ICFP M1 - Phase Transitions – TD n° 7
Mermin-Wagner Theorem and Vortices

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1 Mermin-Wagner theorem

We shall consider a system of spins on a lattice, interacting according to the following ferromagnetic Hamiltonian,

$$H(\underline{\sigma}) = -J \sum_{\langle i,j \rangle} \vec{\sigma}_i \cdot \vec{\sigma}_j - h \sum_{i=1}^{N} \sigma_i^1 \ , \qquad J > 0 \ .$$

The first sum runs over the pairs of nearest neighbor vertices on an hypercubic lattice in dimension d, with distance a between nearest neighbors, and L sites in each direction. We shall denote $N = L^d$ the total number of sites, and assume periodic boundary conditions. The spatial position of site i is denoted $\vec{r}_i$. The degrees of freedom $\vec{\sigma}_i$ on each site are n-component vectors, $\vec{\sigma}_i = (\sigma_i^1, \dots, \sigma_i^n)$, with the contraint $\vec{\sigma}_i^2 = 1$ on their lengths. When $h = 0$ the model is invariant under a simultaneous rotation of all the spins, hence its name of $O(n)$ model, while h is a symmetry breaking magnetic field pointing in the first direction. For $n = 1$ one recovers exactly the Ising model, while the case $n = 2$ is called XY model, and $n = 3$ Heisenberg model. One defines the magnetization as

$$m(T, L, h) = \frac{1}{N} \sum_{i=1}^{N} \langle \sigma_i^1 \rangle \ ,$$

where $\langle \bullet \rangle$ denotes an average over the spin configurations $\underline{\sigma}$ weighted by the Gibbs-Boltzmann factor $e^{-\beta H(\underline{\sigma})}$, and the spontaneous magnetization as

$$m_{\rm sp}(T) = \lim_{h \to 0^+} \lim_{L \to \infty} m(T, L, h) \ .$$

For Ising spins ($n = 1$) we have seen that in dimension $d = 1$ there is no spontaneous magnetization at any finite temperature, while there is a positive spontaneous magnetization at low enough temperature for $d \geq 2$, hence the « lower critical dimension » (below which no spontaneous magnetization can appear) is $d_{\rm lc} = 1$ for discrete spins. On the contrary for continuous spins (i.e. for $n \geq 2$) one has $d_{\rm lc} = 2$, no spontaneous magnetization can occur in $d = 2$ (and also $d = 1$) : this is the content of the Mermin-Wagner theorem (*Phys. Rev. Lett.* **17**, 1133 (1966)).

For simplicity we shall derive this result in the case $n = 2$ (i.e. for XY spins) only, using the parametrization of the spins $\vec{\sigma}_i$ by an angle $\theta_i \in [0, 2\pi]$, i.e.

$$\vec{\sigma}_i = \begin{pmatrix} \sigma_i^1 \\ \sigma_i^2 \end{pmatrix} = \begin{pmatrix} \cos\theta_i \\ \sin\theta_i \end{pmatrix} \ , \qquad H(\underline{\theta}) = -J \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j) - h \sum_{i=1}^{N} \cos(\theta_i) \ , \qquad m(T, L, h) = \frac{1}{N} \sum_{i=1}^{N} \langle \cos\theta_i \rangle \ .$$

1. We shall denote $\langle \bullet \rangle_0$ the average over the spin configurations at $\beta = 0$, i.e. for an arbitrary function $f(\theta_1, \dots, \theta_N)$ which is 2π periodic in each of its arguments,

$$\langle f \rangle_0 = \int_0^{2\pi} \prod_{i=1}^{N} \frac{{\rm d}\theta_i}{2\pi} f(\theta_1, \dots, \theta_N) \ . \qquad (1)$$

What is the consequence of the rotational invariance of this measure for $\left\langle \frac{\partial}{\partial \theta_i} f \right\rangle_0$? Conclude that

$$\left\langle \frac{\partial}{\partial \theta_i} f \right\rangle = \left\langle f \frac{\partial}{\partial \theta_i} (\beta H) \right\rangle \ . \qquad (2)$$

2. Consider the functions

$$X = \sum_{i=1}^{N} e^{i\vec{k}\cdot\vec{r}_i} \sin\theta_i \ , \qquad Y = \sum_{i=1}^{N} e^{i\vec{k}\cdot\vec{r}_i} \frac{\partial}{\partial\theta_i}(\beta H) \ . \tag{3}$$

Give an expression of $\langle fY \rangle$, for an arbitrary function f, using your answer to the previous question. Simplify then the quantities $\langle X^* X\rangle$, $\langle X^* Y\rangle$ and $\langle Y^* Y\rangle$, where * denotes the complex conjugation.

3. The Cauchy-Schwarz inequality implies that $|\langle X^* Y\rangle|^2 \leq \langle X^* X\rangle\langle Y^* Y\rangle$. Deduce from it that

$$m(T,L,h)^2 \leq \beta \left(\frac{1}{N} \sum_{i,j=1}^{N} e^{i\vec{k}\cdot(\vec{r}_i - \vec{r}_j)} \langle \sin\theta_i \sin\theta_j \rangle \right) \left(h + 2J \sum_{\mu=1}^{d} (1 - \cos(ak_\mu)) \right) \ , \tag{4}$$

for $h \geq 0$.

