

Quantum phase transitions and thermodynamic properties in highly anisotropic magnets

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The systems exhibiting quantum phase transitions (QPT) are investigated within the Ising model in the transverse field and Heisenberg model with easy-plane single-site anisotropy. Near QPT a correspondence between parameters of these models and of the quantum ϕ^4 model is established. A scaling analysis is performed for the ground-state properties. The influence of the external “longitudinal” magnetic field on the ground-state properties is investigated, and the corresponding magnetic susceptibility is calculated. Finite-temperature properties are considered with the use of the scaling analysis for the effective classical model proposed by Sachdev. Analytical results for the ordering temperature and temperature dependences of the magnetization and energy gap are obtained in the case of a small ground-state moment. The forms of dependences of observable quantities on the bare splitting (or magnetic field) and renormalized splitting turn out to be different. A comparison with numerical calculations and experimental data on systems demonstrating magnetic and structural transitions (e.g., into a singlet state) is performed. [S0163-1829(98)09329-1]

I. INTRODUCTION

The interest in quantum models of anisotropic spin and pseudospin systems is connected with what they describe as miscellaneous magnetic and structural transitions. Examples of such transitions are transitions into singlet magnetic state in TbSb, Pr, Pr₃Tl (see Ref. 1 and references therein), NiSi₂F₆ (see, e.g., Ref. 2), and orientational and metamagnetic phase transitions under magnetic field.^{3,4}

The simplest model for the systems demonstrating a ground-state quantum phase transition (QPT) is the Ising model in the transverse field. This model is convenient for description of structural transitions in quantum crystals.⁵⁻⁷ It can also be applied to describe magnetic systems where both lowest and next energy levels are singlets. A more complicated first-principles model for spin systems in a strong crystal field is the Heisenberg model with an easy-plane single-site anisotropy; it is applicable in the case where the next-to-lowest energy level is a doublet. As well as the transverse-field Ising model, this model also demonstrates a QPT (the ground-state magnetization vanishes with increasing the anisotropy parameter).

A number of approximate methods were applied to study the transverse-field Ising model⁸⁻¹⁸ at $d > 1$ and the Heisenberg model with easy-axis anisotropy.¹⁹⁻²³ However, most of these methods (except for numerical ones) are applicable only not too close to the QPT. In particular, they lead to Gaussian values of the QPT critical exponents. Thus analytical consideration of the ground-state and finite-temperature properties in the vicinity of the QPT is still an open problem.

The case where the system is close to the QPT is characterized by a small ground-state moment and low transition temperature. Such a situation is reminiscent of weak itinerant magnets.²⁴ An analysis of the ground-state QPT was performed in Refs. 25,26. It was shown that the upper critical dimensionality for such transitions is $d_c^+ = 4 - z$ with z being the dynamical critical exponent. This conclusion has a general character. In the present paper we consider only systems with $z = 1$, which holds for the transverse-field Ising model

and anisotropy-induced QPT in the Heisenberg model. (Note that this is not the case for the QPT induced by magnetic field in degenerate systems with a $n > 1$ component order parameter since here $z = 2$, see Ref. 27.) Thus for $d \geq 3$ the critical exponents are the Gaussian ones, while for $d < 3$ they deviate from the corresponding mean-field values and can be calculated with the use of the $3 - \varepsilon$ expansion. For the critical dimensionality $d = 3$ the ground-state properties contain logarithmic corrections.

Sachdev²⁸ proposed a three-stage method of treating finite-temperature properties of the systems near the QPT. At the first stage, ground-state renormalizations are performed. At the second stage, the nonzero Matsubara frequencies are integrated out to obtain an effective classical action. Finally, perturbation theory for the effective classical model is applied. This method ensures correct analytical properties of the resulting theory. While ground-state renormalizations are nonuniversal, finite-temperature properties, being expressed through quantum-renormalized ground-state parameters, turn out to be universal.

The approach of Ref. 28 is based on a continuum model, namely, the quantum ϕ^4 model. This model is sufficient to express finite-temperature properties near the QPT through the nonuniversal ground-state properties, but insufficient to obtain correct results for the latter properties. A convenient method to consider the lattice spin systems near their critical dimensionality is the expansion in the formal quasiclassical parameter $1/S$. Its applicability is connected with the fact that near d_c the effective interaction of spin waves is small (except for a narrow critical region where the ε expansion can be easily developed to correct the description of the critical behavior). For the Heisenberg model such a situation occurs for temperature transition near the lower critical dimensionality $d_c^- = 2$. This provides for success of the renormalization-group (RG) approach for the description of thermodynamics of $d = 2$ (Ref. 29) and $d = 2 + \varepsilon$ (Refs. 30,29) Heisenberg magnets, and also quasi-two-dimensional (2D) and anisotropic 2D magnets³¹ not too close to T_c .

