Heidelberg University

Seminar-Lecture 5 SS 16

Menelaos Zikidis

Kosterlitz-Thouless Transition

1 Motivation

Back in the 70's, the concept of a phase transition in condensed matter physics was associated with this of a symmetry breaking. After the breakthrough of the Mermin Wanger theorem, i.e. that there cannot be any symmetry breaking in a lattice model of dimension $d \leq 2$ for temperature $T > 0$, physicists thought that there cannot be any phase transition in this 2D model for finite temperature.The main aim of this lecture is to provide an example of a phase transition that is not associated with a symmetry breaking by means of the Mermin Wagner theorem.

In condensed matter physics we classify matter in 3 basic states, in terms of the decay of their correlation functions, that is the physical order that prevails the system:

- Long range ordered state $(LRO) : G(x, x') \longrightarrow c \neq 0$
- Disordered state : $G(x, x') \xrightarrow{\propto exp(|x-x'|)} 0$ (Exponential decay of the correlation function)
- Quasi long range ordered state $(QLRO) : G(x, x') \xrightarrow{\propto |x-x'|^{-\eta}; \eta \in \mathbb{R}^+} 0$ (Algebraic decay of the correlation function)

Jumping from one state to another defines a phase transition for the system.

2 The Heisenberg Model

We introduce now the general lattice model that we will use,to see the destruction of long range order in different dimensions, the so called Heisenberg Model.This is a d-dimensional lattice with spins of n degrees of freedom, $S_i = (s_{i_1}, ..., s_{i_n})$, at each site of the lattice and with the additional constraint that ${S_i}^2 = 1 \; \forall i$. This system respects a $O(n)$-symmetry in a natural way. The Hamiltonian of this model has the form:

$$-\beta H = K \sum_{<i,j>} S_i S_j = -\frac{K}{2} \sum_{<i,j>} [(S_i - S_j)^2 - 2], \; K := \beta J,$$

with $\beta := \frac{1}{k_B T}$, J the spin-spin coupling constant and $\langle i, j \rangle$ indicates the sum operation over the nearest neighbors of every lattice site. Given that for $T = 0$ (ground state) the system has long range order, where all spins are aligned along, lets say, the direction $e_n = (0, ..., 0, 1)$, we see that at the ground state the general $O(n)$-symmetry of the disordered state of the system breaks into a $O(n-1)$-symmetry. We investigate what happens if we start slowly rising the temperature.

•<u>$T > 0$(low)</u>: At low temperatures, low energetic statistical fluctuations arise transverse to the e_n direction,this means that now the spins start to rotate just around this "frozen" direction $(O(n-1) - Symmetry)$. To the continuum approximation we obtain the following form for the Heisenberg-Model Hamiltonian:

$$-\beta H[S] = -\beta E_0 - \frac{K}{2}\int (\nabla S)^2 dx$$

where E_0 is ground state energy and S is now the spin-field of the continuum.For this Hamiltonian the Partition function has the form:

$$\mathcal{Z} = \int \mathcal{D}S(x)\underbrace{\delta(S^2-1)}_{S^2 \overset{!}{=} 1}\delta(S^2-1)e^{-\beta H[S]}$$

which turns out to be our familiar partition function of the NLσM. The next step in our investigation is to parametrize the field $S(x)$ in terms of the transverse fluctuations:

$$S(x) = (\psi_1(x), ..., \psi_{n-1}(x), \sqrt{1-\psi(x)^2}) = (\psi(x), \sqrt{1-\psi(x)^2})$$

and we calculate the average transverse fluctuation using the Gaussian approximation (Landau-Ginzburg expansion until the quadratic term):

$$\langle \psi(x)^2 \rangle = \int \frac{d^dq}{(2\pi)^d}\langle \psi(q)^2 \rangle \overset{\text{GaussAprx}}{=} \int \frac{d^dq}{(2\pi)^d}\frac{n-1}{Kq^2}$$

$$\propto \frac{n-1}{Kq^2}(\alpha^{2-d} - L^{2-d}) \xrightarrow[\text{Thermodynamic limit}]{L\to\infty} \begin{cases} \propto T & d > 2 \\ \to \infty & d \leq 2 \end{cases}$$

where L is the dimensionality of the system and α the Lattice spacing (UV-cutoff)

- $d > 2$: There is always a finite temperature such that fluctuations are small enough to maintain the long range order of the ground state.
- $d \leq 2$:The long range order of the ground state will always get destroyed by the transverse fluctuations.

These results are perfectly in accord with the statement of the Mermin-Wagner Theorem , which does not allow a symmetry breaking in $d \leq 2$ for $T > 0$. This result makes the case $d = 2$ a candidate in our search of a system with phase transition without an association to a symmetry breaking.So we proceed by an exact investigation of this interesting case, so we reduce the general Heisenberg model in 2D.

3 XY-Model

The 2D version of the Heisenberg Model is called XY-model, where te spins can be described as planar rotors $S = (cos\theta, sin\theta)$. The Spin-Hamiltonian will be:

$$-\beta H = K\sum_{\langle i,j\rangle} cos(\theta_i - cos\theta_j)$$

We compare how the correlation function behaves in high and low temperatures.

High Temperature series: The Partition function for the High temperature will be given by:

$$\mathcal{Z} = \int_0^{2\pi} \prod_i \frac{d\theta_i}{2\pi} e^{-\beta H} \overset{\text{K-Exp}}{=} \int_0^{2\pi} \prod_{\langle i,j \rangle} \frac{d\theta_i}{2\pi} [1 + K cos(\theta_i - \theta_j) + \mathcal{O}(K^2)]$$

It is allowed to expand in K , because we deal with high temperatures and K is, per definition, inverse proportianal to the temperature. From the correlation function we can estimate the spin-spin correlation function:

$$\langle S_0 S_x \rangle = < cos(\theta_x - \theta_0) > \propto \left(\frac{K}{2}^{|x|} \right) = \boxed{exp\left(\frac{-|x|}{\xi} \right)} \; ; \; \xi^{-1} := ln\left(\frac{2}{K} \right)$$

This implies an **exponential decay** of the spin-spin correlation function, which indicates that the system finds itself in a disordered state, as we have seen be the classification of the physical orders.

