The Kosterlitz-Thouless transition in the XY Kagomé antiferromagnet

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Abstract

The problem of the Kosterlitz-Thouless (KT) transition in the highly frustrated XY Kagomé antiferromagnet is solved. The problem is mapped onto that of the KT transition in the XY ferromagnet on the hexagonal lattice. The transition temperature is found. It is shown that the spin correlation function exponentially decays with distance even in the low-temperature phase, in contrast to the order parameter correlation function, which decays algebraically with distance.

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Generally, XY spins on two-dimensional lattices undergo a Kosterlitz-Thouless (KT) transition \[1,2\]. As a rule, physics of this transition does not depend on details of lattice structure. In the low temperature phase, pairs of spin direction singularities, vortices, with opposite topological charges form quasi-molecules. Above the transition temperature, the quasi-molecules decay into a vortex gas. In the low-temperature phase, the spin correlations decay algebraically with distance, above the transition temperature, they decay exponentially. Formally, the universality of the KT transition follows from the possibility to describe low-energy states of two-dimensional XY spin systems in terms of the nonlinear \(\sigma\)-model.

The XY antiferromagnet on the two-dimensional Kagomé lattice is an exception from this class. It has infinitely many ground states, therefore its low-temperature properties cannot be described by the nonlinear \(\sigma\)-model. This makes the problem of a KT-like transition in the XY Kagomé antiferromagnet a special one, which is substantially more complicated than the standard theory of the KT transition. The very possibility of a KT transition in such an unusual system is under question.

The problem of the KT transition in the Kagomé antiferromagnet was first addressed by Huse and Rutenberg \[3\]. They suggested that the order parameter for the KT transition is \(e^{3i\theta}\) where \(\theta\) is the angle of a spin. This order parameter is invariant with respect to any arbitrary choice of ground states, which are a subset of local \(2\pi/3\) spin rotations. Therefore this order parameter can change smoothly in the plane even though spins rotate locally at multiple \(2\pi/3\) angles. An indirect evidence of the KT transition in the Kagomé antiferromagnet was obtained from MC simulation \[4\].

A network of Josephson junctions with the \(\pi\)-phase shift can be mapped onto the antiferromagnetic XY model as well. Experimental studies of artificial networks of Josephson junctions on the Kagomé lattice make this problem especially appealing \[5\].

In this paper, we examine the KT-like transition in the XY Kagomé antiferromagnet. We find that the KT transition in the Kagomé antiferromagnet does exist, we evaluate the transition temperature, and we show that the spin correlation function behaves itself in an unusual way.
FIG. 1. The Kagomé lattice (filled dots) with antiferromagnetic bonds (continuous lines) and the dual lattice (circles) and its bonds (dashed lines).

The common treatment of the KT transition in the continuous limit [6,7] does not account for the structure and high degeneracy of the system and therefore it is not applicable in this case. In order to take into account the special structure of the Kagomé lattice we follow the lattice approach developed by Jose, Kadanoff, Kirkpatrick, and Nelson (JKKN) [8]. The Kagomé lattice consists of triangles and hexagons (fig. 1). The Hamiltonian of the Kagomé antiferromagnet can be represented as a sum of squares of the total spins in triangles of the
nearest neighbors, $S_\Delta$:

$$H = \frac{1}{2}J \sum_\Delta (S_\Delta)^2,$$  

(1)

where $\Delta$ numbers the triangles of the nearest neighbors (fig. 1). Each spin participates in two triangles. The ground state energy is equal to zero and there are infinitely many ground states with $S_\Delta = 0$. In any ground state, the angles between neighboring spins are equal to $\pm 2\pi/3$. Vortices are structural defects in the ground state spin pattern with kernels localized in the centers of hexagons or triangles.

