Multicritical behavior of two-dimensional anisotropic antiferromagnets in a magnetic field

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We study the phase diagram and multicritical behavior of anisotropic Heisenberg antiferromagnets on a square lattice in the presence of a magnetic field along the easy axis. We argue that, besides the Ising and *XY* critical lines, the phase diagram presents a first-order spin-flop line starting at $T=0$, as in the three-dimensional case. By using field-theory methods, we show that the multicritical point where these transition lines meet cannot be O(3) symmetric and occurs at finite temperature. We also predict how the critical temperature of the transition lines varies with the magnetic field and the uniaxial anisotropy in the limit of weak anisotropy.

I. INTRODUCTION

Anisotropic antiferromagnets in an external magnetic field have been studied for a long time. In order to determine their phase diagram, they have often been modeled by using the classical *XXZ* model (we only consider the case of a magnetic field along the easy axis)

$$\mathcal{H} = J \sum_{\langle mn \rangle} \vec{S}_n \cdot \vec{S}_m + A \sum_{\langle mn \rangle} S_{m,z} S_{n,z} - H \sum_m S_{m,z}, \quad (1)$$

where $\langle mn \rangle$ indicates a nearest-neighbor pair. Equivalently, one can use the Hamiltonian

$$\mathcal{H} = J \sum_{\langle mn \rangle} \vec{S}_n \cdot \vec{S}_m + D \sum_m S_{m,z}^2 - H \sum_m S_{m,z}, \quad (2)$$

with a single-ion anisotropy term. The most interesting case corresponds to uniaxial systems that show a complex phase diagram. They correspond to Hamiltonians with $A > 0$ or $D < 0$. Several quasi-two-dimensional uniaxial antiferromagnets have been studied experimentally, such as K_2MnF_4, Rb_2MnF_4, and Rb_2MnCl_4.[1–7]

Some general features of the phase diagram of anisotropic antiferromagnets are well known. Their phase diagram in the *T-H* plane presents two critical lines, belonging to the Ising and *XY* universality classes, respectively, which meet at a multicritical point (MCP). The nature of the MCP has been the object of several theoretical studies. In three dimensions (3D), the issue has been recently studied using a field-theory (FT) approach.[8,9] The starting point is the $O(n_1) \oplus O(n_2)$ symmetric Landau-Ginzburg-Wilson (LGW) Φ^4 theory,[10]

$$\mathcal{H}_{LGW} = \int d^d x \left\{ \frac{1}{2} [(\partial_\mu \Phi_1)^2 + (\partial_\mu \Phi_2)^2] + \frac{1}{2} [r_1 \Phi_1^2 + r_2 \Phi_2^2] + \frac{1}{4!} [u_{10}(\Phi_1^2)^2 + u_{20}(\Phi_2^2)^2] + \frac{1}{4} w_0 \Phi_1^2 \Phi_2^2 \right\}, \quad (3)$$

where Φ_1 and Φ_2 are vector fields with n_1 and n_2 real components, respectively. In our case, $n_1 = 2$ and $n_2 = 1$, so that Hamiltonian (3) is symmetric under $\mathbb{Z}_2 \oplus O(2)$ transformations. The renormalization-group (RG) flow has been studied by computing and analyzing high-order perturbative expansions[8,9] to five and six loops. It has been shown that the stable fixed point (FP) of the theory is the biconal FP, and

that no enlargement of the symmetry to O(3) is asymptotically expected because the corresponding O(3) FP is unstable, correcting earlier claims[10] based on low-order ϵ-expansion calculations. The perturbative results allow us to predict that the transition at the MCP is either continuous and belongs to the biconal universality class or that it is of first order—this occurs if the system is not in the attraction domain of the stable biconal FP. Which of these two possibilities occurs is still an open issue. A mean-field analysis[11,10] shows that the MCP is bicritical if $\delta_0 \equiv u_{10} u_{20} - 9 w_0^2 < 0$, and tetracritical if $\delta_0 > 0$. Figures 1 and 2 sketch the corresponding phase diagrams. At one loop in the ϵ expansion, the biconal FP is associated with a tetracritical phase diagram.[10] Since uniaxial antiferromagnets have a bicritical phase diagram, this result predicts a first-order MCP as in Fig. 3. In this case, first-order transitions are also expected along the critical lines that separate the disordered phase from the ordered ones. They start at the MCP, extend up to tricritical points, and are followed by lines of *XY* and Ising transitions.

The nature of the MCP is even more controversial in two dimensions (2D), where different scenarios have been put forward; see, for example, Refs. 1–7 and 12–16. The existence of the Ising and *XY* Kosterlitz-Thouless (KT) critical
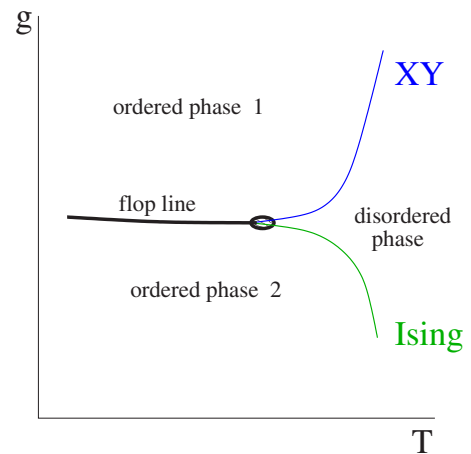

