

Kosterlitz-Thouless and magnetic transition temperatures in layered magnets with a weak easy-plane anisotropy

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The two-dimensional (2D) Heisenberg magnet with a weak easy-plane anisotropy is considered. A renormalization-group analysis in this model is performed for both quantum and classical cases. A crossover from the Heisenberg to 2D XY model is discussed. The magnetic transition owing to the interlayer coupling is considered. Analytical results for the Kosterlitz-Thouless and Curie (Néel) temperatures are derived by taking into account two-loop corrections. The results are compared with experimental data, e.g., on K_2CuF_4 , and turn out to provide a quantitative description, unlike the standard one-loop results. [S0163-1829(99)08725-1]

The interest in the magnetic properties of layered systems has been recently greatly revived. It is well known that even weak magnetic anisotropy can play an important role in such systems. In the present paper we discuss the case of the easy-plane localized-spin system. The simplest classical two-dimensional (2D) XY model was studied in detail,^{1,2} and the relevance of topological (vortex) excitations in thermodynamics was established. In particular, the Kosterlitz-Thouless transition, connected with unbinding of the vortex-antivortex pairs, was found. The transition temperature, where power-law behavior of the spin-correlation function is changed by an exponential one, is estimated as

$$T_{KT} = \frac{\pi}{2} JS^2, \quad (1)$$

where $J > 0$ is the exchange integral. In the quantum XY model the situation is still more complicated, since not only transverse, but also z components of spins should be taken into account.

A different situation takes place in both the quantum and classical Heisenberg 2D model with a weak easy-plane anisotropy, which is a more physically real case.³ A simple expression for the Kosterlitz-Thouless temperature obtained in Ref. 4 reads

$$T_{KT} = \frac{4\pi JS^2}{\ln[\pi^2/(1-\eta)]} \quad (2)$$

($\eta = J^z/J^{x,y}$ is the anisotropy parameter) and has the same form as the result for the magnetic ordering point of the easy-axis layered magnet.³ As well as the latter result (see discussion in Refs. 5–7), the formula (2) is insufficient for a quantitative description of the experimental data (see Ref. 4). Since $T_{KT} \ll JS^2$, one can expect that thermodynamic properties of these systems are determined by usual spin waves, except for a narrow region near T_{KT} . The situation is reminiscent of the easy-axis layered magnet,^{5–7} where the topological (domain-wall) excitations are important only in the vicinity of the Curie (Néel) temperature T_C (T_N). In such a situation, similar to Ref. 7, the renormalization-group (RG) analysis can be performed to calculate T_{KT} with higher accuracy. This analysis is the aim of the present paper. Further

on, we consider effects of interlayer coupling, which lead to occurrence of the true long-range magnetic ordering, and calculate T_C (T_N).

We consider the easy-plane Heisenberg model

$$H = -\frac{1}{2} \sum_{\langle ij \rangle} J_{ij} [S_i^x S_j^x + S_i^y S_j^y + \eta S_i^z S_j^z], \quad (3)$$

where $J_{ij} = J$ [$J > 0$ in the ferromagnetic (FM) case and $J < 0$ in the antiferromagnetic (AF) case] for the nearest-neighbor sites i, j in the same plane, and $J_{ij} = \alpha J$ for i, j in different planes, $\eta < 1$. We suppose $1 - \eta, \alpha \ll 1$. Note that the effect of the single-site anisotropy

$$H_D = D \sum_i (S_i^z)^2, \quad D > 0 \quad (4)$$

is the same as that of exchange anisotropy with $1 - \eta = D(1 - 1/2S)/4|J|$ provided that $D/|J| \ll 1$.

