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

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1 Mermin-Wagner theorem

1. The integral of a derivative being the function evaluated at the boundaries,

$$\left\langle \frac{\partial}{\partial \theta_i} f \right\rangle_0 = \int_0^{2\pi} \prod_{j=1}^N \frac{\mathrm{d}\theta_j}{2\pi} \frac{\partial}{\partial \theta_i} f(\theta_1, \dots, \theta_N) = \int_0^{2\pi} \prod_{j\neq i} \frac{\mathrm{d}\theta_j}{2\pi} \frac{1}{2\pi} \left[f(\theta_1, \dots, \theta_N) \right]_{\theta_i=0}^{\theta_i=2\pi} = 0 \ ,$$

the last step following from the 2π-periodicity of f seen as a function of θ_i. Applying this identity to $fe^{-\beta H}$ we obtain

$$0 = \left\langle \frac{\partial}{\partial \theta_i} \left(f e^{-\beta H} \right) \right\rangle_0 = \left\langle e^{-\beta H} \frac{\partial}{\partial \theta_i} f \right\rangle_0 - \left\langle e^{-\beta H} f \frac{\partial}{\partial \theta_i} (\beta H) \right\rangle_0 \ .$$

Since $\langle \bullet \rangle = \frac{1}{Z} \langle e^{-\beta H} \bullet \rangle_0$, the last equation implies

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

2. By linearity of the average we can apply the previous identity to each term in fY :

$$\langle fY \rangle = \left\langle \sum_{i=1}^N e^{i\vec{k}\cdot\vec{r}_i} f \frac{\partial}{\partial \theta_i} (\beta H) \right\rangle = \sum_{i=1}^N e^{i\vec{k}\cdot\vec{r}_i} \left\langle f \frac{\partial}{\partial \theta_i} (\beta H) \right\rangle = \sum_{i=1}^N e^{i\vec{k}\cdot\vec{r}_i} \left\langle \frac{\partial}{\partial \theta_i} f \right\rangle \ . \tag{1}$$

From the definition of X we obtain immediately

$$\langle X^* X \rangle = \sum_{i,j=1}^N e^{i\vec{k}\cdot(\vec{r}_i - \vec{r}_j)} \langle \sin\theta_i \sin\theta_j \rangle \ .$$

To compute $\langle X^* Y \rangle$ we shall use the identity (1) with $f = X^*$. We first compute its derivative with respect to θ_i,

$$\frac{\partial}{\partial \theta_i} X^* = \frac{\partial}{\partial \theta_i} \sum_{j=1}^N e^{-i\vec{k}\cdot\vec{r}_j} \sin\theta_j = e^{-i\vec{k}\cdot\vec{r}_i} \cos\theta_i \ ,$$

and then conclude with (1) :

$$\langle X^* Y \rangle = \sum_{i=1}^N \langle \cos\theta_i \rangle = N m(T, L, h) \ .$$

Applying the identity (1) with $f = Y^*$ yields

$$\langle Y^* Y \rangle = \sum_{i=1}^N e^{i\vec{k}\cdot\vec{r}_i} \left\langle \frac{\partial}{\partial \theta_i} Y^* \right\rangle = \sum_{i,j=1}^N e^{i\vec{k}\cdot(\vec{r}_i - \vec{r}_j)} \left\langle \frac{\partial^2}{\partial \theta_i \partial \theta_j} (\beta H) \right\rangle \ . \tag{2}$$

Let us compute the derivatives of the Hamiltonian, introducing the notation ∂i for the set of the $2d$ nearest neighbors of the site i :

$$\frac{\partial}{\partial\theta_i} H = J \sum_{k\in\partial i} \sin(\theta_i - \theta_k) + h \sin\theta_i$$

$$\frac{\partial^2}{\partial\theta_i \partial\theta_j} H = \delta_{i,j} \left(J \sum_{k\in\partial i} \cos(\theta_i - \theta_k) + h \cos\theta_i \right) - \mathbb{I}(i,j \text{ n.n.}) J \cos(\theta_i - \theta_j) \ ,$$

where $\mathbb{I}(i,j \text{ n.n.})$ is the indicator function of the event "i and j are nearest negihbors", which is equivalent to $i \in \partial j$ and to $j \in \partial i$. Plugging this formula in (2) leads to