Our plan is as follows. Following JKKN, we represent the partition function in terms of integer-valued currents on the lattice and introduce the dual lattice to the Kagomé lattice, with sites located in the centers of triangles and hexagons. A very important step is to exclude vortices located in the centers of triangles from further consideration because the energy of such vortices is approximately $J \ln (2\sqrt{3})$ higher than that of vortices residing on hexagons. The neglect of such vortices makes sense because, as we show further (Eq. (12)), the KT transition temperature, $T_c = 0.0756J$ is small compared to the energy of a vortex residing on a triangle, and the contribution of such vortices is of order $(2\sqrt{3})^{-J/T_c} \approx 7 \cdot 10^{-8} \ll 1$. This small parameter allows one to integrate out currents in triangles in the partition function. After this step, only currents in hexagons and new variables, chiralities, located on triangles and equal to $\pm 1$ are left. The chirality distinguishes the clockwise and counter-clockwise configurations of spins in each triangle. We show that summation over chiralities renormalizes the partition function expressed in terms of currents in hexagons, however it does not change the low-temperature partition function drastically. We find that the degeneracy of ground states results in a decrease of the transition temperature compared to that of the XY ferromagnet on the hexagonal lattice. The order parameter correlations below the KT transition temperature decay as a power of distance. We show that in the Kagomé antiferromagnet the spin-spin correlations decay exponentially, in contrast with those in “usual”, non-degenerate XY magnets. The reason for such a fast decay of the spin-spin correlations is that the symmetry of the pair spin correlation function is lower than
that of the order parameter and those correlations are sensitive to the multiplicity of ground states, that are mainly disordered.

The partition function of the XY Kagomé antiferromagnet can be represented as a sum over the lattice’s bonds

\[
Z(\beta) = \int e^{-\beta \sum r.a \cos[\theta(r)-\theta(r+a)]} \prod_r d\theta(r),
\]

where \(r\) marks positions on the Kagomé lattice, \(a\) are the three lattice vectors directed along the antiferromagnetic bonds between nearest neighbors, \(\theta_r\) are the spin angles, and \(\beta = JS^2/2T\) is the dimensionless inverse temperature. The \(2\pi\) periodicity of the angle variables allows one to expand \(Z(\beta)\) in Fourier series with the coefficients \(I_n(r,a)(-\beta)\), where \(I_n(x)\) is the modified Bessel function and integer numbers \(n(r,a)\) are located on bonds connecting nearest neighbors \(r\) and \(r+a\).

One can integrate over the angles \(\theta(r)\) in the partition function. This results in the following representation for the partition function:

\[
Z(\beta) = \sum_{\{n(r,a)\}} \prod_{(r,a)} I_n(r,a)(-\beta) \delta \left( \sum_{a=r-r'} n(r,a) \right),
\]

where \(n(r-a,-a) = -n(r,a)\). The numbers \(n(r,a)\) obey the conservation condition at each site of the lattice:

\[
\sum_a n(r,a) = 0.
\]

Following JKKN [8], we introduce the dual lattice to the Kagomé lattice in order to account for the conservation conditions (4). The sites of the dual lattice, \(R\), are located at crossings of lines perpendicular to the bonds that connect nearest neighbors on the Kagomé lattice and cross the bonds in their middle points (fig. 1). This construction provides a one-to-one correspondence between bonds of the Kagomé lattice and bonds of the dual lattice. The conservation conditions (4) can be resolved if one introduces integer-valued currents \(J(R)\) circulating in each triangle and in each hexagon of the the Kagomé lattice. The currents can be assigned to sites \(R\) of the dual lattice located in the centers of triangles and hexagons.
A current along a bond \((\mathbf{r}, \mathbf{a})\), \(n(\mathbf{r}, \mathbf{a})\), is equal to the sum of currents in one triangle and in one hexagon that share the bond \((\mathbf{r}, \mathbf{a})\). The currents \(J(\mathbf{R})\) obey the Kirchhoff’s rule: the sum of currents arriving at each site is equal to the sum of departing ones. Thus, the conservation conditions \([4]\) are fulfilled through the Kirchhoff’s rules.