The partition function of the model (3) can be represented in terms of a path integral over coherent states (see, e.g., Refs. 8,9):

$$\mathcal{Z} = \int D\boldsymbol{\pi} \delta(\pi^2 - 1) \exp(-\mathcal{L}_{\text{dyn}} - \mathcal{L}_{\text{st}}), \quad (5)$$

$$\mathcal{L}_{\text{dyn}} = iS \int_0^{1/T} d\tau \sum_i \mathbf{A}(\boldsymbol{\pi}_i) \frac{\partial \boldsymbol{\pi}_i}{\partial \tau},$$

$$\mathcal{L}_{\text{st}} = \frac{1}{2} S^2 \int_0^{1/T} d\tau \sum_{\langle ij \rangle} J_{ij} [\pi_{xi} \pi_{xj} + \pi_{yi} \pi_{yj} + \eta \pi_{zi} \pi_{zj}],$$

where $\boldsymbol{\pi}$ is the unit-length vector, and $\mathbf{A}(\boldsymbol{\pi})$ is the vector potential of the unit magnetic monopole, which satisfies the equation $\nabla \times \mathbf{A}(\boldsymbol{\pi}) \cdot \boldsymbol{\pi} = 1$.

In the classical case (i.e., with \mathcal{L}_{dyn} being neglected), we have two types of excitations: the field π_y describes the gapless in-plane excitations, and the field π_z describes the out-of-plane excitations with a gap. Expanding Eq. (5) in $\pi_{y,z}, x$ being a (local in the AF case) spin-quantization axis, to leading order in $1/S$ we have

$$\mathcal{L}_{\text{st}} = \frac{1}{2} S^2 \int_0^{1/T} d\tau \sum_{\mathbf{k}} [(J_0 - J_{\mathbf{k}}) \pi_{y\mathbf{k}} \pi_{y,-\mathbf{k}} + (J_0 - \eta J_{\mathbf{k}}) \pi_{z\mathbf{k}+\mathbf{Q}} \pi_{z,-\mathbf{k}-\mathbf{Q}}], \quad (6)$$

where \mathbf{Q} is the wave vector of magnetic structure. The dynamical part \mathcal{L}_{dyn} , which is present in the quantum case, results in (i) quantum renormalizations of the Hamiltonian parameters (in the AF case only), which are supposed to be already performed and (ii) the summations over wave vectors are bounded by $\sqrt{T/J_S}$ in the FM case or T/c in the AF case (c is the quantum-renormalized spin-wave velocity) rather than by the Brillouin-zone boundary (see Ref. 7).

The interaction of spin waves, which occurs in higher orders in $1/S$, leads to temperature renormalizations of the Hamiltonian parameters. Due to the smallness of the anisotropy, large logarithms occur in these renormalizations: $\ln|T/(1-\eta)J|$ in the quantum FM case, $\ln[T^2/(1-\eta)J^2]$ in the quantum AF case, and $\ln[1/(1-\eta)]$ in the classical case. It is natural to sum up these logarithms within the RG approach. However, there exists the difficulty owing to that gapless π_y excitations are present too. In the absence of the interlayer coupling, they lead to infrared divergences in some quantities like the in-plane magnetization. In the presence of interlayer coupling, another type of logarithms occur, $\ln(T/\alpha J)$, $\ln(T^2/\alpha J^2)$, or $\ln(1/\alpha)$, depending on the case. The situation, where two types of excitations with different characteristic scales are present, is typical for systems demonstrating a crossover.¹⁰ In our model this is the crossover from the Heisenberg (almost isotropic) behavior to the XY behavior.

To describe correctly this crossover we include anisotropy in all the renormalization factors.¹⁰ We also introduce the scaling factors of the field π . Because of anisotropic character of the model, we have two such factors: Z_{xy} and Z_z , so that $\pi_{xR}/\pi_x = \pi_{yR}/\pi_y = Z_{xy}$ and $\pi_{zR}/\pi_z = Z_z$. We use the normalization condition $\Gamma_{zz}^{(2)}(0) = 1 - \eta$ (which fixes the gap of z excitations) instead of the standard one, $d\Gamma_{zz}^{(2)}(q)/d(q^2) = 1$, $\Gamma_{zz}^{(2)}(q)$ being the two-point vertex function (inverse Green's function) of the field π_z . Then we have $Z_z \equiv 1$. For other Hamiltonian parameters we obtain the following system of RG equations:

$$\mu \frac{d(1/t_\mu)}{d\mu} = (1+t_\mu)f(\eta_\mu, \mu) + \mathcal{O}(t_\mu^2), \quad (7a)$$

$$\mu \frac{d \ln Z_{xy}}{d\mu} = t_\mu [1 + f(\eta_\mu, \mu)] + \mathcal{O}(t_\mu^3), \quad (7b)$$

$$\mu \frac{d \ln \eta_\mu}{d\mu} = 2t_\mu f(\eta_\mu, \mu) + \mathcal{O}(t_\mu^2), \quad (7c)$$

$$\mu \frac{d \ln \alpha_\mu}{d\mu} = -t_\mu + \mathcal{O}(t_\mu^2), \quad (7d)$$

where μ is the scale parameter, $f(\eta_\mu, \mu) = \eta_\mu \mu^2 / (\eta_\mu \mu^2 + 1 - \eta)$,

$$t = \begin{cases} T/(2\pi JS^2) & \text{FM,} \\ T/(2\pi \rho_s) & \text{AF} \end{cases}$$

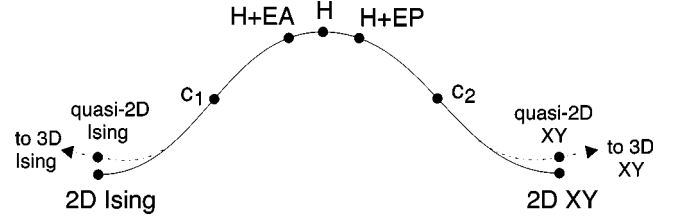


FIG. 1. Schematic picture of the RG trajectories in layered magnets. Left-hand side: the flow from the 2D easy-axis Heisenberg (H+EA) to the 2D Ising model. Right-hand side: the flow from the 2D easy-plane Heisenberg (H+EP) to the 2D XY model. The inflection points c_1, c_2 mark the crossover regions. The dashed lines are for the corresponding quasi-2D models.

is the dimensionless temperature, $\rho_s \approx S(S+0.079)|J|$ being the spin stiffness.¹¹ The first two equations in Eq. (7) are written to two-loop order, while the last two are in one-loop order, which is sufficient to obtain the final results to the two-loop order accuracy. The initial scale μ_0 for these equations is

$$\mu_0 = \begin{cases} \sqrt{32} & \text{classical regime } (T \gg |J|S), \\ T/c & \text{quantum regime } (T \ll |J|S), \text{AF,} \\ \sqrt{T/J_S} & \text{quantum regime } (T \ll JS), \text{FM} \end{cases}$$

for the details see, e.g., Ref. 7.

The flow of RG parameters is shown schematically in Fig. 1 (for comparison, the easy-axis case $\eta > 1$ is depicted too). From Eqs. (7a) and (7c) we obtain

$$\frac{1}{t_\mu} = \frac{1}{t} + \frac{1}{2} \ln \frac{\eta \mu^2 t_\mu^2 + t^2(1-\eta)}{\eta \mu_0^2 t_\mu^2 + t^2(1-\eta)} + \ln \frac{t}{t_\mu} + \Phi(\mu), \quad (8)$$

where the function $\Phi(\mu) = \mathcal{O}(t_\mu)$ comes from \mathcal{O} terms in Eqs. (7) and corresponds to the contribution of higher-order loops. For $\mu \gg \sqrt{1-\eta}$ the effective temperature t_μ is small (which guarantees that the spin-wave theory works well), so that we have $\Phi(\mu) \ll 1$ and

