The Mermin-Wagner theorem and the Kosterlitz-Thouless transition

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1 Mermin-Wagner Theorem

Before talking about the Mermin-Wagner theorem, we first have to clarify the connection between spontaneous symmetry breaking and phase transitions. For that, let's remember the Hamiltonian of a spin magnet, where the spins are vectors of size n

$$H = -J \sum_{i,j} s_i \cdot s_j$$

The Hamiltonian is invariant under the $O(n)$ group, because the scalar product of two rotated vectors does not change. If we start bringing the temperature of the spin system down, what happens is that below the Curie temperature they begin to align in a certain direction and the mean magnetisation $\langle M \rangle \neq 0$. This direction is random and in the case of a two dimensional system could be any angle $\theta \in (0, 2\pi)$. The important observation is, that the Hamiltonian from above is still valid and dictates the behaviour of the system, but the newly occupied ground state of the system has lost the symmetry of the Hamiltonian, namely the $O(n)$ symmetry. This is easy to see, as a spin field aligned in the x-direction is in a different state than one aligned in the y-direction. Thus by choosing a ground state (this is what the *spontaneous* refers to) the system broke the original symmetry it had before the phase transition (here from para- to ferromagnetic).

We can now state the theorem.

Theorem (Mermin-Wagner)**.** *There is no spontaneous symmetry breaking in systems with short-range interactions and a continuous symmetry in $d \leq 2$.*

There are two important points to observe. First, that the interactions have to be short-range. Second, the symmetry has to be a continuous one. This makes sense, because as we know from the solution of the Ising model by Onsager [1], there is a phase transition for $d = 2$. This difference in behaviour arises from the fact the in the Ising model the spins can only point in two directions. Instead of rotating, we are just allowed to flip the spins, which is a discrete symmetry (the group $\mathbb{Z}/2$).

Now we will give an overview of the original paper [2]. The Hamiltonian, the authors start from, is

$$H = -\sum_{i,j} J_{ij} s_i \cdot s_j - h \sum_i (s_i)_z e^{-ik\cdot r_i}$$

Apart from the internal interaction there is also an external field h that interacts through the z-component of the spins. The vector k serves the purpose of accounting for both ferro- and antiferromagnetism ($e^{-ik\cdot r_i} = \pm 1$). The next step is the usage of the Bogoliubov inequality

$$\frac{1}{2}\langle\{\hat{A}, \hat{A}^\dagger\}\rangle \geq k_B T |\langle[\hat{C}, \hat{A}]\rangle|^2 / \langle[[\hat{C}, \hat{H}], \hat{C}^\dagger]\rangle,$$

with a smart choice of operators $\hat{A}$ and $\hat{C}$. After a series of calculations the new inequality reads

$$|s_z| \leq \frac{\text{const.}}{T^{1/2}} \frac{1}{|\ln(|h|)|^{1/2}}.$$

The interpretation is, that for a finite temperature $T > 0$, in the limit of a vanishing external field $h \to 0$, the spin expectation value also vanishes and therefore we observe no magnetisation. Put differently, there is no symmetry breaking. The proof can be adapted to many different physical systems (e.g. superfluids) as the procedure does not change much as long as the symmetries remain similar. There also exists a more general field theoretic proof by Coleman, in which is shown that there are no Goldstone bosons in two dimensions [3].

2 Kosterlitz-Thouless

2.1 XY model

The XY model is a generalisation of the Ising model, in the sense that spins can now rotate in two dimensions $s = (\cos(\theta), \sin(\theta))$. Further, we just take into account next neighbour interactions.

$$\begin{aligned} H &= -J \sum_{\langle ij \rangle} s_i \cdot s_j = -J \sum_{\langle ij \rangle} \Big(\cos(\theta_i)\cos(\theta_j) - \sin(\theta_i)\sin(\theta_j)\Big) \\ &= -J \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j) \end{aligned}$$

2.2 No spontaneous symmetry breaking

The Mermin-Wagner theorem tells us that the XY model, due to its continuous $O(2)$ symmetry, cannot exhibit spontaneous symmetry breaking at finite temperatures. Redoing the proof for this case is much simpler and gives a good idea of the general procedure. It suffices to consider the Schwarz inequality

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

and to make the following choice for the operators

$$\begin{aligned} A &= \frac{1}{N} \sum_j e^{-iq\cdot r_j} \sin\theta_j \\ B &= \frac{1}{N} \sum_l e^{-iq\cdot r_l} \frac{\partial H}{\partial \theta_l}. \end{aligned}$$

Now, the individual expectation values (with respect to Boltzmann weight) have to be calculated. As an example, we evaulate the term $\langle AB^* \rangle$.

$$\langle AB^* \rangle = \frac{1}{N^2} \sum_{j,l} e^{-iq(r_j - r_l)} \langle \sin\theta_j \frac{\partial H}{\partial \theta_l} \rangle .$$