FIG. 1. (Color online) Phase diagram with a bicritical point where an Ising line and an *XY* line meet. Here, *T* is the temperature and *g* is a second relevant parameter. The thick black line ("flop line") corresponds to a first-order transition.
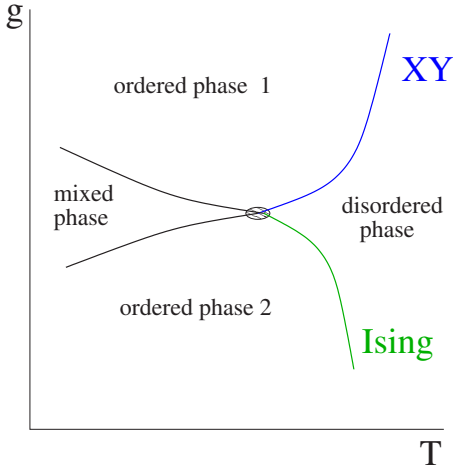
FIG. 2. (Color online) Phase diagram with a tetracritical point where an Ising line and an *XY* line meet. Here, *T* is the temperature and *g* is a second relevant parameter.

lines is well established. However, other features, such as the existence of the spin-flop line, the nature of the MCP, and the MCP temperature, are still the object of debate. For example, the two different phase diagrams sketched in Fig. 4 have apparently been both supported by recent numerical Monte Carlo (MC) analyses: Ref. 15 claims that MC data are in agreement with the phase diagram reported on the top, while Ref. 16 supports that reported on the bottom. Similar contradictions appear in the analyses of the experimental data.[1–7]

In this paper, we study the nature of the MCP in 2D within the FT approach. Our main findings are the following:

(i) The MCP cannot be O(3) symmetric even at $T=0$. Indeed, the magnetic field and the anisotropy give rise to an *infinite* number of relevant perturbations of the O(3) FP. Moreover, since at $T=0$ the order parameter is discontinuous as H is varied,[12,17] we expect a first-order spin-flop line. We thus predict a finite-temperature MCP.

(ii) We study the limit of weak anisotropy. In this limit, we determine how the critical temperature of the Ising and KT transition lines and of the MCP vary with H and A.
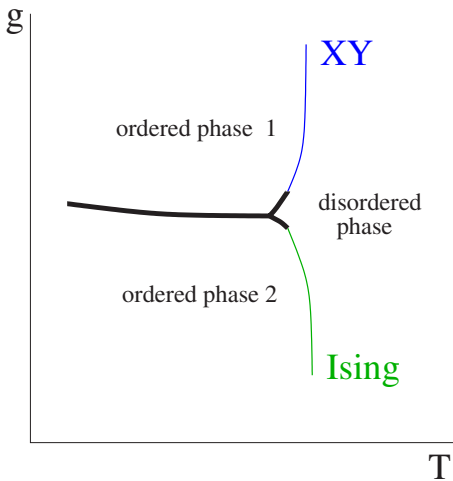

FIG. 3. (Color online) Phase diagram with a first-order bicritical point. The thick black lines correspond to first-order transitions.

Our results on the phase diagram of the classical *XXZ* model (1) are also relevant for the phase diagram of quantum spin-*S* *XXZ* models[18,19] and related systems, such as the hard-core boson Hubbard model.[20,21]

The paper is organized as follows. In Sec. II, we summarize some general predictions for the isotropic model. In Sec. III, we investigate the stability of the O(3) FP by using field theory and give predictions for the critical temperature as a function of H and A for small A and H. Finally, in Sec. IV, we discuss the implications of the FT results and discuss the possible phase diagrams that are compatible with them.

II. ISOTROPIC ANTIFERROMAGNET IN TWO DIMENSIONS

For $H=A=0$, the critical behavior of model (1) is well known. Indeed, if we perform the change of variables

$$\vec{\sigma}_n = (-1)^{[n]}\vec{S}_n, \tag{4}$$

where $[n]\equiv n_x+n_y$ $[n=(n_x,n_y)]$ in 2D $([n]\equiv n_x+n_y+n_z$ $[n=(n_x,n_y,n_z)]$ in 3D), we obtain the ferromagnetic Heisenberg model, for which several results are known.[22,23] In particular, if we define the two-point function

$$G(n) = \langle\vec{S}_0 \cdot \vec{S}_n\rangle, \tag{5}$$

a universal critical behavior is observed for the staggered susceptibility

$$\chi_s = \sum_n (-1)^{[n]}G(n) \tag{6}$$

and for the staggered second-moment correlation length

$$\xi_s^2 = \frac{1}{4\chi_s}\sum_n (-1)^{[n]}|n|^2G(n). \tag{7}$$

Under the mapping (4), χ_s and ξ_s go over to the standard susceptibility and correlation length of the ferromagnetic model. In 2D, the perturbative RG allows one to derive the critical behavior of these two quantities for $T\to 0$.[23] Using the results of Refs. 24 and 25, we obtain

$$\chi_s = C_\chi\xi_s^2\left(\frac{T}{2\pi}\right)^2[1 + 0.181\,69T + 0.1334T^2$$
$$+ 0.1346T^3 + O(T^4)],$$
$$\tag{8}$$
$$\xi_s = C_\xi e^{2\pi/T}\left(\frac{T}{2\pi}\right)[1 - 0.0914T - 0.1969T^2 + O(T^3)].$$

The constants C_ξ and C_χ cannot be determined in perturbation theory. Numerical values are reported in Ref. 26:

$$C_\chi = 93.25(3), \quad C_\xi = 0.012\,478\,3(12). \tag{9}$$

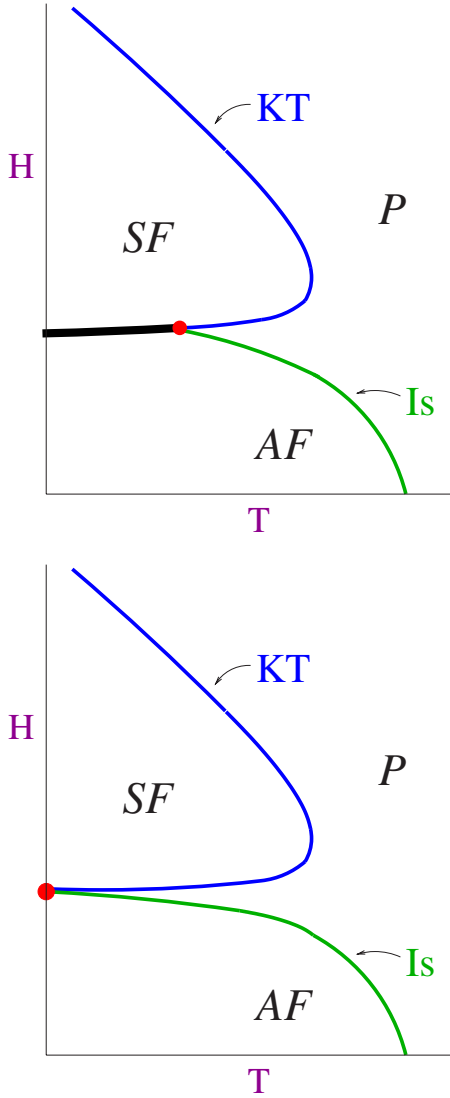The asymptotic expansions (8) are quite accurate for $T \lesssim 0.3$, within a few percent at most.[27,28]

FIG. 4. (Color online) Phase diagrams in the *T*-*H* plane in the presence of easy-axis anisotropy $A>0$ in 2D. The top figure shows a first-order transition line separating the antiferromagnetic (AF) and spin-flop (SF) phases, with a bicritical point where the Ising (Is) and the *XY* Kosterlitz-Thouless (KT) critical lines meet. In the bottom figure, the Ising and KT lines meet at a zero-temperature O(3)-symmetric MCP.

III. CRITICAL AND MULTICRITICAL BEHAVIORS FOR SMALL *A* AND *H*

A. General results

We consider the O(3) isotropic model at $H=0$ and add terms that break the O(3) symmetry down to $\mathbb{Z}_2 \otimes$ O(2) (for instance, the magnetic field or the anisotropy). The corresponding general Hamiltonian is

$$\mathcal{H}_{\text{gen}} = J \sum_{\langle nm \rangle} \vec{S}_n \cdot \vec{S}_m + \lambda Q(S). \tag{10}$$

If $Q(S)$ is a relevant perturbation of the O(3) FP, the O(3) critical point is a MCP in the full theory. In 3D, we can write the singular part of the free energy[10] for $\lambda \to 0$ as

$$\mathcal{F}_{\text{sing}} \sim u_t^{2-\alpha} B(X), \quad X = u_\lambda u_t^{-\phi}, \tag{11}$$

where α and ϕ are the O(3) specific-heat and crossover exponents, respectively, $B(X)$ is a universal scaling function, and u_t and u_λ are the scaling fields associated with the temperature and with λ. In general, we expect

$$u_t = t + k\lambda, \tag{12}$$

where k is a constant, $t \equiv T/T_{O(3)} - 1$ is the reduced temperature, and $T_{O(3)}$ is the critical temperature of the isotropic model. No such mixing between t and λ occurs in u_λ, since u_λ vanishes for $\lambda = 0$. Hence, we can take $u_\lambda = \lambda$. The crossover exponent ϕ is related to the RG dimension y_λ of the operator Q that represents the perturbation of the MCP: $\phi \equiv y_\lambda \nu$. Suppose now that the system has a continuous transition for $\lambda \neq 0$ at $T_c(\lambda)$. Since the singular part of the free energy close to a critical point behaves as $(T-T_c)^{2-\alpha}$, we must have $B(X_c) = 0$, where X_c is the value of X obtained by setting $T = T_c(\lambda)$. This equation is solved by $X_c = X_\pm$, where $X_\pm$ are two constants that depend on the sign of λ, such that $X_+ > 0$, $X_- < 0$. Hence, we obtain

$$\lambda \left[\frac{T_c(\lambda)}{T_{O(3)}} - 1 + k\lambda \right]^{-\phi} = X_\pm. \tag{13}$$

It follows that

$$T_c(\lambda) = T_{O(3)}[1 + (\lambda/X_+)^{1/\phi} - k\lambda + \cdots], \quad \lambda > 0,$$

$$T_c(\lambda) = T_{O(3)}[1 + (\lambda/X_-)^{1/\phi} - k\lambda + \cdots], \quad \lambda < 0. \tag{14}$$

These expressions provide the λ dependence of the critical temperature for λ small. Note that, depending on the sign of λ, $T_c(\lambda)$ varies differently. The sign of λ may also be relevant to the nature of the phase transition. Indeed, the low-temperature phase may be different depending on this sign: in this case, one observes critical behaviors belonging to different universality classes for $\lambda > 0$ and $\lambda < 0$.

One can generalize these considerations to the case in which there are two relevant perturbations Q_1 and Q_2 with parameters λ_1 and λ_2. In this case, we can write

$$\mathcal{F}_{\text{sing}} \sim u_t^{2-\alpha} B(X_1, X_2), \tag{15}$$

with

$$X_1 \equiv u_1 u_t^{-\phi_1}, \quad X_2 \equiv u_2 u_t^{-\phi_2},$$

$$u_1 = \lambda_1 + c_1 \lambda_2, \quad u_2 = \lambda_1 + c_2 \lambda_2, \tag{16}$$

$$u_t = t + k_1 \lambda_1 + k_2 \lambda_2,$$

where k_1, k_2, c_1, and c_2 are constants. We assume here that there are two RG relevant operators that break the O(3) invariance, with RG dimensions $y_1 > y_2 > 0$, as is the case for anisotropic systems in the presence of a magnetic field. The crossover exponents are $\phi_1 = \nu y_1$ and $\phi_2 = \nu y_2$. The scaling fields u_1 and u_2 are linear combinations (and, beyond linear order, generic functions) of λ_1 and λ_2, due to the fact that the lattice operators Q_1 and Q_2 generically couple both RG operators.