For the QPT in highly anisotropic spin systems the $1/S$ expansion works well near the *upper* critical dimensionality $d_c^+ = 3$. In this case there are excitations, which are almost gapless near the QPT (they are analogous to the spin-wave excitations in Heisenberg magnets). Besides that, for the ordered degenerate systems (with $n \geq 2$) there are always Goldstone modes with zero energy gap and the $1/S$ expansion becomes applicable at arbitrary anisotropy below its critical value. The situation is more complicated for finite temperatures, since close to the temperature transition the system behaves as a corresponding classical magnet and therefore the picture of excitation spectrum differs from that at $T=0$.

The aim of the present paper is to apply the above-discussed concepts for calculating ground-state and finite-temperature properties of the transverse-field Ising model ($n=1$) and Heisenberg model with strong easy-plane anisotropy ($n=2$). To this end we apply perturbation theory (which is in fact an expansion in $1/S$) to the original lattice models (not to their continuum analogs), which enables us to calculate nonuniversal ground-state quantum renormalizations. After that we combine perturbation results for short-wave fluctuations with the results of the $3-\varepsilon$ RG approach for the long-wave fluctuations to correct the results of perturbation theory. Finally, we consider finite-temperature properties within the RG approach for the effective continuum classical model.

The plan of the paper is as follows. In Sec. II we discuss the Ising model in the transverse field. We consider corresponding mean-field results, construct the perturbation theory in $1/S$, and apply a scaling approach to investigate ground-state and thermodynamic properties, in particular the influence of external magnetic field. In Sec. III the Heisenberg model with easy-plane anisotropy is considered in a similar way. In Sec. IV we discuss the results obtained and compare them with experimental data on systems exhibiting structural and magnetic transitions. Some details of calculations are presented in Appendixes.

II. TRANSVERSE-FIELD ISING MODEL

A. The formulation of the model and the mean-field approximation

We consider the Hamiltonian of the Ising model in the transverse field Ω

$$\mathcal{H} = -\frac{I}{2} \sum_{\langle ij \rangle} S_i^x S_j^x - \Omega \sum_i S_i^z, \quad (1)$$

where I is the exchange parameter. This model can describe singlet magnetic systems. A derivation of such a model for Heisenberg magnets with strong single-site anisotropy is presented in Appendix A. The model (1) also describes structural transition in quantum crystals (cooperative Jahn-Teller effect, see Ref. 7) where the two lowest energy levels are singlets. In this case $I = \Delta_2$, $\Omega = \Delta_1$, where $\Delta_{1,2}$ is the energy-level splitting at $T=0$ and $T > T_c$, respectively. For further purposes it will be useful to consider the model (1) for arbitrary values of (pseudo-) spin S .

At $\Omega=0$ the model (1) coincides with the Ising model and thus the order parameter $\bar{S} \equiv \langle S^x \rangle = S$ in the ground state.

With increasing Ω , model (1) demonstrates a quantum phase transition where \bar{S} vanishes. The one-dimensional $S=1/2$ transverse-field Ising model in the ground state can be solved rigorously.³² In particular, it can be reduced to the two-dimensional Ising problem at finite temperatures,³³ so that critical exponents for both the phase transitions coincide. The transverse-field Ising model with $d > 1$ requires approximate methods.