The expectation value on the right, after integration by parts reads

$$Z^{-1} \int_0^{2\pi} \prod_i d\theta_i \, e^{-\beta H} \sin\theta_j \frac{\partial H}{\partial \theta_l} = \frac{T}{Z} \int_0^{2\pi} \prod_i d\theta_i \, e^{-\beta H} \cos\theta_j \, \delta_{lj} ,$$

where we used $e^{-\beta H} \partial H / \partial \theta_l = \beta^{-1} \partial e^{-\beta H} / \partial \theta_l$. The boundary terms vanish due to the symmetry of the model. Finally we arrive at

$$\langle AB^* \rangle = \frac{T}{N^2} \sum_j \langle \cos\theta_j \rangle \equiv \frac{Tm}{N^2} .$$

Simplifying the other terms we get the following expression for the inequality

$$1 \leq \frac{T}{N} m^2 \sum_q \frac{1}{Jq^2 + h} \longrightarrow T m^2 \int \frac{d^2 q}{(2\pi)^2} \frac{1}{Jq^2 + h} ,$$

having taken the thermodynamic limit the the last line. For $h \to 0$ the integral has a logarithmic divergence and hence for the inequality to be valid, m also has to go to zero, meaning that there is no magnetisation.

2.3 Differing correlation lengths

Numerical simulations of the XY model have shown that at low and high temperature the system behaves differently. In fact, at low temperatures the spins start to align in macroscopic regions, i.e. they are correlated. In the light of the previous section, this seems surprising as we are used to equate phase transitions – in this case a shift from an unordered to an ordered phase – to the breaking of a symmetry. To investigate this further we compute the correlation of two spins between the origin and the position r. Since an exact calculation is not possible we restrict ourselves to cases of high and low temperature. We start at high temperature and take advantage of the fact, that the Boltzmann factor becomes very small, which allows us to Taylor expand it. Setting $K \equiv -\beta J$

$$\begin{aligned}
\langle s_0 \cdot s_r \rangle &= \langle \cos(\theta_0 - \theta_r) \rangle \\
&= \frac{1}{Z} \prod_{i=1}^{N} \left(\int_0^{2\pi} \frac{d\theta_i}{2\pi} \right) \cos(\theta_0 - \theta_r) e^{K \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j)} \\
&= \frac{1}{Z} \prod_{i=1}^{N} \left(\int_0^{2\pi} \frac{d\theta_i}{2\pi} \right) \cos(\theta_0 - \theta_r) \prod_{\langle i,j \rangle} \left[1 - K \cos(\theta_i - \theta_j) + \mathcal{O}(K^2) \right]
\end{aligned}$$

Neglecting terms of order K^2 the integrand becomes a product of the form

$$[1 - K\cos(\theta_1 - \theta_2)][1 - K\cos(\theta_2 - \theta_3)] \cdots ,$$

so by multiplying out we either get a one or a cosine. But due to

$$\int_0^{2\pi} \frac{d\theta_1}{2\pi} \cos(\theta_1 - \theta_2) = 0$$

$$\int_0^{2\pi} \frac{d\theta_2}{2\pi} \cos(\theta_1 - \theta_2) \cos(\theta_2 - \theta_3) = \frac{1}{2} \cos(\theta_1 - \theta_3)$$

any term that got multiplied by at least a factor of one is zero after integration. Only terms with exclusively cosines survive and contribute a factor $K/2$. This procedure goes under the name of high temperature expansion and can be represented graphically. The result is therefore

$$\langle s_0 \cdot s_r \rangle \approx \left(\frac{K}{2}\right)^r = e^{-r/\xi},$$

with $\xi = \ln(2/K)^{-1}$. As we expected, in the high temperature regime the correlation decays exponentially. This is due to large fluctuations which destroy any long-range order.

Now we try to find the correlation at low temperature. For that, we employ the so called spin-wave approximation. As the fluctuations are weak we assume that the angle between neighbours doesn't vary too much. Then we can Taylor expand the cosine and take the continuum limit

$$\cos(\theta_i - \theta_j) \approx 1 - \frac{1}{2}(\theta_i - \theta_j)^2 \to 1 - \frac{a^2}{2}(\nabla\theta)^2,$$

where a stands for the lattice spacing (which we set to one for simplicity). For the energy then follows

$$H = \frac{K}{2}\int d^2x(\nabla\theta)^2 = \frac{K}{2}\int \frac{d^2q}{(2\pi)^2} q^2 \tilde{\theta}(q)\tilde{\theta}(-q),$$

which looks like an ordinary free field Hamiltonian. There is one important difference though, the variable θ has physical meaning only modulo 2π. Further we write

$$\langle \cos(\theta_0 - \theta_r)\rangle = \mathfrak{Re}\langle \exp\{i(\theta_0 - \theta_r)\}\rangle = \mathfrak{Re}\exp\{i\langle(\theta_0 - \theta_r)^2\rangle\}$$

where in the last step we used results from Gaussian integration. Continuing

$$\langle(\theta_r - \theta_0)^2\rangle = \int \frac{dq_1 dq_2}{(2\pi)^2}(e^{-iq_1 r} - 1)(e^{-iq_2 r} - 1)\langle\tilde{\theta}(q_1)\tilde{\theta}(q_2)\rangle$$

