Kosterlitz-Thouless Phase Transition in 2d-xy Heisenberg Ferromagnet

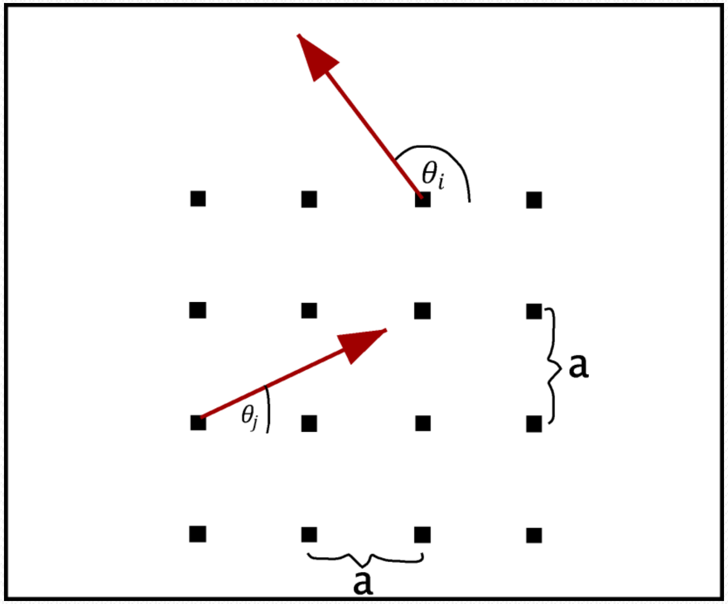
Martin Schäffer
06/09/2009

Structure

- **2d-xy Heisenberg ferromagnet**
- **Spin wave approximation**
- **Correlation functions**
- **Discussion on the result**
- **Vortex postulation**
- **Interesting analogue**

2d-xy Heisenberg ferromagnet

Consider a 2d-xy ferromagnet. It may consist of a number n of spins residing on a square lattice with lattice constant a.



$$\vec{S}_i = (S_i^x, S_i^y)$$

$$\vec{S}_i^{\,2} = 1$$

$$S_i^x = \cos\theta_i\,,\quad S_i^y = \sin\theta_i$$

2d-xy Heisenberg ferromagnet

Neglect all spin interactions but ones between nearest neighbours. The Hamiltonian of the ferromagnet can be written (J>0)

$$H = -J \cdot \sum_{<i,j>} \left(\vec{S}_i \cdot \vec{S}_j - 1\right) = J \cdot \sum_{<i,j>} [1 - \cos(\theta_i - \theta_j)]$$

It is natural to define the generating functional for correlation functions, W[h]

$$W[h] = \frac{1}{Z} \cdot \prod_i \int_{-\pi}^{+\pi} d\theta_i e^{-\beta H + \theta_i h_i} \; ; \quad h = (h_1, h_3, h_2 \ldots h_n)$$

$$W[h = 0] = 1,\; Z = Z(\beta) \; ; \; \left(\frac{\partial^n W}{\partial h_k \partial h_l \partial h_m \ldots \partial h_u}\right)_{h=0} = \langle \theta_k \theta_l \theta_m \ldots \theta_u \rangle$$

Spin wave approximation

At low temperature, it is reasonable to assume short-range order of the spins.
More precisely, the orientation angles of nearest neighbours are supposed to differ only very little, so that in good approximation

$$\cos(\theta_i - \theta_j) \cong 1 - \frac{1}{2}(\theta_i - \theta_j)^2$$

Furthermore, it appears natural to extend the range of the value of the orientation angle.

$$-\pi < \theta_i < +\pi \;\; \rightarrow \;\; -\infty < \theta_i < \infty$$

This leads to the further replacement,

$$\frac{1}{Z}\prod_i d\theta_i \;\; \rightarrow \;\; d\mu[\theta]$$

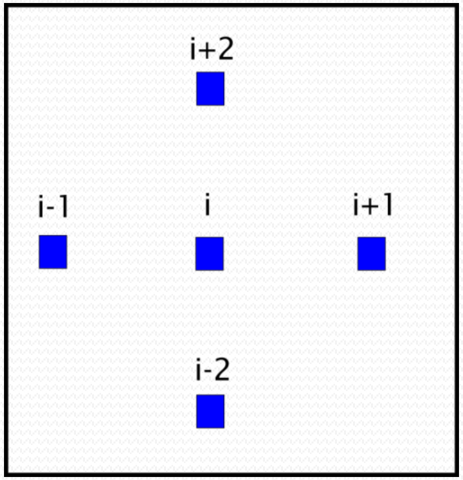
with $d\mu[\theta + \bar{\theta}] = d\mu[\theta]$, due to continuous symmetry of the system.