Let us now assume that, for λ_1 and λ_2 small, the model shows generically two types of phase transitions belonging to different universality classes and that, for specific values of the ratio λ_1/λ_2, multicritical transitions occur. As before, we wish to derive the dependence of the critical temperature as a function of λ_1 and λ_2 for $\lambda_1, \lambda_2 \to 0$. Since

$$X_2 = u_2 |u_1|^{-\phi_2/\phi_1} |X_1|^{\phi_2/\phi_1}, \quad (17)$$

we can rewrite Eq. (15) as

$$\mathcal{F}_{\text{sing}} \sim u_t^{2-\alpha} \mathcal{B}_{\pm}(X_1, u_2 |u_1|^{-\phi_2/\phi_1}), \quad (18)$$

where we have introduced two different functions depending on the sign of u_1. If $u_1 > 0$, the relevant function is $\mathcal{B}_+(x,y)$; if $u_1 < 0$, one should consider $\mathcal{B}_-(x,y)$. At the critical point, we must have

$$\mathcal{B}_{\pm}(X_{1c}, u_2 |u_1|^{-\phi_2/\phi_1}) = 0, \quad (19)$$

which implies

$$X_{1c} = F_{\pm}(u_2 |u_1|^{-\phi_2/\phi_1}), \quad (20)$$

with $F_+(x) > 0$ and $F_-(x) < 0$. We obtain

$$\frac{T_c}{T_{O(3)}} - 1 \approx \left[\frac{u_1}{F_{\pm}(u_2 |u_1|^{-\phi_2/\phi_1})} \right]^{1/\phi_1} - k_1 \lambda_1 - k_2 \lambda_2. \quad (21)$$

Let us now discuss some limiting cases. First, assume that $u_2 |u_1|^{-\phi_2/\phi_1} \ll 1$. This implies that X_2 is small compared to X_1, so that we can neglect X_2. We are back to the case considered before, so that we can use Eq. (14). Depending on the sign of u_1, we have

(1) if $u_1 > 0$, the phase transition is located at

$$\frac{T_c}{T_{O(3)}} - 1 \approx \left(\frac{u_1}{X_+} \right)^{1/\phi_1} - k_1 \lambda_1 - k_2 \lambda_2, \quad (22)$$

where $X_+ > 0$;

(2) if $u_1 < 0$, there is a phase transition located at

$$\frac{T_c}{T_{O(3)}} - 1 \approx \left(\frac{u_1}{X_-} \right)^{1/\phi_1} - k_1 \lambda_1 - k_2 \lambda_2, \quad (23)$$

where $X_- < 0$.

By comparing with Eq. (21), we obtain $F_{\pm}(0) = X_{\pm}$.

The second interesting limiting case corresponds to $u_1 \to 0$. In this case, X_1 can be neglected and we need to consider only X_2. Therefore, depending on the sign of u_2, we have a MCP located at

$$\frac{T_c}{T_{O(3)}} - 1 \approx \left(\frac{u_2}{X_{\text{mc},\pm}} \right)^{1/\phi_2} - k_1 \lambda_1 - k_2 \lambda_2, \quad (24)$$

where $X_{\text{mc},+} > 0$ and $X_{\text{mc},-} < 0$. Consistency with Eq. (21) requires

$$F_{\pm}(x) \approx \pm (x/X_{\text{mc},+})^{-\phi_1/\phi_2} \quad (25)$$

for $x \to +\infty$, and

$$F_{\pm}(x) \approx \pm (x/X_{\text{mc},-})^{-\phi_1/\phi_2} \quad (26)$$

for $x \to -\infty$. One may devise simple interpolations that are exact for $x \to 0$ and $x \to \infty$. If, for instance, $u_1 > 0$ and u_2

> 0, we may consider the approximate expression

$$\frac{T_c}{T_{O(3)}} - 1 \approx \left(\frac{u_1 + b u_2^{\phi_1/\phi_2}}{X_+} \right)^{1/\phi_1} - k_1 \lambda_1 - k_2 \lambda_2, \quad (27)$$

where $b = X_+ X_{\text{mc},+}^{-\phi_1/\phi_2}$. The functions $F_{\pm}(x)$ are crossover functions that interpolate between the two regimes, in which only one of the relevant operators is present. As far as the nature of the transition is concerned, the relevant quantity is the sign of u_1. In general, we expect that the transition belongs to different universality classes depending on the sign of u_1. For $u_1 = 0$, the leading relevant operator decouples and, thus, we obtain a MCP whose nature may depend on the sign of u_2.

The previous results apply to the three-dimensional model, but cannot be used directly in 2D, since in this case $T_{O(3)} = 0$ and the correlation-length exponent ν is not defined (the correlation length increases exponentially, as $\xi_s \sim e^{2\pi/T}$ for $\lambda = 0$). In order to investigate the two-dimensional case, let us consider again Hamiltonian (10); let us assume that $Q(S)$ renormalizes multiplicatively under RG transformations and that its RG dimension is 2 with logarithmic corrections (as we shall see, this is the case of interest). The perturbative analysis of the scaling behavior of the free energy is analogous to that presented in Ref. 29. The correct scaling variable is

$$Y = u_\lambda \left(\frac{T}{2\pi} \right)^p e^{4\pi/T} \sim u_\lambda \left(\frac{T}{2\pi} \right)^{p-2} \xi_s^2, \quad (28)$$

where we used Eq. (8), and p is a power that can be computed by using the one-loop expression of the anomalous dimension of Q. Then, the singular part of the free energy is given by

$$\mathcal{F}_{\text{sing}} \approx \xi_s^{-2} B(Y). \quad (29)$$

The critical line is again characterized by $Y = Y_{\pm}$, i.e., by

$$\lambda \left(\frac{T_c}{2\pi} \right)^p e^{4\pi/T_c} = Y_{\pm}, \quad (30)$$

with $Y_+ > 0$ and $Y_- < 0$. Solving this equation for T_c, we obtain

$$T_c = \frac{4\pi}{\ln(Y_{\pm}/\lambda)} \left[1 - p \frac{\ln \frac{1}{2} \ln(Y_{\pm}/\lambda)}{\ln(Y_{\pm}/\lambda)} + \cdots \right]. \quad (31)$$