4. We define B as the set of N vectors $\vec{k} = \frac{2\pi}{aL}(n_1, \dots, n_d)$ with each n_μ taking L integer values between $-\frac{L}{2}$ and $\frac{L}{2}$. Show that $\frac{1}{N} \sum\limits_{\vec{k}\in B} e^{i\vec{k}\cdot\vec{r}} = \delta_{\vec{r},\vec{0}}$ if $\vec{r}$ is a vector of the lattice.

5. Dividing the left hand side of (4) by the second term of its right hand side and summing over the N values of $\vec{k}$ in B, show that

$$m(T,L,h)^2 \leq \frac{\beta}{\frac{1}{N} \sum\limits_{\vec{k}\in B} \frac{1}{h + 2J \sum\limits_{\mu=1}^{d} (1 - \cos(ak_\mu))}} \ . \tag{5}$$

6. Conclude by taking the limit $L \to \infty$, and then $h \to 0^+$.

2 Vortices

We study now the effect of vortices on the energy of configurations of the bidimensional XY model. Neglecting the effect of the lattice we approximate the energy of a configuration for a domain Ω of the plane as

$$H = \frac{J}{2} \int_{\Omega} d\vec{r}\ (\vec{\nabla}\theta)^2 \ ,$$

where $\theta(\vec{r})$ is defined modulo 2π and is assumed to be smooth except at some isolated singularities, which will be regularized by excluding from Ω a small disk of radius a around them. The singularities correspond to the center of the vortex spin configurations considered in the following.

The motivation for this exercise is to understand what are the valid spin configurations in the low temperature phase. In this phase single vortices cannot survive since their energy diverges with the system size (as will be seen in question 1) and the entropy contribution cannot counterbalance this divergence at low enough temperatures. Valid spin configurations therefore must have a bounded energy and its explicit form will be investigated in questions 2 to 4, in a special case.

We recall some formulas of vectorial analysis in the plane. In polar coordinates (r, φ) the gradient of a scalar function $f(r,\varphi)$ is $\vec{\nabla} f = \frac{\partial f}{\partial r}\vec{e}_r + \frac{1}{r}\frac{\partial f}{\partial \varphi}\vec{e}_\varphi$, and the Laplacian of a radial function $f(r)$ is $\Delta f(r) = \frac{1}{r}\frac{d}{dr}\left(r\frac{df}{dr}\right)$. Moreover for two functions $f(\vec{r})$ and $g(\vec{r})$ one has

$$\int_{\Omega} d\vec{r}\ (\vec{\nabla} f)\cdot(\vec{\nabla} g) = \int_{\partial\Omega} d\vec{r}\ f\ \vec{n}\cdot(\vec{\nabla} g) - \int_{\Omega} d\vec{r}\ f\Delta g \ ,$$

with $\partial\Omega$ the boundary of Ω and $\vec{n}$ the normal unit vector oriented towards the exterior of Ω.

1. Consider a configuration containing a single vortex of charge $q \in \mathbb{Z}$ at the origin, i.e. such that $\theta(\vec{r}) = \theta_0 + q\,\varphi(\vec{r})$. Give an order of magnitude of the energy of such a configuration in a domain that can be approximated as a disk with radius L around the vortex.

2. In all the following we consider a configuration containing two vortices of charges q_1 and q_2 at two positions $\vec{r}_1$ and $\vec{r}_2$, the field $\theta(\vec{r})$ is thus the sum of the fields of the two individual vortices. We require that the energy of this configuration does not diverge when the size of the domain Ω becomes very large. Give a condition on q_1 and q_2 that ensures this requirement, that will be understood in the following questions.

3. Give a function $\Phi(\vec{r}) = \Phi_1(\vec{r})+\Phi_2(\vec{r})$ such that $\vec{\nabla}\theta = \vec{e}_z \wedge \vec{\nabla}\Phi$, with $\vec{e}_z$ the unit vector completing the direct orthonormal basis $(\vec{e}_r, \vec{e}_\varphi, \vec{e}_z)$. Check that $\Delta\Phi = 0$ outside the singularities of Φ, and conclude that

$$H = \frac{J}{2} \int_{\partial\Omega} \mathrm{d}\vec{r}\ \Phi\ \vec{n} \cdot \vec{\nabla}\Phi\ .$$

4. Assuming that the distance $|\vec{r}_1 - \vec{r}_2|$ between the centers of the vortices is much larger than the cutoff a, evaluate the contributions of the different pieces of $\partial\Omega$ to this integral, and show that for this configuration

$$H = -\pi J(q_1^2 + q_2^2) \ln a - 2\pi J q_1 q_2 \ln(|\vec{r}_1 - \vec{r}_2|)\ .$$