Spin wave approximation

Upon defining $K \coloneqq \beta J$, the Hamiltonian can now be written in the employed spin wave approximation as follows

$$\beta H_S := K \sum_{<i,j>} (\theta_i - \theta_j)^2 =: \frac{K}{2} \sum_{i,j} \theta_i \Delta_{ij} \theta_j =: \frac{K}{2} (\theta, \Delta\theta)$$

The definition of Δ_{ij} is illustrated below.



$$\Delta_{ij} \coloneqq 4\delta_{i,j} - \sum_{\alpha=1,2} \left(\delta_{i+\alpha,j} + \delta_{i-\alpha,j}\right) = \Delta_{ji}$$

$$\sum_j \Delta_{ji} = 0$$

Spin wave approximation

In the approximation of small lattice constant a, one may introduce a continuous description, namely

$$\Delta_{ij} \;\to\; -a^2\nabla^2; \qquad (\theta, \Delta\theta) \;\to\; -\int d^3r\, \theta\nabla^2\theta$$

Note that the symmetry property, $d\mu[\theta + \bar{\theta}] = d\mu[\theta]$, is still valid.

Now that the specification of the employed idealizations is complete, the explicit evaluation of the correlation functions shall be tackled.

Correlation functions

In the new notation, the correlations generating functional reads

$$W_S[h] = \int d\mu[\theta] e^{-\frac{K}{2}(\theta,\Delta\theta)+(\theta,h)}$$

Performing the transformation,

$$\theta_i = \bar{\theta}_i + \varphi_i \, ; \qquad \sum_i \bar{\theta}_i = 0$$

the argument of the above exponential is given

$$-\frac{K}{2}(\theta,\Delta\theta) + (\theta,h) = -\frac{K}{2}(\varphi,\Delta\varphi) - \frac{K}{2}(\bar{\theta},\Delta\bar{\theta}) - \frac{K}{2}(\varphi,\Delta\theta) + (\bar{\theta},h) + (\varphi,h)$$

Introduce new variables,

$$h_i \coloneqq K \textstyle\sum_j \Delta_{ij} \bar{\theta}_j + \frac{1}{N} \sum_j h_j \qquad\qquad G_{ij} : \; \sum_l \Delta_{il} G_{lj} = \delta_{ij} - \frac{1}{N}; \;\; \sum_j G_{lj} = 0$$

Correlation functions

Substituting these variables, the generating functional factorizes beautifully to give

$$W_S[h] = e^{\frac{1}{2K}(h,Gh)} \underbrace{\int d\mu[\bar{\theta} + \varphi] e^{-\frac{K}{2}(\varphi,\Delta\varphi)}}_{=1}$$

Now one evaluates

$$\langle \sum_i \theta_i \rangle_{H_S} = 0; \quad h_j = h \neq 0 \qquad\qquad \langle \theta_i \theta_j \rangle_{H_S} = \frac{k_B T}{J} G_{ij}$$

It is left to calculate explicitly the numbers G_{ij}
This is done most efficiently in Fourier space.

$$G_{lj} = \frac{1}{V} \sum_{\vec{k}} \tilde{G}(\vec{k})\, e^{i\vec{k}(\vec{r}_l - \vec{r}_j)}; \qquad V = na^2$$

Correlation functions

As well-known from solid state physics, the range of the wave vector can be confined to the first Brillouin zone.

$$-\frac{\pi}{a} \leq k_{x,j}, k_{y,j} < \frac{\pi}{a}$$

Consider the sum

$$\sum_l \Delta_{il} G_{lj} = \frac{1}{V} \sum_{\vec{k}} \tilde{G}(\vec{k})\, e^{i\vec{k}(\vec{r}_i - \vec{r}_j)} (4 - 2e^{ik_x a} - 2e^{ik_y a})$$

Using previous definitions,

$$\sum_l \Delta_{il} G_{lj} \equiv \delta_{ij} - \frac{1}{N} = \frac{1}{N} \sum_{\vec{k}} e^{i\vec{k}(\vec{r}_i - \vec{r}_j)} (1 - \delta_{k,0})$$

one can identify $\tilde{G}(\vec{k})$.