The mean-field (MF) approximation^{6,8} yields the critical field $\Omega_0 \equiv I_0 S$, and the equation for the order parameter at $\Omega < \Omega_0$ reads

$$\frac{\Omega_0}{H_e} B_S(H_e/T) = 1, \quad (2)$$

where

$$B_S(x) = (1 + 1/2S) \coth(1 + 1/2S)x - (1/2S) \coth(x/2S),$$

$$B_{1/2}(x) = (1/2) \tanh(x/2), \quad (3)$$

is the Brillouin function, $H_e = (\Omega^2 + \Omega_0^2 \bar{S}^2 / S^2)^{1/2}$, $I_0 = 2Id$. Owing to the field Ω , the value of $\langle S^z \rangle$ is finite in both ordered and disordered phase and reads

$$\langle S^z \rangle = \frac{\Omega S}{H_e} B_S(H_e/T). \quad (4)$$

It should be noted that at $\Omega < \Omega_0$ we have simply $\langle S^z \rangle = S\Omega/\Omega_0$. The critical temperature where \bar{S} vanishes is determined for the physically important case $S=1/2$ by

$$T_c^{\text{MF}} = \frac{\Omega}{2 \tanh^{-1}(\Omega/\Omega_0)} \simeq \frac{\Omega}{\ln[2/(1 - \Omega/\Omega_0)]} \quad (5)$$

(the last approximation is valid for $1 - \Omega/\Omega_0 \ll 1$). Thus the MF theory predicts a very weak inverse-logarithmic dependence for the critical temperature near the QPT in arbitrary dimensionality. This contradicts the results of the scaling approach^{26,28} both above and below the upper critical dimensionality $d_c^+ = 3$.

To improve the MF approximation, one has to take into account the collective excitations which are analogous to spin-wave excitations in Heisenberg magnets. The spectrum of these excitations in the random-phase approximation has the form⁶

$$E_{\mathbf{q}}^2 = \Omega[\Omega - I_{\mathbf{q}} \langle S^z \rangle] + I_0^2 \bar{S}^2 \quad (6)$$

in both ordered and disordered phases. Near the QPT [$\bar{S}(T=0) \ll 1$], these excitations become almost gapless and give dominant contributions to physical properties.

The result of account of the collective excitations to first order in $1/\mathcal{R}$ (where \mathcal{R} is the radius of exchange interaction)¹⁵ for $d=3$ reads

$$T_c \sim \mathcal{R}^{3/2} \sqrt{1 - \Omega/\Omega_0}. \quad (7)$$

This has a correct square-root behavior (see, e.g., Ref. 28). However, the logarithmic corrections, that occur for $d=3$, are not reproduced by the result (7). Besides that, the $1/\mathcal{R}$ expansion does not enable one to determine correctly the coefficient in Eq. (7) for not too large \mathcal{R} .

Another approach used in Ref. 11 is to consider the excitations (6) self-consistently within the random-phase-approximation (RPA) decoupling scheme for the sequence of equations of motion. Unlike the $1/\mathcal{R}$ expansion, this procedure gives the possibility of taking into account the reaction of the RPA excitation spectrum (6) on the deviation of the critical field from Ω_0 . Corrections to mean-field ground-state parameters turn out to be small enough, but at finite temperatures the RPA magnetization shows a double-value behavior with first-order temperature phase transition. Authors of Ref. 11 consider also a generalization of RPA, the two-site self-consistent approximation (TSCA) which gives the possibility of including partially correlation effects. This approximation gives more satisfactory results than RPA. However, it predicts first-order character not only for the temperature transition, but also for the QPT.

One should mention also the papers^{12,13} where high-temperature series expansions (HTSE) and ground-state perturbation theory (GSPT) were used. Although these expansions gives consistent results for the critical field, their applicability near the QPT is questionable. Recently some results of GSPT and HTSE have been confirmed by numerical correlated-basis-function analysis.^{17,18}

Below we use the $1/S$ expansion to treat ground-state and finite-temperature properties of the transverse-field Ising model. Unlike the $1/\mathcal{R}$ expansion, it takes into account the ‘‘spin-wave’’ excitations already in the zeroth-order of perturbation theory. Contrary to the RPA,¹¹ this is a systematic expansion, and therefore scaling corrections can be easily calculated. It should be also noted that the $1/S$ expansion differs from the ground-state perturbation theory used in Ref. 13 where the expansions in powers of Ω/I and I/Ω are used for the ordered and disordered phases, respectively. Indeed, the $1/S$ expansion treats both the terms in the Hamiltonian (1) on equal footing and thus yields physically correct results already in the first order in $1/S$.