$$\begin{aligned}
\langle Y^* Y \rangle &= \beta \sum_{i,j=1}^N e^{i\vec{k}\cdot(\vec{r_i}-\vec{r_j})} \left\langle \delta_{i,j} \left(J \sum_{k\in\partial i} \cos(\theta_i - \theta_k) + h\cos\theta_i \right) - \mathbb{I}(i,j \text{ n.n.}) J \cos(\theta_i - \theta_j) \right\rangle \\
&= \beta h \sum_{i=1}^N \langle \cos\theta_i \rangle + \beta J \sum_{i=1}^N \sum_{k\in\partial i} \langle \cos(\theta_i - \theta_k) \rangle - \beta J \sum_{\langle i,j \rangle} \left(e^{i\vec{k}\cdot(\vec{r_i}-\vec{r_j})} + e^{-i\vec{k}\cdot(\vec{r_i}-\vec{r_j})} \right) \langle \cos(\theta_i - \theta_j) \rangle \\
&= \beta h \sum_{i=1}^N \langle \cos\theta_i \rangle + 2\beta J \sum_{\langle i,j \rangle} \left(1 - \cos(\vec{k}\cdot(\vec{r_i}-\vec{r_j})) \right) \langle \cos(\theta_i - \theta_j) \rangle \ . \qquad (3)
\end{aligned}$$

In the last step we used the fact that the sum over i, then over $k \in \partial i$, counts each edge twice, hence the factor 2.

3. We first derive an upperbound on $\langle Y^* Y \rangle$ from (3). As $\langle \cos\theta_i \rangle$ and $\langle \cos(\theta_i - \theta_j) \rangle$ are ≤ 1, and as these quantities are multiplied by positive terms in (3), we can write

$$\langle Y^* Y \rangle \leq N\beta h + 2\beta J \sum_{\langle i,j \rangle} \left(1 - \cos(\vec{k}\cdot(\vec{r_i}-\vec{r_j})) \right) \ .$$

Moreover,

$$\begin{aligned}
2 \sum_{\langle i,j \rangle} \left(1 - \cos(\vec{k}\cdot(\vec{r_i}-\vec{r_j})) \right) &= \sum_{i=1}^N \sum_{j\in\partial i} \left(1 - \cos(\vec{k}\cdot(\vec{r_i}-\vec{r_j})) \right) \\
&= N \left(2d - 2\sum_{\mu=1}^d \cos(ak_\mu) \right) = 2N \sum_{\mu=1}^d (1 - \cos(ak_\mu)) \ ,
\end{aligned}$$

as for every site i its $2d$ neighbors $j \in \partial i$ are at distance a in all directions. We thus have

$$\langle Y^* Y \rangle \leq N\beta \left(h + 2J \sum_{\mu=1}^d (1 - \cos(ak_\mu)) \right) \ .$$

Using the Cauchy-Schwartz inequality and the expressions of $\langle X^* X \rangle$ and $\langle X^* Y \rangle$ previously obtained we finally get

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

4. As a vector of the lattice $\vec{r}$ can be written $\vec{r} = a(m_1, \dots, m_d)$ with integer coefficients m_μ. Hence

$$\frac{1}{N} \sum_{\vec{k}\in B} e^{i\vec{k}\cdot\vec{r}} = \prod_{\mu=1}^d \left(\frac{1}{L} \sum_{n_\mu} (e^{i\frac{2\pi}{L} m_\mu})^{n_\mu} \right) = \prod_{\mu=1}^d \delta_{m_\mu,0} = \delta_{\vec{r},\vec{0}} \ ,$$

as the sum over n_μ runs over L successive integer values. Note that the the condition $m_\mu = 0$ has to be understood modulo L, hence $\vec{r} = \vec{0}$ modulo the translations of La in each direction, in agreement with the periodic boundary conditions.

5. Following the indication of the text, which is legitimate as we divide by a positive constant,

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

Dividing again by a positive quantity yields

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

6. In the $L\to\infty$ limit the sum over $\vec{k}$ becomes an integral, more precisely $\frac{1}{N}\sum\limits_{\vec{k}\in B} f(\vec{k}) \to \int\limits_{[-\pi/a,\pi/a]^d} \mathrm{d}\vec{k}\, f(\vec{k})$.