The summation over currents \(\{n(\mathbf{r}, \mathbf{a})\}\) with the conservation laws \([1]\) in the partition function \([3]\) is equivalent to summation over currents \(\{J(\mathbf{R})\}\) located on sites of the dual lattice

\[
Z(\beta) = \sum_{\{J(\mathbf{R})\}} \prod_{(\mathbf{R}, \mathbf{A})} I_{J(\mathbf{R}+\mathbf{A})+J(\mathbf{R})}(-\beta), \tag{5}
\]

where \(\mathbf{A}\) are the lattice vectors of the dual lattice.

From this point, our way deviates from that by JKKN. The product \(\prod_{(\mathbf{R}, \mathbf{A})}\) over the bonds can be factorized as a product over all triangles of the Kagomé lattice and triple products of the Bessel’s functions corresponding to the bonds in each triangle because each bond of the Kagomé lattice belongs to one and only one triangle. This allows one to represent the partition function as follows:

\[
Z(\beta) = \sum_{\{J(\mathbf{R}_h)\}} \prod_{(\mathbf{R}_t)} \sum_{h=1}^3 I_{J(\mathbf{R}_t+\mathbf{A}_{h'})+J(\mathbf{R}_t)}(-\beta). \tag{6}
\]

Here we separate the sums over hexagon and triangle currents, \(J(\mathbf{R}_h)\) and \(J(\mathbf{R}_t)\), with centers \(\mathbf{R}_h\) and \(\mathbf{R}_t\), and \(h'\) numbers three hexagons surrounding each triangle \(\mathbf{R}_t\).

We consider sums of the triple products of the Bessel functions that appear in Eq. \([3]\) and recall that \(I_n(-\beta)\) is \(n\)-th Fourier harmonic of \(e^{-\beta \cos \phi}\). In the low-temperature limit \((\beta \gg 1)\), the integrand in each triple product has extrema at \(\phi_h = 2\pi \sigma_h/3\), \(\sigma_h = \pm 1\) \((h = 1, 2, 3)\). Thus, one arrives at the following asymptotic formula

\[
\sum_{J(\mathbf{R}_t)} \prod_{h'=1}^3 I_{J(\mathbf{R}_t+\mathbf{A}_{h'})+J(\mathbf{R}_t)}(-\beta) \sim \\
\sum_{\sigma(\mathbf{R}_t)=\pm 1} \exp \left\{ \frac{i 2\pi \sigma(\mathbf{R}_t)}{3} \sum_{h'=1}^3 J_{\mathbf{R}_t+\mathbf{A}_{h'}} \right\} \left( 1 + O\left( \frac{1}{\beta} \right) \right). \tag{7}
\]
We note that in addition to hexagon currents, new variables, $\sigma = \pm 1$, which reside in triangles, appear. These variables count the multiple ground states. Now we return to calculation of the partition function (6). We substitute the asymptotic formula for the triple products of Bessel functions (7) into Eq. (6) and rewrite the product of exponentials over the triangles as an exponential of the sum over the triangles. We also use the Poisson summation formula. Finally, we arrive at the following expression for the partition function

$$Z(\beta) = \sum_{\{\sigma(R_t)\}, \{m(R_h)\}} \int \exp \left[ 2\pi i \sum_{R_h} J(R_h) Q(R_h) \right. \left. - \frac{2}{3 \beta} \sum_{R_h, B_h} (J(R_h) - J(R_h + B_h))^2 \right] \prod_{R_h} dJ(R_h), \quad (8)$$

$$Q(R_h) = m(R_h) + \frac{1}{3} \sum_{A_t} \sigma(R_h + A_t) \quad (9)$$

Here $A_t$ runs over all six triangles surrounding each hexagon with the centers $R_h$, $B_h$ are six vectors that connect the centers of nearest hexagons. Note that centers of hexagons form a triangular lattice which is dual to the hexagonal lattice.