$$\frac{1}{t_\mu} = \frac{1}{t} + \ln \frac{\mu t}{\mu_0 t_\mu}. \quad (9)$$

For $\mu \ll \sqrt{1-\eta}$ we obtain

$$\frac{1}{t_\mu} = \frac{1}{t} - \ln \frac{\mu_0}{\sqrt{1-\eta}} + 2 \ln \frac{t}{t_\mu} + \Phi(\mu), \quad (10)$$

and in this regime t_μ is μ dependent only through the function $\Phi(\mu)$. The scale $1/\sqrt{1-\eta}$ is just a characteristic scale for the crossover from the Heisenberg to XY behavior and Eq. (10) describes t_μ in the XY regime. On the other hand, in this regime only vortices contribute to the temperature renormalization since such a renormalization owing to spin waves is absent (the interaction of spin waves in the XY model is due to topological effects only). Thus for the temperature renormalization we have the system of RG equations,^{1,2} which in our notations can be written as

$$\mu \frac{d(1/t_\mu)}{d\mu} = 32\pi^2 y_\mu^2, \quad (11a)$$

$$\mu \frac{dy_\mu}{d\mu} = -y_\mu \left(2 - \frac{1}{2t_\mu} \right). \quad (11b)$$

It should be noted that the coupling constant for the vortex system is not t (as for spin waves), but $y = \exp(-E_0/T)$ where E_0 is the energy of a vortex core. Therefore, Eqs. (11) are applicable for small enough μ . Let $\mu_1 \ll \sqrt{1-\eta}$ be the scale where we pass to scaling (11). Then the solution of Eqs. (11) for $t > t_{\text{KT}}$ reads

$$\frac{1}{t_\mu} = 4 + 2C_1 \tan \left(C_1 \ln \frac{\mu}{\mu_1} + C_2 \right), \quad (12)$$

where

$$C_1 = \sqrt{(8\pi y_1 t_1)^2 - (4t_1 - 1)^2} / (2t_1)$$

$$\tan C_2 = \frac{1 - 4t_1}{\sqrt{(8\pi y_1 t_1)^2 - (4t_1 - 1)^2}}, \quad (13)$$

and $t_1 \equiv t_{\mu_1}, y_1 \equiv y_{\mu_1}$ are determined by

$$\frac{1}{t_1} = \frac{1}{t} - \ln \frac{\mu_0}{\sqrt{1-\eta}} + 2 \ln \frac{t}{t_1} + \Phi(\mu_1) \quad (14)$$

$$y_1 = \frac{1}{4\pi} \left[\frac{\mu}{2} \frac{d\Phi(\mu)}{d\mu} \right]_{\mu=\mu_1}^{1/2}.$$

It should be stressed that even if the original model is a quantum one, the resulting XY model is classical since $\mu_1 \ll \sqrt{1-\eta} \ll L_\tau^{-1}$ ($L_\tau = JS/T$ for FM case and $L_\tau = c/T$ for AF case is a characteristic length for quantum effects), and at scales much larger than L_τ quantum and classical systems becomes indistinguishable. Thus all the quantum effects are already taken into account at the scales $\mu \gg \sqrt{1-\eta}$, where the behavior of RG trajectories is a Heisenberg one.

The Kosterlitz-Thouless temperature T_{KT} is determined by the equation of the separatrix line for Eqs. (11)

$$8\pi y_1 = 1/t_1 - 4, \quad t = t_{\text{KT}}. \quad (15)$$

This line separates the low- and high-temperature phases. For small enough μ we have $\Phi(\mu) \rightarrow \text{const}$, $d\Phi(\mu)/d\mu \rightarrow 0$ and we have for $t_{\text{KT}} = T_{\text{KT}}/(2\pi JS^2)$ (or $T_{\text{KT}}/(2\pi \rho_s)$ in the AF case)

$$t_{\text{KT}} = [\ln(\mu_0/\sqrt{1-\eta}) + 2 \ln(2/t_{\text{KT}}) + C]^{-1} \quad (16)$$

where $C = 4 - 6 \ln 2 - \Phi(\mu \rightarrow 0)$ is a universal constant. This result is identical with that for the Curie (Néel) temperature of an easy-axis magnet,⁷ except for the constant C , which need not be the same as for the easy-axis case.