The case of two relevant perturbations can be treated analogously. We define two scaling variables Y_1 and Y_2 as

$$Y_i = u_i \left(\frac{T}{2\pi} \right)^{p_i} e^{4\pi/T}, \quad i = 1, 2, \quad (32)$$

and write the free energy as

$$\mathcal{F}_{\text{sing}} = \xi_s^{-2} B(Y_1, Y_2). \quad (33)$$

If $p_1 < p_2$, the critical behavior depends on the sign of u_1: For $u_1 > 0$ and $u_1 < 0$, one obtains different critical behaviors. In the limit in which Y_2 is small and can be neglected, we can write

$$T_c = \frac{4\pi}{\ln(Y_\pm/u_1)}\left[1 - p_1\frac{\ln\frac{1}{2}\ln(Y_\pm/u_1)}{\ln(Y_\pm/u_1)}\right], \quad (34)$$

where $Y_\pm$ are two constants such that $Y_+ > 0$ and $Y_- < 0$. As observed in the three-dimensional case, Eq. (34) [it is the analog of Eqs. (22) and (23)] holds only if Y_2 can be neglected. Since

$$Y_2 = \frac{u_2}{u_1}Y_1\left(\frac{T}{2\pi}\right)^{p_2-p_1} \approx \frac{u_2}{u_1}Y_1\left[\frac{1}{2}\ln\left(\frac{Y_1}{u_1}\right)\right]^{p_1-p_2}, \quad (35)$$

Eq. (34) holds only in the parameter region in which

$$u_2 \ll u_1\left[\frac{1}{2}\ln\left(\frac{Y_\pm}{u_1}\right)\right]^{p_2-p_1}, \quad (36)$$

i.e., far from the MCP at $u_1 = 0$. For $|u_1| \to 0$, this region shrinks to zero and, thus, a correct formula requires the full crossover function.

For $u_1 = 0$, we have a MCP at

$$T_c = \frac{4\pi}{\ln(Y_{mc,\pm}/u_2)}\left[1 - p_2\frac{\ln\frac{1}{2}\ln(Y_{mc,\pm}/u_2)}{\ln(Y_{mc,\pm}/u_2)}\right], \quad (37)$$

depending on the sign of u_2.

B. Effective Hamiltonians

In order to apply the results of the previous section to the *XXZ* model, let us now derive an effective ferromagnetic Hamiltonian for model (1). For this purpose, we consider the ferromagnetic Hamiltonian corresponding to Eq. (1) under the mapping (4),

$$\mathcal{H}_f = -\sum_{\langle nm \rangle}\vec{\sigma}_n \cdot \vec{\sigma}_m - A\sum_{\langle nm \rangle}\sigma_{n,z}\sigma_{m,z} + H\sum_n(-1)^{[n]}\sigma_{n,z}, \quad (38)$$

where we set $J = 1$ for convenience. We argue that Hamiltonian (38) is equivalent to the Hamiltonian

$$\mathcal{H}^* = -\sum_{\langle nm \rangle}\vec{\sigma}_n \cdot \vec{\sigma}_m + \sum_{l \geq 1}\alpha_l(T,h,a)\mathcal{O}_{2l}(\sigma), \quad (39)$$

where $\mathcal{O}_{2l}(\sigma)$ are the zero-momentum dimension-zero spin-$2l$ perturbations of the O(3) FP, $h \equiv H/T$, $a \equiv A/T$ (note that the partition function depends on h and a). The operators $\mathcal{O}_{2l}(\sigma)$ can be constructed starting from the symmetric traceless operators of degree $2l$, see, e.g., Ref. 30. Explicitly, for $l = 1, 2$, we have

$$\mathcal{O}_2(\sigma) = \sum_n\left(\sigma_{n,z}^2 - \frac{1}{3}\right),$$

$$\mathcal{O}_4(\sigma) = \sum_n\left(\sigma_{n,z}^4 - \frac{6}{7}\sigma_{n,z}^2 + \frac{3}{35}\right). \quad (40)$$

The functions $\alpha_l(T,h,a)$ are smooth and vanish for $h \to 0$ and $a \to 0$. It should be stressed that the two Hamiltonians are equivalent only for the computation of the leading critical behavior of long-distance quantities.

The equivalence of $\mathcal{H}_f$ and $\mathcal{H}^*$, for what concerns the critical behavior, can be justified on the basis of the results of

Ref. 10 obtained in the usual LGW approach. In the absence of anisotropy and magnetic field, i.e., for $A = H = 0$, model (1) is O(3) invariant and, thus, its critical behavior is described by the usual LGW Hamiltonian

$$\mathcal{H}_{\Phi^4} = \int d^dx\left[\frac{1}{2}\sum_\mu(\partial_\mu\Phi)^2 + \frac{r}{2}\Phi^2 + \frac{u}{4!}\Phi^4\right], \quad (41)$$

where $\vec{\Phi}$ is a three-component vector. The magnetic field and the anisotropy break the O(3) invariance. If we define $\vec{\Phi} = (\vec{\phi}, \varphi)$, where $\vec{\phi}$ is a two-component vector and φ a scalar, the LGW Hamiltonian (3) corresponding to Eq. (1) can be written as[10]

$$\mathcal{H} = H_{\Phi^4} + \int d^dx[f_{22}P_{22} + f_{42}P_{42} + f_{44}P_{44}], \quad (42)$$