Now one can integrate the partition function (8) over the currents in hexagons, $J(R_h)$. This results in the expression for the partition function of the 2D Coulomb gas with quasi-charges $Q(R_h)$ (Eq. (9)) positioned on sites of the triangular lattice $R_h$. Quasi-charges are $1/3$-multiple, this corresponds to the $2\pi/3$-multiplicity of vortex rotations.

At zero temperature, the integration over $J(R_h)$ in (8) yields conservation conditions $\prod_{R_h} \delta(Q(R_h))$, i.e., in any ground state, the sum of chiralities of triangles surrounding each hexagon is a multiple of 3. The problem of counting ground states is mapped onto that of coloring of the hexagonal lattice [3] which was solved exactly [4]. The exact number of ground states, $Z_N$, is equal to $1.46099^{N/3}$, where $N$ is the number of spins. A naive approximation that assumes that chiralities of triangles surrounding each hexagon are independent and equally probable gives a good estimate $Z_N \approx (11/8)^{N/3} = 1.375^{N/3}$ for the number of the ground states. In this estimate we neglect correlations between chiralities of triangles surrounding neighboring hexagons and farther correlations. The effect of those correlations can be estimated as the inverse number of the nearest neighbors on the triangular lattice,
At finite temperatures, excitations against ground states, vortices with nonzero quasi-charges $Q$, appear. Both integration over hexagon currents, $J(R_h)$, and summation over chiralities of triangles surrounding each hexagon contribute to the probability of vortex formation. Therefore, in addition to the standard estimate of the probability of vortex formation in unfrustrated XY magnets, one has to find the contribution due to various chirality configurations. This accounts for the high degeneracy of ground states in the Kagomé antiferromagnet. The lowest energy vortices have quasi-charges $Q = \pm 1/3$. States with the sum of chiralities of triangles surrounding a certain hexagon equal to $\pm 1$ and $\pm 4$ contribute to formation of such $Q = \pm 1/3$ vortices. The number of such configurations, $Z_{1,N}$, differs from the number of ground states, $Z_N$, by some numerical factor, $w_1$. We estimate the factor $w_1$ the same naive way as we estimated the number of ground states, i.e. we assume that chiralities $\pm 1$ have equal and independent probabilities, $w_1 \approx 21/22$. The precision of this estimate is again of order $1/6$.

Thus, the low-temperature partition function is the sum over states with zero quasi-charge and over states with quasi-charges equal to $\pm 1/3$. It is convenient to redefine $\Psi(R_h) = J(R_h)/(3K)$ and $K = \beta/12$. In terms of new fields $\Psi(R_h)$, the partition function reads

$$Z = \int e^{-K/2\sum R_h \cdot b_h \left[\Psi(R_h) - \Psi(R_h + b_h)\right]^2}$$

$$\times \left[1 + 2w_1 \sum_{R_h} \cos(2\pi K \Psi(R_h))\right] \prod_{R_h} d\Psi(R_h). \quad (10)$$

This expression coincides with that obtained by JKKN [8]. The quantity $w_1$ plays the role of magnetic field $y_0$ in Ref. [8]. In our case, the lattice $R_h$ is dual to the lattice of hexagons, which corresponds to the initial hexagonal lattice. Hence, the problem of the KT transition on the Kagomé lattice with the antiferromagnetic interaction is mapped onto that of the KT transition in a ferromagnet on the hexagonal lattice.

In order to find the transition temperature and to estimate the role of chiralities we extract the short-distance part of the Green’s function in the hexagonal ferromagnet (10). In the continuous limit, we obtain
\[ Z = \int \mathcal{D}\Psi(r)e^{-\int d^2r \left[ \frac{\nabla_k}{2}(\nabla \Psi)^2 - h a^{-2} \cos(2\pi K \Psi) \right]} , \]  

(11)

where \( h = 2w_1 e^{-K \pi^2/2} = 2w_1 e^{-\beta \pi^2/24} \). At the KT transition temperature, this is a small field, therefore it can be neglected according to reasoning by JKKN. From the usual renormalization [6–8] we find that the KT transition on the hexagonal lattice occurs when \( \sqrt{3}/(2K_c) = \pi/2 \), i.e.

\[ T_c/J S^2 = \sqrt{3}\pi/72 = 0.0756 . \]  

(12)

Note that recent Monte Carlo simulations of the KT transition in the Kagomé antiferromagnet [4] yield \( T_c/J S^2 \approx 0.078 \). This is in a very good agreement with our exact result (12).