Low Temperature series: Now the cost of small fluctuations around the direction of the ordered ground state is obtained within a quadratic expansion (we also assume that the direction of the rotors varies smoothly):

$$cos(\theta_i - \theta_j) = 1 - \frac{1}{2}(\underbrace{\theta_i - \theta_j}_{\partial_x})^2 \; ; \; \partial_x \text{ by means of the discrete Laplacian}$$

which expansion leads to the continuum expression for the Hamiltonian in low temperature , as we have seen for the general case of the Heisenberg model:

$$-\beta H = \frac{K}{2} \int dx (\nabla\theta)^2$$

Which in the Gaussian approximation gives the correlation function:

$$\langle S(0)S(x) \rangle = \mathfrak{Re} \, \langle exp[i(\theta(0) - \theta(x))] \rangle = \mathfrak{Re} \left[exp\left(-\frac{\langle (\theta(0) - \theta(x))^2 \rangle}{2} \right) \right]$$

and in 2 dimensions the Gaussian fluctuations grow logarithmically as:

$$\frac{\langle (\theta(0) - \theta(x))^2 \rangle}{2} \simeq \frac{ln\left(\frac{|x|}{\alpha} \right)}{2\pi K}$$

We obtain from this analysis that the correlation function of the low temperature case **decays algebraically** as:

$$\langle S(0)S(x) \rangle \simeq \boxed{\left(\frac{\alpha}{|x|} \right)^{\frac{1}{2\pi K}}}$$

something that indicates that the system has a quasi long range order on such low temperatures.

The Problem: The difference of the order of the system between high temperatures and low temperatures is somehow peculiar because it looks like a phase transition is happening somewhere in between. One could thing, that our Gaussian approximation may failed us at some point, this has been later calculated by Winger,in terms of RG,and got the same results.
Let us try to understand what could happened by going back to our familiar Heisenberg Model. There we have seen that the phase transition in the Heisenberg model was associated with a symmetry breaking

$$\begin{array}{ccc} \text{Disorder} & & O(n) \\ {\scriptstyle\text{Phase Tr.}}\big\downarrow & & \big\downarrow{\scriptstyle SymmetryBreaking} \\ \text{LRO} & & O(n-1) \end{array}$$

Could the phase transition in the XY Model be also associated with a symmetry breaking?NO! Now a symmetry breaking is forbidden by the statement of Mermin-Wagner Theorem. $\Longrightarrow$ **Symmetry braking $\nsim$ Phase transition**.

The solution: Then Kosterlitz and Thouless proposed a solution: Topological defects explain the Phase transition! The theory of topological defects was a new idea back in the late 70's. These defects are solutions of the Model, that are topologically distinct from the ground state solution.This means that there cannot be found a continuous perturbation that turns the soliton solution into the ground state solution. In general topological defects arise in any Model with a compact group describing the order parameter,as for example a "Skyrmion" in a O(3) Heisenberg-Ferromagnet.

4 The Defects:Vortices

In the XY Model the spin are planar rotors and therefore is the spin-orientation defined up to an integer multiple of 2π. The idea is that there are spin configurations in which the traversal of a closed path sees the spin-angle rotate by $2n\pi; n \in \mathbb{Z}$:

$$\oint_\gamma \nabla\theta dl = 2n\pi \implies \nabla\theta = \frac{n}{r}\mathbf{e}_r \times \mathbf{e}_z;$$

for γ-closed path of radius r that encloses the defect and by symmetry $\nabla\theta$ is uniform and points along the azimuthal direction.For r small the continuum approximation fails and the Lattice structure becomes important.In our framework,we call the defect with topological charge $n = \pm 1$ a vortex.The discreteness of n is the one that gives away the nature of a topological defect over this configuration,whereby we will call the number $n-$**topological charge** of the defect.

We can calculate the energy cost for the formation of a single defect of charge n.The for the total contribution we have to take into account both the core region as well as the distortions away from the center.Without loss of generality we take a radius α that distinguishes the range of the two contributions,

$$\beta E_n = \beta E_n^0(\alpha) + \frac{K}{2}\int_\alpha dx(\nabla\theta)^2 = E_n^0(\alpha) + \pi K n^2 \ln\left(\frac{L}{\alpha}\right)$$

This obviously implies a logarithmic divergence of $\Delta E = E_n - E_n^0$ Now let us estimate the entropy of the elementary defect ($n = 1$), from the number of places one can locate the vortex center on the lattice namely $\left(\frac{L}{\alpha}\right)^2$, that is the number of all elementary plaquettes of the lattice.Then the configurational entropy is given by:

$$S = k_B \ln\left(\frac{L}{\alpha}\right)^2$$

This gives us an expression for the free energy:

$$F = E_1 - TS = E_0^1 + (\pi K - 2k_B T)\left(\frac{L}{\alpha}\right) \xrightarrow[\text{Thermodynamic limit}]{L\to\infty;\ T\propto K^{-1}} \begin{cases} \to +\infty & ;\ \text{for} T\text{-low} \implies K\text{-large} \\ \to -\infty & ;\ \text{conversly} \end{cases}$$

This indicates finally the existence of the a phase transition, the so called Kosterlitz-Thouless Transition, by the critical temperature $T_c = \pi\frac{K}{2k_B}$.