Correlation functions

$$\ldots\ \tilde{G}(\vec{k}) = \frac{a^2}{4 - 2\cos k_x a - 2\cos k_y a} \quad ; \qquad \vec{k} \neq 0$$

Inserting this result in the previous expression, one can define

$$G_{m0} = \sum_{\vec{k}\neq 0}^{1.BZ} \frac{a^2 e^{i\vec{k}\cdot\vec{r}_m}}{4 - 2\cos k_x a - 2\cos k_y a} =: G(\vec{r}_m)$$

Now the work is almost done. Specifying

$$C(\vec{r}_m) \coloneqq \langle \vec{S}(\vec{r}_m)\vec{S}(0)\rangle = \langle e^{i(\theta_m - \theta_0)}\rangle = \langle e^{i(h,\theta)}\rangle \, ; \qquad h_j \coloneqq i\left(\delta_{jm} - \delta_{j0}\right)$$

one finds in the continuous approximation

$$C(\vec{r}) = e^{-\frac{1}{K}[G(0)-G(\vec{r})]} = e^{-\frac{1}{2}\langle(\theta(\vec{r})-\theta(0))^2\rangle_{H_S}}$$

Correlation functions

It is of interest to check for long-range order (LRO). Thus, assume $r \gg \bar{a}$ for some cut-off distance $\bar{a}$ .Thus,

$$G(0) - G(r) \sim \frac{1}{2\pi} \int_0^{1/\bar{a}} kdk \int_0^{2\pi} d\vartheta \, \frac{1 - e^{ikr\cos\vartheta}}{k^2} = \frac{1}{2\pi} \int_0^{1/\bar{a}} dk \, \frac{1 - J_0(kr)}{k}$$

In the considered region $r >> \bar{a}$, the Bessel function is negligible, therefore

$$\boldsymbol{G(0) - G(r) \approx \frac{1}{2\pi} ln\left(\frac{r}{\bar{a}}\right) + const}$$

Note that the deviation of the orientation of the spins increase without limit with increasing distance!

Correlation functions

It follows that the correlation function is of the form

$$\boldsymbol{C_S(r) \sim \left(\frac{r}{\bar{a}}\right)^{-\eta(T)}} \quad ; \quad \boldsymbol{r \gg \bar{a}}$$

with the exponent

$$\boldsymbol{\eta(T) = \frac{k_B T}{2\pi J} > 0}$$

The exponent is not universal in this case!

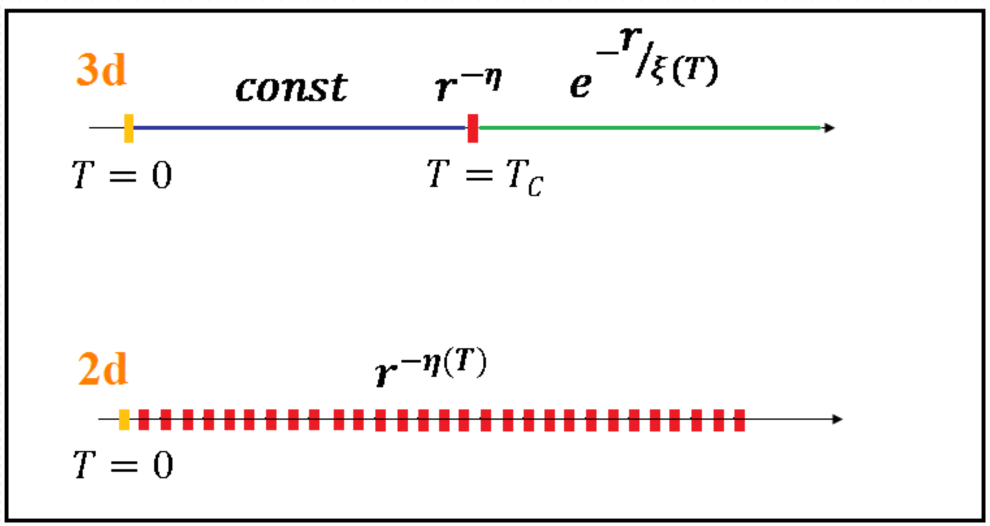
Discussion on the result

There exists no LRO in the system (no broken symmetry).

Instead, the angular deviations increase unlimited with distance .

The correlation function decays algebraically with a non-universal exponent.

Compare the 3d case.



LRO below some critical temperature.

universal exponent .

exponential decay of correlations above the critical temperature.

like lines of critical points.