In the critical region above t_{KT} ,

$$\frac{1}{8\pi} (t_{\text{KT}}^{-1} - t^{-1}) \ll 1, \quad (17)$$

the expression for the correlation length obtained from Eq. (12) reads

$$\xi = \frac{1}{\mu_1} e^{-C_2/C_1} \approx \frac{1}{\sqrt{1-\eta}} \exp \left(\frac{A}{2\sqrt{t_{\text{KT}}^{-1} - t^{-1}}} \right), \quad (18)$$

and has the same form as for the XY model (A is a constant). Under the condition, opposite from Eq. (17), we have the standard Heisenberg behavior¹¹

$$\xi = (C_\xi/\mu_0) t \exp(1/t). \quad (19)$$

In the presence of interlayer coupling, the magnetic ordering at low enough temperatures occurs. Due to topological effects, the transition temperature grows up from T_{KT} , and not from zero. Note that in this case T_{KT} plays the role of a crossover temperature from 2D to 3D XY behavior rather than a critical temperature, and the only true phase transition is connected with the magnetic ordering at $T_C(T_N)$.

In the case $\alpha \ll 1 - \eta$ we choose μ_1 such that $\alpha^{1/2} \ll \mu_1 \ll (1-\eta)^{1/2}$. In terms of RG transformation (see Fig. 1), at $\mu = \mu_1$ we have not 2D, but a quasi-2D XY effective model with the lattice constant μ_0/μ_1 and the interlayer coupling $(\mu_0/\mu_1)^2 \alpha_1$ where, as follows from Eq. (7d),

$$\alpha_1 \equiv \alpha_{\mu_1} = \alpha t / t_1. \quad (20)$$

With further flow of the RG transformation we should arrive at the 3D XY model. However, this part of the RG transformation meets with difficulties owing to a complicated geometry of vortex loops (see Ref. 12, and references therein). Instead of a direct calculation of RG trajectories, we use the same scaling arguments as in Ref. 4. The transition temperature can be estimated from the requirement that the correlation length of the model without interlayer coupling ($\alpha = 0$) coincides with the characteristic scale of the crossover from the 2D to 3D XY model, $1/\alpha_1^{1/2}$ (in the units of the lattice constant of original lattice). Then we have for the critical temperature $t_c = T_C/(2\pi JS^2)$ [or $T_N/(2\pi \rho_s)$] in the case $\alpha \ll 1 - \eta$

$$t_c = \left\{ \ln \frac{\mu_0}{\sqrt{1-\eta}} + 2 \ln \frac{2}{t_{\text{KT}}} + C - \frac{A^2}{\ln^2[(1-\eta)/\alpha]} \right\}^{-1}. \quad (21)$$

The last term in the denominator determines the difference between t_c and t_{KT} . Since this term cannot be too small, we do not expand Eq. (21) in it.

The result (21) is qualitatively valid up to α of order of $1 - \eta$ (in this case, the last term in the denominator leads to renormalization of C only). Consider now briefly the case $\alpha \gg 1 - \eta$. Then the corrections to the RG result for the quasi-2D magnets,⁷ owing to the easy-plane anisotropy, are given by

$$t_c = \left[\ln \frac{\mu_0}{\sqrt{\alpha}} + 2 \ln \frac{2}{t_c} + C' + \mathcal{O} \left(\frac{(1-\eta)^{1/\psi}}{\alpha^{1/\psi}} \right) \right]^{-1}, \quad (22)$$