Taking advantage of the diagonal Hamiltonian in k-space we can directly write

$$\langle\tilde{\theta}(q_1)\tilde{\theta}(q_2)\rangle = \frac{(2\pi)^2}{K}\delta(q_1 + q_2) = \frac{(2\pi)^2 T}{J}\delta(q_1 + q_2)$$

After some further calculations (for details see [4, 5]) we arrive at the result

$$\langle s_0 \cdot s_r \rangle \approx r^{-T/2\pi J}.$$

In contrast to the high temperature regime, we now get an algebraic decay. Further the exponent is not universal but depends on the temperature. This confirms the numerical results mentioned above but also shows that this is not the usual correlated phase that has a constant universal exponent, but one that varies. This phase is called *quasi-ordered*. The low temperature approximation cannot be valid at all T because we know from earlier that at high T the spin correlation has to decay exponentially. We infer that the spin-wave approximation becomes invalid at a certain temperature. Intuitively this makes sense as high temperatures lead to more fluctuations which perturb the uniformity of the spin field.

What other solutions for the spin field could exist? Minimizing the energy $\delta H/\delta\theta$ leads to the Laplace equation $\nabla^2\theta = 0$, which apart from the uniform solution (spin-wave) also permits singular solutions in the form of vortices (see Fig. 1)

$$\theta(r, \phi) = n\phi + c,$$

where n is called the winding number and describes how many times a spin arrow winds around itself, going around clockwise the vortex center.

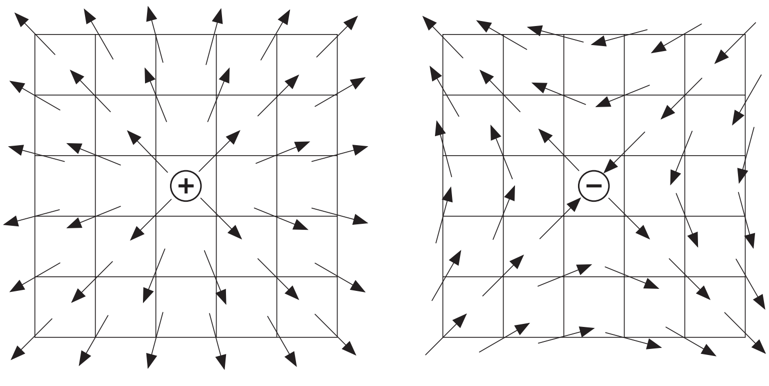

Figure 1: Two vortex configurations with positive and negative winding number [5]

2.4 Vortices

Kosterlitz and Thouless discovered that these vortices are the origin of the unusual behaviour of the system [6]. Their work was the starting point of the study of what is known as topological defects. The energy of a vortex can be calculated by noting that

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

Hence, inserting into the Hamiltonian

$$E = \frac{J}{2}\int \frac{n^2}{r^2} r\,dr\,d\phi = n^2\pi J \ln\frac{R}{r_0} + E_C.$$

To get a finite energy we introduce a cutoff radius (or vortex radius) r_0 and absorb the missing energy into the core energy E_C. The entropy of a vortex is given by the number of possibilities to place a vortex into our system. From above, the vortex area is proportional to r_0^2 and the whole are of course is R^2. Then

$$S = \ln\left(\frac{R}{r_0}\right)^2 = 2\ln\left(\frac{R}{r_0}\right).$$

The free energy of one isolated vortex is

$$F_1 = (\pi J - 2T)\ln\frac{R}{r_0}.$$

This shows that F_1 is positive for $T < T_{KT} = \pi J/2$ and negative for $T > T_{KT}$. Since thermodynamic systems minimize their free energy, it is energetically favourable to generate vortices once the system surpasses the temperature T_{KT}. This further confirms the breakdown of the spin-wave approximation at high temperatures as vortices represent a large perturbation of the spin field and their number grows with increasing temperature. In our calculation we neglected the interaction between vortices which gets more important with higher vortex numbers. Nonetheless we get a qualitative understanding for the phase transition.

Taking into account multiple vortices the energy becomes

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

where we sum over the winding number of all vortices. This shows, that vortices with opposite winding numbers can cancel their energy contribution, such that $E = 0$. Therefore, as long as the system generates a matching vortex and anti-vortex pair, vortices can also exist below the temperature T_{KT}. We can think of the system as a sea of vortex pairs whose number is not conserved but which are spatially bound to each other. Increasing the temperature leads to the creation of single vortices interacting with the background sea. At a certain temperature the interactions become too large and the pairs unbind, leading to long-range disorder.

The above formula suggests that we can interpret the winding number as a kind of charge. Indeed, one can show that there exists a mapping between the XY model and a two dimensional Coulomb gas, with the electric charges replaced by the winding numbers [4, 5]. The resulting potential is

$$E = -\pi J \sum_{i \neq j} n_i n_j \log \frac{|r_i - r_j|}{r_0} + E_C ,$$

where r_i are the positions of the vortex centers. Additionally this expression is also much more suited for renormalization group techniques, which confirm the validity of our rough estimate of T_{KT}.

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