The existence of a new set of variables, chiralities, qualitatively changes the spin correlation function compared to that in “normal” XY magnets. Returning to the initial formulation of the problem (2), we consider the correlation function \( K(r_0) = \langle \exp (i\theta(0) - i\theta(r_0)) \rangle \). In terms of the integer-valued variables, \( n(r, a) \) (see (3)), we arrive at an expression that differs from (3), only by arguments of the \( \delta \)-functions. Namely, for sites 0 and \( r_0 \) we get

\[ \sum_a n(0, a) = -\sum_a n(r_0, a) = 1 . \]  

(13)

instead of the conservation condition (4). This condition is equivalent to a pattern of currents which is a superposition of currents \( J(R_A) \), that flow in the Kagomé lattice and obey the condition (4), and an unit current which is created in the point 0 and is annihilated in the point \( r_0 \). Thus, the correlation function \( K(r_0) \) has the form

\[ K(r_0) = \frac{1}{Z(\beta)} \sum_{\{J(R)\}} \prod_{(R \neq R^*, A \neq A^*)} I_J(R^* + A^*) + J(R^*) + J + 1(\beta) , \]  

(14)

analogous to that of Eq. (3). Here \( (R^*, A^*) \) are sites and vectors of the dual lattice such that \( A^* \) crosses the path \((0, r_0)\) on the initial kagomé lattice. Now we integrate over currents in the triangles in Eq. (14) as we did it before using the asymptotic formula (7). Instead of
Eq. (8) we get \( K(r_0) = Z(\beta, r_0)/Z(\beta) \) where \( Z(\beta) \) is given by Eq. (8) and \( Z(\beta, r_0) \) differs from \( Z(\beta) \) by the additional contribution from the unit current running along the path \( (0, r_0) \).

The vertex contribution in the large \( r_0 \) asymptotics of the spin correlation function \( K(r_0) \) below the KT-transition point is negligible because the renormalization-group flow at \( T < T_c \) yields that the effective constant \( h \) in (11) is equal to zero. This is equivalent to the neglect of the first term in square brackets in Eq. (8) in the expression for \( Z(\beta, r_0) \). Neglecting constraints on chiralities of triangles as we did before we immediately get a factor \((\cos 2\pi/3)^{r_0/a} = (-1)^{r_0/a}2^{-r_0/a}\) in the correlation function, where \( a \) is the Kagomé lattice constant. The integration over \( J(R_h) \) in the \( r_0 \to \infty \) limit can be done in the spin-wave approximation and the result coincides with that by JKKN [8]. Thus, in the low-temperature phase \( T \leq T_c \) in the long-distance limit \( r_0/a \gg 1 \) the spin correlation function reads

\[
K(r_0) \propto (-1)^{r_0/a}2^{-r_0/a}(r_0/a)^{-T/36T_c}.
\]

(15)

It decays exponentially with distance. The true order parameter of the KT-transition is the cubed spin [3], \( \eta(r) = \exp(3i\theta(r)) \). The correlation function of this order parameter at \( T < T_c \) decays as a power of distance

\[
< \eta(0)\eta(r) > \sim (r_0/a)^{-T/4T_c}.
\]

(16)

In conclusion, it is shown that the XY antiferromagnet on the two-dimensional Kagomé lattice exhibits a Kosterlitz-Thouless transition and the transition temperature, \( T_c \), is evaluated (Eq. (12)). It is found that the spin correlation function decays exponentially with distance even below the transition temperature (Eq. (15)). Nevertheless, the order parameter correlations decay as a power of the distance in the low-temperature phase (Eq. (16)).

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