where

$$P_{22} = \varphi^2 - \frac{1}{3}\Phi^2,$$

$$P_{42} = \Phi^2 P_{22}, \quad (43)$$

$$P_{44} = \varphi^4 - \frac{6}{7}\Phi^2\varphi^2 + \frac{3}{35}(\Phi^2)^2,$$

and f_{ij} are coupling constants depending on a, h^2, and T. We have introduced here the homogeneous polynomial P_{ml}. The polynomial P_{ll} has degree l and transforms irreducibly as a spin-l representation of the O(3) group.[31] Polynomials P_{ml}, $m > l$, are defined as $P_{ml} \equiv (\Phi^2)^{(m-l)/2}P_{ll}$. The classification of the zero-momentum perturbations in terms of spin values is particularly convenient, since polynomials with different spins do not mix under RG transformations and the RG dimensions y_{ml} do not depend on the particular component of the spin-l representation. We refer to Ref. 8 for details. Thus, in the LGW approach, the O(3) Hamiltonian is perturbed by spin-2 and spin-4 perturbations. If one considers higher powers of the fields, also spin-6, spin-8,…, perturbations appear. They are irrelevant in 3D and can, thus, be neglected. In 2D, instead, they should be kept into account, since the field Φ is dimensionless and any polynomial of the fields is relevant.[32]

C. Three-dimensional behavior

In 3D, the critical behavior is well known:

(i) In the absence of anisotropy, i.e., for $A = 0$, there is an *XY* critical line $T_{XY}(H)$ ending at the O(3) critical point for $H = 0$. The phase diagram is symmetric under $H \to -H$.

(ii) In the absence of magnetic field, i.e., for $H = 0$, there are two critical lines: an *XY* critical line for $A < 0$ and an Ising critical line for $A > 0$, which meet at the O(3) critical point as $A \to 0$.

(iii) If A and H are both present, one observes two different phase diagrams depending on the sign of A. If A is negative, there is an *XY* transition. If A is positive, there is an Ising critical line for small values of H and an *XY* critical line for large H; the two lines meet at a MCP corresponding to a nonvanishing value of H.
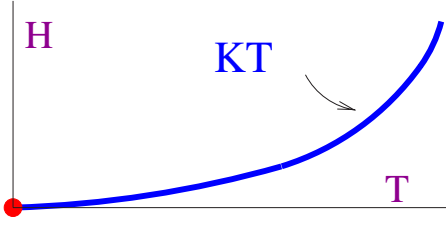
FIG. 5. (Color online) Phase diagram of isotropic antiferromagnets in the T-H plane ($A=0$).

We wish now to determine the dependence of the critical temperatures on A and H close to the O(3) point. For this purpose, we investigate the relevance of the perturbations. In 3D, we expect that only polynomials of degree 2 or 4 are relevant. Thus, P_{22}, P_{42}, and P_{44} are the only quantities that should be considered. The RG analysis is reported in Ref. 8 and indicates that P_{42} is irrelevant, while P_{22} and P_{44} are relevant. Perturbative FT calculations provide estimates of the corresponding RG dimensions:[8,33] $y_{22} \approx 1.79$, $y_{44} \approx 0.01$, and $y_{42} \approx -0.55$. The relevant scaling fields are $u_1 = a + c_1 h^2$ associated with P_{22} and $u_2 = a + c_2 h^2$ associated with P_{44}. The scaling fields depend on h^2, because of the symmetry under $H \rightarrow -H$ transformations. Since P_{22} is the most relevant operator, the critical behavior depends on the sign of u_1. We obtain XY behavior for $a + c_1 h^2 < 0$ and Ising behavior for $a + c_1 h^2 > 0$. Since for $A=0$ only the XY transition is observed, the constant c_1 must be negative. Hence, Ising behavior can only be observed if a is positive and h^2 is not too large, in agreement with experiments. The critical temperatures behave as

$$T_{c,XY} - T_{O(3)} = b_{XY}(-a - c_1 h^2)^{1/\phi_{22}} - k_1 a - k_2 h^2,$$

$$T_{c,\text{Is}} - T_{O(3)} = b_{\text{Is}}(a + c_1 h^2)^{1/\phi_{22}} - k_1 a - k_2 h^2, \quad (44)$$

where b_{XY}, b_{Is}, k_1, and k_2 are constants, with $b_{XY} > 0$ and $b_{\text{Is}} > 0$. Here,[8] $\phi_{22} = 1.260(11)$ and $1/\phi_{22} = 0.794(7)$.

Multicritical behavior is observed for $a = -c_1 h^2$. Note that, since c_1 is negative, this equality can only occur for $a > 0$. Since $1/\phi_{44} \gtrsim 100$, the leading nonanalytic term with exponent $1/\phi_{44}$ cannot be observed in practice, and therefore,

$$T_{c,\text{MC}} - T_{O(3)} = -k_1 a - k_2 h^2. \quad (45)$$

D. Two-dimensional behavior

The critical behavior in 2D is analogous to that observed in 3D. For $A < 0$, there is an XY KT transition for any H, while for $A > 0$, there is an Ising transition for small $|H|$, an XY transition for large $|H|$, and a MCP in between. The phase diagram in the two limiting cases $A=0$ and $H=0$ is reported in Figs. 5 and 6.