We obtain in this way

$$\lim_{L\to\infty} m(T,L,h)^2 \leq \frac{\beta}{\int\limits_{[-\pi/a,\pi/a]^d} \frac{d\vec{k}}{(2\pi)^d} \frac{1}{h+2J\sum_{\mu=1}^d (1-\cos(k_\mu))}} \ ; \qquad (4)$$

to be completely precise we have not proven that the limit in the left hand side exists, we could nevertheless write the previous inequality with a lim sup and finish the argument in the same way.

It remains to understand the behavior of the right hand side of this inequality in the limit $h\to 0^+$. One observes that for $h=0$ the integrand diverges at the origin, as $2J\sum_{\mu=1}^d (1-\cos(k_\mu)) \sim Jk^2$. Depending on the dimension this singularity can be integrable or not. In polar coordinates the integral around the origin becomes, up to some irrelevant constants, $\int \mathrm{d}k \frac{k^{d-1}}{k^2}$ which converges if and only if $d>2$. On the contrary for $d\in\{1,2\}$ the integral diverges to $+\infty$ when $h\to 0^+$, hence the right hand side of (4) goes to zero in this limit. As the left hand side is positive we can conclude that

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

we have thus proven the absence of spontaneous magnetization in dimensions 1 and 2 for continuous (XY) spins.

2 Vortices

1. Using the formulas recalled in the text one has for this function $\vec{\nabla}\theta = q\frac{1}{r}\vec{e}_\varphi$, hence $(\vec{\nabla}\theta)^2 = q^2\frac{1}{r^2}$. Taking for simplicity the domain Ω as a disk of radius L centered at the origin, deprived of the small disk of radius a around the singularity at the origin, and integrating in polar coordinates yields $H = \frac{J}{2}2\pi\int_a^L \mathrm{d}r\, r\, q^2\frac{1}{r^2} = \pi J q^2 \ln(L/a)$.
2. Far from the positions $\vec{r}_1$ and $\vec{r}_2$ the field $\theta(\vec{r})$ is equivalent to the one of a single vortex of charge $q=q_1+q_2$. As seen in the previous question the corresponding energy diverges with L, unless $q_1=-q_2$, which will be assumed in the next questions.

   More precisely, we start from $\theta(\vec{r}) = \theta_0^{(1)} + q_1\varphi(\vec{r}) + \theta_0^{(2)} + q_2\varphi(\vec{r}+\vec{r}_1-\vec{r}_2)$, where we took one of the vertices to be the origin. Then

$$\vec{\nabla}\theta = q_1\frac{1}{|\vec{r}|}\vec{e}_\varphi(\vec{r}) + q_2\frac{1}{|\vec{r}+\vec{r}_1-\vec{r}_2|}\vec{e}_\varphi(\vec{r}+\vec{r}_1-\vec{r}_2), \qquad (5)$$

   which for $|\vec{r}_1-\vec{r}_2| \ll \vec{r}$ can be Taylor expanded. In this case the vectors $\vec{e}_\varphi(\vec{r})$ and $\vec{e}_\varphi(\vec{r}+\vec{r}_1-\vec{r}_1)$ will almost point in the same direction. Setting $q_1=-q_2$ we find

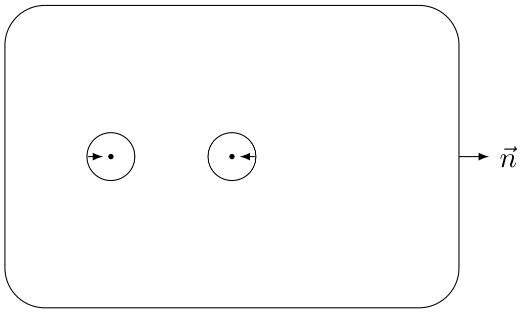
$$\frac{1}{|\vec{r}|} - \frac{1}{|\vec{r}+\vec{r}_1-\vec{r}_2|} \approx \frac{(\vec{r}_1-\vec{r}_2)\cdot\vec{r}}{|\vec{r}|^3}$$

   so $|\vec{\nabla}\theta| \propto \frac{1}{r^2}$ at large distance from the center of the vortices, hence $(\vec{\nabla}\theta)^2 \propto \frac{1}{r^4}$ is integrable when $r\to\infty$.

