fig. 7.8).

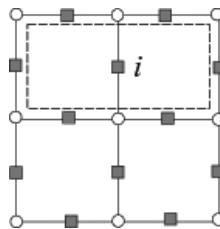


Fig. 7.8 An example of a sublattice C_i , which includes bond i , is shown as a dashed contour.

It is convenient to rename the fields in the following way: $\phi_l = \psi_l$ if $l \notin C_i$ and $\phi_i = \eta_i$ if $i \in C_i$. Then, we can separate the variables to write $\langle f(\phi_i) \rangle_{h,N}$ as

$$\langle f(\phi_i) \rangle_{h,N} = \frac{\sum_{\{\phi_l\}} f(\phi_i) e^{-\beta(H(\{\phi_l\})+h \sum_l \phi_l)}}{\sum_{\{\phi_l\}} e^{-\beta(H(\{\phi_l\})+h \sum_l \phi_l)}} \quad (7.70)$$

$$= \frac{\sum_{\{\psi_l\}} z_{\{\psi\}} e^{-\beta h \sum_{l \notin \mathcal{C}_i} \psi_l} g(\{\psi_l\})}{\sum_{\{\psi_l\}} z_{\{\psi\}} e^{-\beta h \sum_{l \notin \mathcal{C}_i} \psi_l}}, \quad (7.71)$$

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$$z_{\{\psi\}} = \sum_{\{\eta_i\}} e^{-\beta(H(\{\psi_l, \eta_i\}) + h \sum_{i \in \mathcal{C}_i} \eta_i)}, \quad (7.72)$$

and

$$g(\{\psi_l\}) = \frac{\sum_{\{\eta_i\}} f(\eta_i) e^{-\beta(H(\{\psi_l, \eta_i\}) + h \sum_{i \in \mathcal{C}_i} \eta_i)}}{z_{\{\psi\}}}. \quad (7.73)$$

From eqn (7.71), since $z_{\{\psi\}} e^{-\beta h \sum_{l \notin \mathcal{C}_i} \psi_l}$ is positive definite, $\langle f(\phi_i) \rangle_{h,N}$ can be bounded as follows

$$|\langle f(\phi_i) \rangle_{h,N}| \leq |g(\{\bar{\psi}_l\})|, \quad (7.74)$$

where $\{\bar{\psi}_l\}$ is the particular configuration of fields ψ_l that maximizes $g(\{\psi_l\})$ in eqn (7.71). The quantity $H(\{\psi_l, \eta_i\})$ is a zero-dimensional Hamiltonian in that it involves only a finite number of bonds as far as the field variables η_i are concerned. This zero-dimensional Hamiltonian $H(\{\psi_l, \eta_i\})$ is invariant under the global symmetry group of transformations \mathfrak{S} over the fields η_i , e.g. $S_i \rightarrow -S_i$ ($\forall i$) in the Z_2 gauge theory.

Let us define $H(\{\eta_i\}) \equiv H(\{\bar{\psi}_l, \eta_i\})$. The range of the interactions between the η -fields in $H(\{\eta_i\})$ is clearly the same as the range of the interactions between the ϕ -fields in the original Hamiltonian $H(\{\phi_l\})$. Since $H(\{\eta_i\})$ is a zero-dimensional Hamiltonian with only a finite number of variables, $g(\{\bar{\psi}_l\})$ is an analytic function of h for any N including the thermodynamic limit. The exponential in the numerator of eqn (7.73) is invariant under the global transformation \mathfrak{S} in the limit $h \rightarrow 0$ after $N \rightarrow \infty$ but the function $f(\eta_i)$ changes the sign in the Z_2 gauge theory e.g. $f(\eta_i)$ may be S_i , which changes as $S_i \rightarrow -S_i$. In the case of the $U(1)$ gauge theory the phase changes like $f(\eta_i) = e^{i\phi_i} \rightarrow e^{i(\phi_i + \phi)}$. Thus, $g(\{\bar{\psi}_l\}) = -g(\{\bar{\psi}_l\})$ for the Ising (\mathbb{Z}_2) case and $g(\{\bar{\psi}_l\}) = e^{i\phi} g(\{\bar{\psi}_l\})$ for the $U(1)$ gauge theory, any one of which is satisfied only if $g(\{\bar{\psi}_l\}) = 0$. This completes the proof.

Notice that the frozen variables $\bar{\psi}_l$ act like external fields in $H(\{\eta_i\})$, which do not break the global symmetry group of transformations \mathfrak{S} . From a physics standpoint, a gauge symmetry involves a few degrees of freedom and it costs only a finite amount of energy to change a stable state to another one, which is in marked contrast to the case of global symmetry depicted in Fig. 5.2. This is the essence of the above proof.