To compute the position of the critical point, we should investigate the relevance of the perturbations P_{ml}. As shown in Ref. 32, in 2D, any spin-l perturbation P_{ll} is relevant at the O(3) FP, since the corresponding RG dimension y_{ll} is positive: $y_{ll} = 2$ apart from logarithms which can be computed by using perturbation theory. One can also argue that perturba-
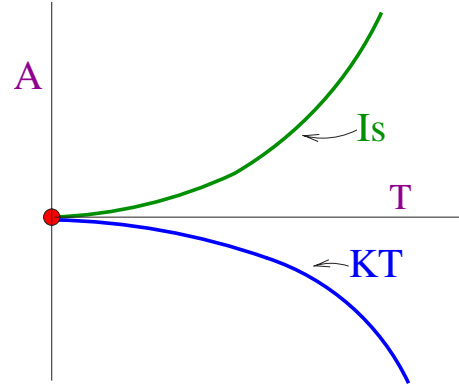

FIG. 6. (Color online) Phase diagram of anisotropic antiferromagnets in the T-A plane for $H=0$.

tions P_{ml} with $m > l$ can be neglected. Indeed, spin waves, which are rotations of the spins, are the critical modes of the ferromagnetic O(3) model. Changes in the size of the field Φ should not be critical. Therefore, $P_{ml} \equiv (\Phi^2)^{(m-l)/2} P_{ll}$ should be equivalent to $(\Phi_0^2)^{(m-l)/2} P_{ll} \sim P_{ll}$, where Φ_0^2 is the average of Φ^2. Thus, one should only consider the operators P_{ll}. Equation (39) then follows immediately. The equivalence of model (1) with Hamiltonian (39) was already conjectured in Ref. 34, even though there only the leading spin-2 term was explicitly considered.

The relevant scaling variables are

$$Y_{2l} = u_l \left(\frac{T}{2\pi} \right)^{l(2l+1)+2} e^{4\pi/T}, \quad (46)$$

which are associated with the spin-$2l$ perturbation. The power $l(2l+1)+2$ of T, which is universal, has been determined by using the perturbative results of Ref. 32, which provide the anomalous dimension of any zero-dimension spin-l perturbation of the 2D N-vector model. The scaling fields u_l are linear combinations of the parameters that break the O(3) invariance. As before, we write them as $u_l = a + c_l h^2$. As a consequence, the free energy can be written as

$$\mathcal{F}_{\text{sing}} \approx \xi^{-2} \hat{F}(Y_2, Y_4, \dots). \quad (47)$$

Note that different powers of T appear in definition (46). The most relevant term for $T \rightarrow 0$ corresponds to the spin-2 operator, since $Y_{2l} \sim Y_2 T^{l(2l+1)-3}$ and $l(2l+1)-3$ is positive for $l \geq 2$. Next, one should consider the spin-4 scaling variable Y_4. If one considers the scaling limit at fixed $Y_2 \neq 0$ or $Y_4 \neq 0$, the higher-order spin variables go to zero as $T \rightarrow 0$ and, thus, represent corrections to scaling proportional to powers of T. Thus, in the scaling limit one can neglect $Y_6, Y_8, \dots$, and write

$$\mathcal{F}_{\text{sing}} \approx \xi^{-2} F_2(Y_2, Y_4), \quad (48)$$

which coincides with Eq. (33). We can thus use the above-obtained results.

(i) For $u_1 < 0$, i.e., $a + c_1 h^2 < 0$, there is a KT transition at

$$T_{c,XY} = \frac{4\pi}{\ln(Y_{XY}/u_1)}\left[1 - 5\frac{\ln\frac{1}{2}\ln(Y_{XY}/u_1)}{\ln(Y_{XY}/u_1)}\right], \quad (49)$$

where $Y_{XY}<0$. Note that the occurrence of an *XY* transition for $a=0$ implies $c_1<0$ as in the three-dimensional case.

(ii) For $u_1>0$, i.e., $a+c_1h^2>0$, there is an Ising transition at

$$T_{c,Is} = \frac{4\pi}{\ln(Y_{Is}/u_1)}\left[1 - 5\frac{\ln\frac{1}{2}\ln(Y_{Is}/u_1)}{\ln(Y_{Is}/u_1)}\right], \quad (50)$$

where $Y_{Is}>0$. Since $c_1<0$, this transition can only occur for $a>0$ and small h^2.

(iii) For $u_1=0$, i.e., $a+c_1h^2=0$, there is a MCP at

$$T_{c,MC} = \frac{4\pi}{\ln(Y_{MC}/h^2)}\left[1 - 12\frac{\ln\frac{1}{2}\ln(Y_{MC}/h^2)}{\ln(Y_{MC}/h^2)}\right], \quad (51)$$

where $Y_{MC}>0$. Note that since the MCP occurs for $a=-c_1h^2$, we can replace $u_2=a+c_2h^2$ simply with h^2.

Note that, as discussed before, Eqs. (49) and (50) are valid only as long as condition (36) is satisfied, i.e., far from the MCP $u_1=0$.

IV. DISCUSSION AND CONCLUSIONS

In Sec. III D, we discussed the behavior of the classical two-dimensional *XXZ* model (1) on a square lattice in the presence of a magnetic field along the easy axis, for A and H small, focusing on the dependence of the critical temperature on A and H. In this section, we wish to discuss the possible scenarios for the nature of the MCP.

First, we exclude the possibility that the MCP is O(3) symmetric and located at $T=0$, as shown on the bottom in Fig. 4. This is implicit in the results of Sec. III D, but we wish to present here an extended discussion. There are essentially two observations that exclude an O(3) MCP.

(i) For $T=0$, the *XXZ* model (1) on a square lattice can be easily solved.[12,17] At fixed $A>0$, one finds two critical values of the magnetic field:

$$H_{c1} = 4J\sqrt{2A + A^2},$$
$$H_{c2} = 4J(2 + A). \quad (52)$$

For $|H|<H_{c1}$, the system is in a fully aligned antiferromagnetic configuration; for $H_{c1}<|H|<H_{c2}$, the system is in a spin-flop configuration; while for $|H|>H_{c2}$, all spins are aligned with the magnetic field. The spin-flop transition at $|H|=H_{c1}$ is of first order, since the order parameter, the staggered magnetization, has a discontinuity. If the transition were at $T=0$, the MCP should coincide with the spin-flop point $|H|=H_{c1}$. Thus, the magnetization, the susceptibility, and all critical quantities would have a discontinuity at $T=0$ when varying H. It is unclear how an O(3) critical behavior might be consistent with this discontinuity. On the other hand, the first-order behavior at $T=0$ is consistent with the existence of a first-order spin-flop line.