B. Ground-state properties within the $1/S$ perturbation theory

To construct perturbation expansion in a convenient form we use the spin coherent-state approach.³⁴ The partition function is presented in terms of a path integral,

$$\mathcal{Z} = \int D\boldsymbol{\pi} \exp[-(\mathcal{S}_{\text{dyn}} + \mathcal{S}_{\text{st}})], \quad (8)$$

where

$$\begin{aligned} \mathcal{S}_{\text{dyn}} &= iS \sum_i \int_0^{1/T} d\tau (1 - \cos \vartheta_i) \frac{\partial \varphi_i}{\partial \tau}, \\ \mathcal{S}_{\text{st}} &= - \int_0^{1/T} d\tau \left[\frac{IS^2}{2} \sum_{\langle ij \rangle} \pi_{xi} \pi_{xj} + \Omega S \sum_i \pi_{zi} \right], \end{aligned} \quad (9)$$

are static and dynamic parts of the action, $\boldsymbol{\pi}_i = \{\pi_{xi}, \pi_{yi}, \pi_{zi}\}$ is a three-component vector field with $\pi_i^2 = 1 + 1/S$, ϑ_i and φ_i are the polar and azimuthal angles of $\boldsymbol{\pi}_i$ in an arbitrarily chosen coordinate system (which does not need to coincide with the $\pi_x - \pi_y - \pi_z$ coordinate system). Further we additionally rotate the coordinate system through the angle θ determined by

$$\sin \theta = \langle \pi_x \rangle / \langle |\boldsymbol{\pi}| \rangle \quad (10)$$

around the π_y axis (in the disordered phase $\theta=0$ and the rotated coordinate system coincides with the original one).

The calculation of the two-point vertex function $\Gamma(\mathbf{q}, \omega)$ of the fields $\tilde{\pi}_x, \tilde{\pi}_y$ (the tilde sign is referred to the rotated coordinate system), which is connected with matrix Green's function G of these fields by the relation $\Gamma(\mathbf{q}, \omega) = G^{-1}(\mathbf{q}, \omega)$, is performed for both ordered and disordered phases in Appendix B and yields to first order in $1/S$ the result

$$\begin{aligned} \Gamma_{\pm}(\mathbf{q}, \omega_n) &= \begin{pmatrix} S^2(I_0 - I_{\mathbf{q}} + I_0 \Delta_{\pm}^2) & iS\omega_n(w_S + X_0/2 + Y_0/2) \\ iS\omega_n(w_S + X_0/2 + Y_0/2) & I_0 S^2 D_{\pm} \end{pmatrix}, \end{aligned} \quad (11)$$

where $w_S = (1 + 1/2S)^{-1}$,

$$X_0 = \frac{1}{2S} \sum_{\mathbf{q}} \frac{1}{\sqrt{1 - I_{\mathbf{q}}/I_0}}, \quad Y_0 = \frac{1}{2S} \sum_{\mathbf{q}} \sqrt{1 - I_{\mathbf{q}}/I_0}, \quad (12)$$

Δ_{\pm} and D_{\pm} are the dimensionless temperature-dependent energy gap and the renormalization factor for the exchange parameter in the disordered and ordered phases, respectively, their concrete expressions being specified below. The matrix static uniform spin susceptibility in the rotated coordinate system is expressed in terms of Γ as

$$\tilde{\chi}^{ij} = S^2 \Gamma_{ij}^{-1}(0,0), \quad (13)$$

where $i, j = x, y$. The renormalized spin-wave spectrum is determined by the condition $\det \Gamma(\mathbf{q}, -iE_{\mathbf{q}}) = 0$ and has the form

$$\tilde{E}_{\mathbf{q}} = S[1 + 1/2S - (X_0 + Y_0)/2] \sqrt{I_0 D_{\pm}(I_0 - I_{\mathbf{q}} + I_0 \Delta_{\pm}^2)}. \quad (14)$$

The quantum-renormalized critical field Ω_c is given by

$$\frac{\Omega_c}{I_0} = 1 + \frac{1}{2S} - \frac{1}{4S} \sum_{\mathbf{q}} \frac{2I_0 + I_{\mathbf{q}}}{\sqrt{I_0(I_0 - I_{\mathbf{q}})}}. \quad (15)$$

The last two terms in this expression yield the first-order $1/S$ correction to the mean-field value of Ω_c . For $S=1/2$ the numerical calculation of the integral in Eq. (15) yields the result $\Omega_c = 2.44I$ in the 3D case and $\Omega_c = 1.10I$ in the 2D case. Thus the critical field is strongly renormalized by quantum fluctuations both in the 3D and 2D cases. The critical field values obtained are considerably smaller than the corresponding RPA results,¹¹ $\Omega_c = 2.88I$ and $\Omega_c = 1.83I$, and somewhat smaller than those obtained by HTSE (Ref. 12) and GSPT,¹³ $\Omega_c = 2.58I$ and $\Omega_c = 1.54I$. This demonstrates that the considered first-order $1/S$ perturbation theory overestimates the effects of quantum fluctuations (especially in the 2D case), but treats these fluctuations more correctly than RPA.