7.7.3 Phase transitions in the lattice gauge theory

The three-dimensional Z_2 gauge theory of eqn (7.61) is dual (i.e. essentially equivalent) to the three-dimensional Ising model, as explained in Section 10.2. The latter has a phase transition at finite temperature. This means that the free energy of the Z_2 gauge theory shows the same singularity at the critical temperature T_c as the conventional Ising model. However, the phase transition in the Z_2 gauge theory does not manifest itself as a spontaneous symmetry breaking in the local spin variables due to Elitzur's theorem; the Z_2 gauge theory does not have a Landau-type local order parameter.¹⁷⁷

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To characterize the low- and high-temperature phases, one must use a correlation function that is gauge invariant. A well-known physical quantity used to characterize the phases of gauge models is the *Wilson loop*, constructed for the Z_2 gauge theory for example, as

$$W_\Gamma = \left\langle \prod_{i \in \Gamma} S_i \right\rangle, \quad (7.75)$$

where i runs over the bonds forming a closed path or loop Γ as in Fig. 7.9. This quantity W_Γ is gauge invariant. For example, if one changes the signs of S_i 's connected to a vertex \mathcal{J} located on Γ , two of the S_i 's on bonds emanating from \mathcal{J} and on Γ change the sign and thus W_Γ remains invariant.

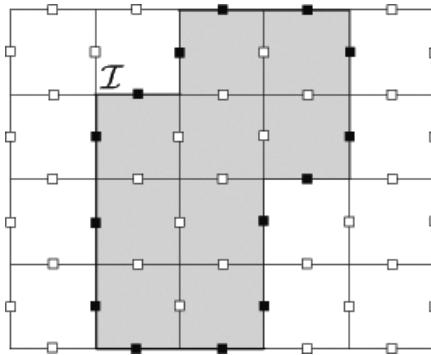


Fig. 7.9 A Wilson loop consists of the product of variables along a closed path Γ (thick lines). In this figure the variables on Γ are denoted in black squares. A gauge transformation of variables around a vertex \mathcal{J} on Γ keeps W_Γ invariant.

From the dependence of W_Γ on Γ in the limit of large loops, one can determine the nature of the phases of the model. In the high-temperature phase, the Wilson loop has an exponential decay controlled by the area of the loop, an *area law* $W_\Gamma \approx e^{-c|A|}$ ($c > 0$), where $|A|$ is the size of the area surrounded by Γ (shown in gray in Fig. 7.9). At low temperatures, it is controlled by the length of the loop, a *perimeter law* $W_\Gamma \approx e^{-c|\Gamma|}$ ($c > 0$), where $|\Gamma|$ is the length of Γ . The temperature at which there is a change in the asymptotic behavior of W_Γ defines the transition point T_c .

The two-dimensional version of the Z_2 gauge theory is trivially solvable by a high-temperature expansion, as elucidated in Section 10.2. It displays no finite-temperature phase transition, and the lower critical dimension of the Z_2 gauge theory is $d_{lc} = 2$.

Notes

- 1 This simple evaluation fails to take into account the avoidance condition of overlaps with more than a few steps before. A more accurate estimate leads to $a^{\lceil N \rceil}$ possibilities with a slightly less than 3, which, however, does not affect our conclusion qualitatively.
- 2 There are examples of classical systems with short-range interactions, such as Kittel's zipper model, that display true thermodynamic phase transitions in $d = 1$. Typically, these short-range models include hard-core interactions.
- 3 Integration by parts in the third expression of eqn (7.4) changes the integrand to $-\phi \nabla^2 \phi$. Functional variation of this expression yields the result.
- 4 A more rigorous evaluation of the integral leads to the same conclusion that the lower critical dimension of the XY model is two.
- 5 We normalize the lattice constant to unity, i.e. $a = 1$.
- 6 Rigorously speaking, long-range order is not identical to spontaneous magnetization, the former being defined by the limiting value of a correlation function as discussed at the end of Section 5.6. We, however, often use these two names interchangeably in this book because they are physically equivalent.
- 7 J. M. Kosterlitz and D. J. Thouless, J. Phys. C **6** (1973) 1181. A similar idea was proposed by V. L. Berezinskii in Sov. Phys. JETP 34 (1972) 610.
- 8 Strictly speaking, a fixed point should be distinguished from a critical point. Thus, K appearing here is not the interaction constant before renormalization $K = J/T$ (*bare coupling*) but is the variable after many steps of renormalization (*renormalized coupling*). The difference between these two concepts will be explained in more detail later.
- 9 The scaling fields of the two-dimensional XY model are often written as x and y for historical reasons. This notation may be confused with the scaling dimension or the exponent of the renormalization group eigenvalue. In this book we write u_x and u_y for the scaling dimension and exponent, respectively, of the vortex numbers. Do not confuse this notation with the Cartesian components of the velocity field u of the previous section.
- 10 Do not confuse the constant a of this section with the lattice constant.
- 11 Sometimes, a gauge symmetry is referred to as a gauge structure instead of a symmetry since two states related by this gauge transformation are the same state but with a different label.
- 12 The group $U(1)$ is composed of rotations on the complex plane.
- 13 A bond is often called a *link* in gauge theories.

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