(2) The second objection is based on the LGW analysis presented in Sec. III B. The O(3) FP is unstable under an infinite number of perturbations. Thus, an infinite number of tunings is needed to recover the O(3) symmetry.

On the basis of these remarks, a phase diagram with a zero-temperature O(3)-symmetric MCP, as put forward in some analyses[5,16] of experimental and numerical MC results, appears untenable. These conclusions are analogous to those that hold in 3D.[8,9] It should be noted that in 2D the argument is much stronger. While in 3D these conclusions are based on the numerical determination of the RG dimension of the spin-4 perturbation, in 2D they follow from the relevance of the spin-*l* perturbations, which is an *exact* result. Moreover, while in 3D the O(3) behavior can be obtained by tuning a single additional parameter in such a way as to decouple both the spin-2 and spin-4 operators, in 2D the O(3) behavior can never be obtained at finite A, since an infinite number of tunings is needed.

Since the two-dimensional MCP cannot have O(3) symmetry, its nature is an open problem. We can show that the decoupled FP, corresponding to a multicritical behavior in which the two order parameters are effectively uncoupled, is stable. The stability of the decoupled FP can be proven by nonperturbative arguments.[35] Indeed, the RG dimension y_w of the operator $\Phi_1^2\Phi_2^2$ that couples the two order parameters in the LGW theory (3) is given by

$$y_w = \frac{1}{\nu_{KT}} + \frac{1}{\nu_{Is}} - 2 = -1 < 0, \quad (53)$$

since $\nu_{KT}=\infty$ and $\nu_{Is}=1$. Therefore, the perturbation is irrelevant and the decoupled FP is stable. Note that a decoupled MCP is always tetracritical, as in Fig. 2.

The stability of the decoupled FP and the instability of the O(3) FP are also consistent with some general arguments.[36] At a MCP, the exponent η describing the critical behavior of the correlation function of the order parameter is replaced by a matrix η_{ij}, see, e.g., Ref. 10. The conjecture of Ref. 36 states that Tr η should have a maximum at the stable FP. This indeed occurs in the present case: at the decoupled FP, we have Tr $\eta=3/4$, while at the O(3) FP, Tr $\eta=0$.

In Fig. 7, we show a plausible phase diagram, with three transition lines: a spin-flop first-order transition line, an Ising line, and a KT critical line. The phase diagram inside the blob is an open issue. Some possibilities are shown in Fig. 8:

(1) Figure 8(a) presents a bicritical point, which may be associated with a stable biconal FP with symmetry $\mathbb{Z}_2 \oplus O(2)$, whose attraction domain is in the bicritical region of the bare parameters of the LGW Φ^4 theory. We should say that we do not have any evidence for the existence of such a FP.

(2) In Fig. 8(b), we show a tetracritical point, where the Ising and KT lines intersect each other. In this case, the MCP may be controlled by the stable decoupled FP discussed above.

(3) In Fig. 8(c), the transition at the MCP is of first order. Starting from the MCP, the first-order transitions extend up to tricritical points, where the Ising and KT critical lines start. This occurs if the system is outside the attraction domain of the stable FP of the RG flow. This is the phase diagram expected in 3D and shown in Fig. 3.
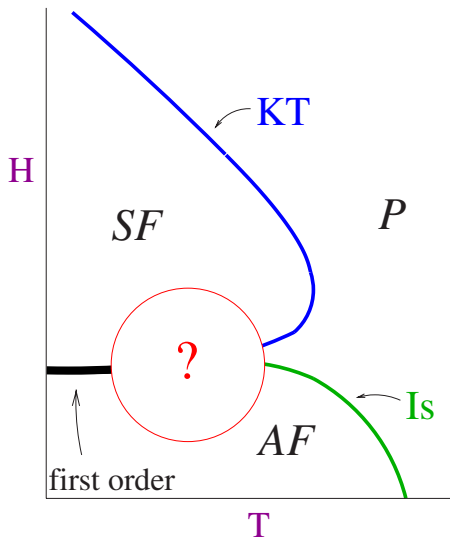
FIG. 7. (Color online) Phase diagram in the T-H plane in the presence of uniaxial anisotropy $A > 0$. See Fig. 4 for the explanation of the symbols.

FIG. 8. (Color online) Some possible phase diagrams inside the blob appearing in Fig. 7.

(4) Finally, we cannot exclude phase diagrams like those shown in Figs. 8(d) and 8(e). Figure 8(d) is apparently observed in antiferromagnets with single-ion anisotropy and more than nearest-neighbor interactions,[37] and also in hard-core boson systems,[21] which are equivalent to anisotropic spin-1/2 *XXZ* systems in a magnetic field.
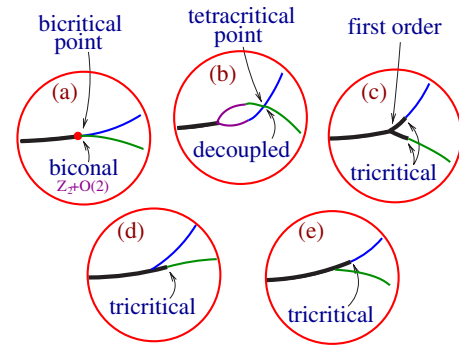
Of course, further experimental and theoretical investigations are called for to conclusively settle this issue.

We finally mention that the results presented here are expected to apply to the *XXZ* model on generic bipartite lattices. On the other hand, the *XXZ* model (1) on a triangular lattice or on a stacked triangular lattice (and, more generally, on lattices that are not bipartite) is expected to show a different multicritical behavior, essentially because of frustration. Reference 38 reports a study of the possible phase diagrams in the mean-field approximation and a FT study of the three-dimensional RG flow.

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