where $\psi = \nu_3(2 - \gamma_\eta)$ is the crossover exponent, ν_3 is the corresponding critical exponent for the 3D Heisenberg model, and γ_η is the anomalous dimensionality of the anisotropy parameter near the 3D Heisenberg fixed point, see, e.g., Ref. 10. The ε expansion in the anisotropic $4 - \varepsilon$ -dimensional ϕ^4 model for $\varepsilon = 1$ (which has the same symmetry as the model under consideration) yields $\psi \approx 0.83$, see Ref. 10. For an antiferromagnet, the constant $C' \approx -0.066$ was calculated within the $1/N$ expansion.⁵ Unlike Eq. (21), the last term in the denominator of Eq. (22) has

not an inverse-logarithmic form. This is a consequence of the fact that the correlation length in the 3D Heisenberg model does not demonstrate the exponential behavior (ν_3 is finite). For this reason the correction in the denominator of Eq. (22) is small and can be neglected.

Finally, we consider the experimental situation for layered magnets. The mostly investigated easy-plane system is the compound K_2CuF_4 . This is a $S=1/2$ ferromagnet with $T_{\text{KT}}=5.5$ K, $T_C=6.25$ K and the parameters $J=20$ K, $1-\eta=0.04$, $\alpha=6\times 10^{-4}$ (see, e.g., Ref. 3). Substituting these values into Eqs. (16) and (21) we obtain $C\approx -0.5$ and $A\approx 3.5$. Note that the formula (2) yields the value $T_{\text{KT}}=11.4$ K which is much larger than the experimental one.

Another example of a quasi-2D FM XY -like system is the stage-2 NiCl_2 graphite interlayer compound with $S=1$. According to Ref. 3, $J=20$ K, $1-\eta=8\times 10^{-3}$, and $\alpha=5\times 10^{-5}$. Using the same values of A and C as for K_2CuF_4 , we calculate $T_{\text{KT}}=17.4$ K and $T_C=18.7$ K, which is in agreement with experimental data (both values T_{KT} and T_C lie in the region 18–20 K). At the same time, using formula (2) yields $T_{\text{KT}}=35.3$ K, which is again twice larger as compared to the experimental value.

We have also applied our results to the compound $\text{BaNi}_2(\text{PO}_4)_2$ which is a $S=1$ antiferromagnet with $|J|=22.0$ K and easy-plane anisotropy $1-\eta=0.05$, $\alpha=1\times 10^{-4}$, see Ref. 3. We obtain $T_{\text{KT}}=23.0$ K which coincides

with the experimental value and $T_N=24.3$ K, again in excellent agreement with $T_N^{\text{exp}}=24.5\pm 1$ K. Note that in spite of $T_{\text{KT}}\sim |J|S$ for this compound, the true criterion of the quantum regime is $(T/JS)^2\ll 32$ (see Ref. 7), and this case also should be considered a quantum one.

To conclude, we have investigated the Heisenberg model with a weak easy-plane anisotropy. We have performed the two-loop RG transformation with unknown function $\Phi(\mu)$ (which takes into account the contribution of higher loops and non-spin-wave excitations) and joined the results with well-known behavior of the RG trajectories in the 2D XY model. In such a way we have obtained simple analytical expressions for the Kosterlitz-Thouless and Curie (Néel) temperatures. These expressions contain two constants A, C which are still indeterminate within the RG approach. The calculation of these constants, as well as of the corresponding parameters for the isotropic quasi-2D and easy-axis 2D Heisenberg model,⁷ is possible by numerical (e.g., by the quantum Monte-Carlo) methods.¹³ At the same time, our results already enable one to estimate the Kosterlitz-Thouless temperature [and also to determine the difference $T_C(T_N)-T_{\text{KT}}$] with an accuracy which is sufficient to fit experimental data on layered magnets, unlike the simplest expression (2).

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¹³In the AF case one can use also the $1/N$ expansion. However, unlike the isotropic quasi-2D case (Ref. 5), in the presence of anisotropy this expansion becomes inapplicable in the critical region (which gives a considerable contribution to C) because of small values $N=1$ and $N=2$ for the Ising and XY models.