Discussion on the result

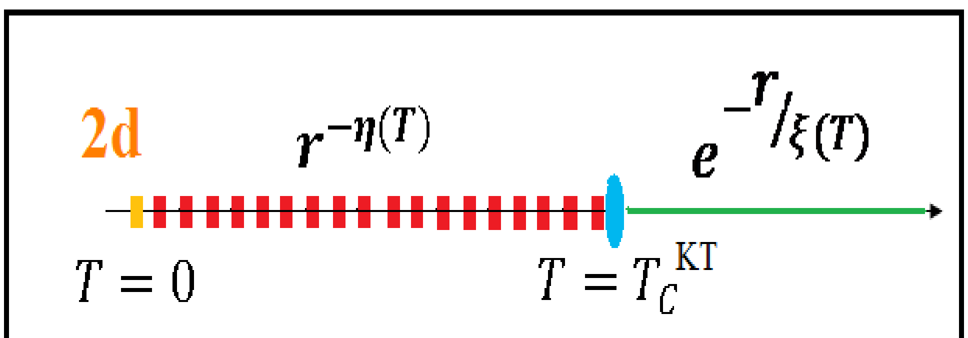
Note that the 2d discussion was carried out in spin wave approximation.

This approximation is valid only in the regime of low temperatures.

The correlations must decrease exponentially for high temperatures (paramagnetic phase).

There apparently exist excitations of the system besides spin waves, which must be taken into account to describe correctly the physical properties of this system.

Educated guess of the true correlations behaviour.



quasi-LRO below some critical temperature .

phase transition
without broken symmetry.

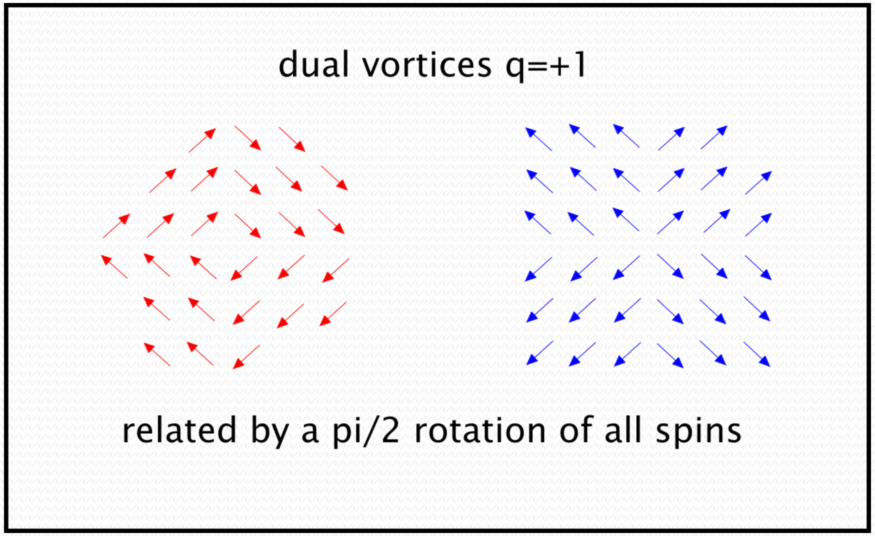
exponential decay of correlations
above the critical temperature.

Vortex postulation

Berezinskii, Kosterlitz and Thouless proposed, that this phase transition occurs due to the unbinding of vortex states at some critical temperature T_C^{KT} .

Vortices are configurations with the property that along any path enclosing the so called vortex core,

$$\oint \nabla\theta(r) \cdot d\vec{r} = 2\pi q, \quad q = \pm 1, \pm 2, \pm 3 \ldots \text{(winding number)}$$



Vortex postulation

For vortex configurations, it follows for the gradient of the orientation angle, $\nabla\theta_v(r)$,