3. For a single vertex of unit charge at the origin one has $\vec{\nabla}\theta = \frac{1}{r}\vec{e}_\varphi = \vec{e}_z \wedge \left(\frac{1}{r}\vec{e}_r\right) = \vec{e}_z \wedge \vec{\nabla} \ln r$, and one checks with the formula recalled in the text that $\Delta \ln r = 0$ for $r \neq 0$. For the configuration with two vortices one can thus take $\Phi(\vec{r}) = \Phi_1(\vec{r}) + \Phi_2(\vec{r}) = q_1 \ln(|\vec{r} - \vec{r}_1|) + q_2 \ln(|\vec{r} - \vec{r}_2|)$ to have $\vec{\nabla}\theta = \vec{e}_z \wedge \vec{\nabla}\Phi$. This function satisfies $\Delta\Phi = 0$ when $\vec{r} \notin \{\vec{r}_1, \vec{r}_2\}$. Noting that if $\vec{a}, \vec{b}$ are two vectors of the plane then $(\vec{e}_z \wedge \vec{a}) \cdot (\vec{e}_z \wedge \vec{b}) = \vec{a} \cdot \vec{b}$, we have

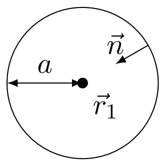
$$H = \frac{J}{2} \int_\Omega \mathrm{d}\vec{r}\, (\vec{\nabla}\theta)^2 = \frac{J}{2} \int_\Omega \mathrm{d}\vec{r}\, (\vec{e}_z \wedge \vec{\nabla}\Phi) \cdot (\vec{e}_z \wedge \vec{\nabla}\Phi) = \frac{J}{2} \int_\Omega \mathrm{d}\vec{r}\, (\vec{\nabla}\Phi) \cdot (\vec{\nabla}\Phi)$$
$$= \frac{J}{2} \int_{\partial\Omega} \mathrm{d}\vec{r}\; \Phi\; \vec{n} \cdot \vec{\nabla}\Phi \;,$$

where in the last step we used the integral formula recalled in the text with $f = g = \Phi$ whose Laplacian vanishes in the domain Ω that excludes the disks of radius a around $\vec{r}_1$ and $\vec{r}_2$:



Ω

4. The boundary $\partial\Omega$ is made of three parts, the external boundary $\partial\Omega_{\text{ext}}$ and the two circles of radius a around $\vec{r}_1$ and $\vec{r}_2$, denoted $\partial\Omega_1$ and $\partial\Omega_2$ respectively. Thanks to the condition $q_1 = -q_2$ the contribution of $\partial\Omega_{\text{ext}}$ vanishes when the boundary is far away from the vortices, as discussed previously. Consider now the contribution of $\partial\Omega_1$, on which the following figure zooms in :



As $|\vec{r}_1 - \vec{r}_2| \gg a$ one can take $(\vec{\nabla}\Phi_2)(\vec{r}) \approx$ constant when $\vec{r}$ travels along $\partial\Omega_1$. Moreover $\Phi(\vec{r}) = q_1 \ln(a) + q_2 \ln(|\vec{r} - \vec{r}_2|) \approx q_1 \ln(a) + q_2 \ln(|\vec{r}_1 - \vec{r}_2|)$ is approximately constant for $\vec{r} \in \partial\Omega_1$. As $\int_{\partial\Omega} \mathrm{d}\vec{r}\; \vec{n} \cdot \vec{C} = 0$ by symmetry when $\vec{C}$ is a constant vector, we can simplify the contribution of the integral on $\partial\Omega_1$ as

$$\int_{\partial\Omega_1} \mathrm{d}\vec{r}\; \Phi\; \vec{n} \cdot \vec{\nabla}\Phi = \int_{\partial\Omega_1} \mathrm{d}\vec{r}\; \Phi\; \vec{n} \cdot \vec{\nabla}\Phi_1 \;.$$

Noting that $(\vec{\nabla}\Phi_1)(\vec{r}) = -q_1 \frac{1}{a}\vec{n}$ when $\vec{r} \in \partial\Omega_1$ this last integral is seen to be $(q_1 \ln(a) + q_2 \ln(|\vec{r}_1 - \vec{r}_2|)) \times (-2\pi\, q_1)$. Adding the contribution of $\partial\Omega_2$, multiplying by $J/2$ and using the relationship $q_1 = -q_2$ yields

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