$$|\nabla\theta_v(r)| = |q| \cdot \frac{1}{r}$$

The energy of a vortex can be calculated to be

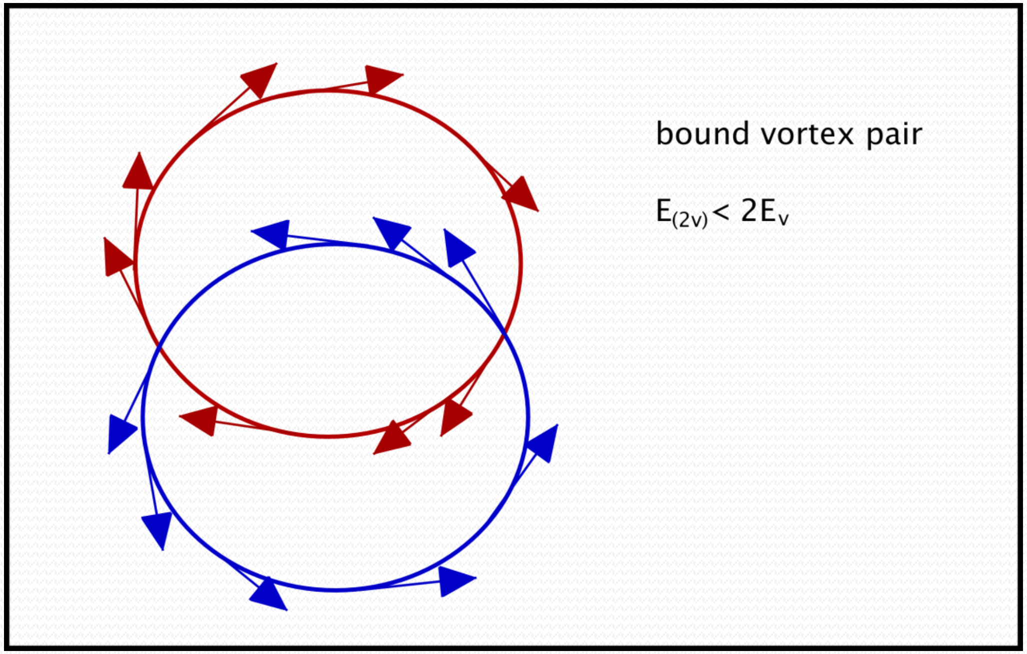
$$E_v = \frac{J}{2}\int d^2r(\nabla\theta_v)^2 \approx \frac{2\pi J}{2}\int_{\bar{a}}^{L=V^{1/2}} \frac{q^2}{r^2} rdr + E_{core} = E_{core} + \pi q^2 J \cdot \ln(\frac{L}{\bar{a}})$$

Having calculated the energy cost of a vortex, the reasoning of Kosterlitz and Thouless can be duplicated naturally.

At low temperature, the creation of a single vortex is too costly.
However, bound pairs of vortices (q,-q) will appear and lead to quasi-LRO.
At T_C^{KT} , these pairs break up and quasi-LRO is destroyed.

Vortex postulation

A bound pair of the class (1,-1) is illustrated below.



The critical temperature

The critical temperature T_C^{KT} is calculated from a consideration on the free energy of a vortex. The core of the vortex can equally likely reside on any of $(L/\bar{a})^2$ positions.

Therefore the entropy is given

$$S_v = k_B \ln(L/\bar{a})^2$$

The free energy reads

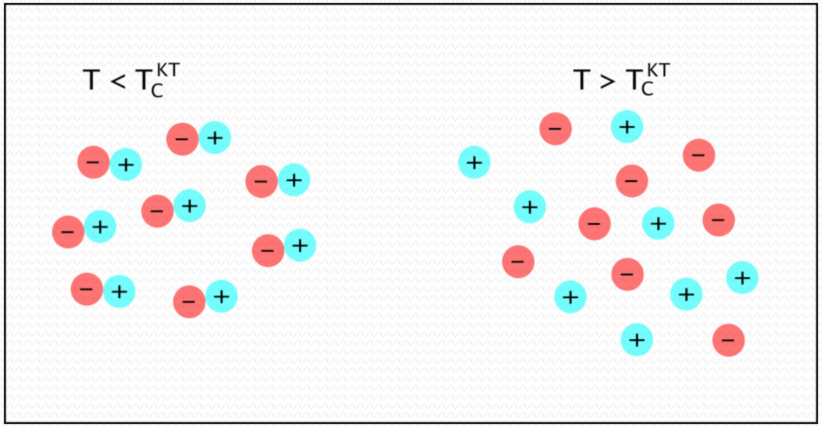
$$F_v = E_v - TS_v = (\pi J - 2k_B T)\ln\left(\frac{L}{\bar{a}}\right)$$

The free energy turns positive at the temperature

$$\mathbf{k_B T_C^{KT} = \frac{\pi J}{2}}$$

Interesting analogue

The previous discussion is comparable to the treatment of a 2d Coulomb gas. The Kosterlitz-Thouless phase transition can be naturally interpreted in this case. Consider vortices with positive (negative) winding number as positive (negative) charges.



Below the critical temperature, condensation occurs. Single charges tend to form bound states (microscopic dipoles).