In the disordered phase with $\langle \pi_x \rangle = 0$ ($\Omega > \Omega_c$) the expressions for the ground-state energy gap and factor D_{\pm} have the form

$$\Delta_+^2(t_+,0) = \frac{t_+}{1-t_+} (1-X'_0)[1+A_+(t_+)],$$

$$A_+(t) = \frac{1}{4St} \sum_{\mathbf{q}} \left\{ \frac{2I_0+I_{\mathbf{q}}(1+t)}{\sqrt{I_0[I_0-I_{\mathbf{q}}(1-t)]}} - \frac{2I_0+I_{\mathbf{q}}}{\sqrt{I_0(I_0-I_{\mathbf{q}})}} \right\}, \quad (16)$$

and

$$D_+(t_+) = \frac{1+Y_0-X_0}{1-t_+} [1+t_+A_+(t_+)], \quad (17)$$

where

$$t_+ = 1 - \Omega_c/\Omega \quad (18)$$

and

$$X'_0 = \frac{1}{2S} \sum_{\mathbf{q}} \frac{I_{\mathbf{q}}}{\sqrt{I_0(I_0-I_{\mathbf{q}})}}.$$

In the ordered phase ($\Omega < \Omega_c$) we obtain

$$\Delta_-^2(t_-,0) = t_- (1-X'_0)[1+A_-(t_-)],$$

$$A_-(t) = -2(1-t)A_+(t) - \frac{1-t}{8S} \sum_{\mathbf{q}} \frac{[2I_0+I_{\mathbf{q}}(1+t)]^2}{I_0^{1/2}[I_0-(1-t)I_{\mathbf{q}}]^{3/2}}, \quad (19)$$

and

$$D_-(t_-) = 1+Y_0-X_0, \quad (20)$$

where

$$t_- = 1 - (\Omega/\Omega_c)^2. \quad (21)$$

Consider now the observable quantities. The expression for the order parameter $\bar{S}(t_-,T) \equiv S\langle \pi_x \rangle$ at $T=0$, $\Omega < \Omega_c$ reads

$$\bar{S}(t_-,0) = St_-^{1/2} [1+B(t_-)]^{1/2} [1+1/2S - (X_0+Y_0)/2],$$

$$B(t) = -2(1-t)A_+(t). \quad (22)$$

In the limiting case of zero transverse field we have the trivial result $\bar{S}=S$, and the energy spectrum reduces to its mean-field form, $\tilde{E}_{\mathbf{q}} = \Omega_0$. At very large $\Omega \gg \Omega_c$ we reproduce again the mean-field result $\tilde{E}_{\mathbf{q}} = \Omega$. This is a consequence of the fact that in both the limits $\Omega=0$ and $\Omega \rightarrow \infty$ quantum fluctuations are absent. Thus the $1/S$ expansion gives the possibility of obtaining the correct values of the ground-state parameters for an arbitrary $\Omega \geq 0$, except for the region $\Omega \approx \Omega_c$ where the quantum fluctuations are strong enough to modify considerably the results. A more detailed consideration of this region will be performed below in Sec. II D.

For the longitudinal susceptibility we have

$$\chi^{xx} = \cos^2 \theta \tilde{\chi}^{xx} + \sin \theta \cos \theta (\tilde{\chi}^{xz} + \tilde{\chi}^{zx}) + \sin^2 \theta \tilde{\chi}^{zz}, \quad (23)$$

where the tilde sign refers to susceptibilities in the rotated coordinate system (recall that for the disordered phase

$\theta=0$). For the ordered phase the first summand in Eq. (23) gives a dominant contribution near the QPT, and using the relation (13) yields in both the ordered phase near the QPT and disordered phase the expression for the ground-state spin susceptibility through the gap in the excitation spectrum

$$\chi^{xx} = \frac{1}{I_0 \Delta_{\pm}^2(t_{\pm},0)}. \quad (24)$$

C. Influence of longitudinal magnetic field

To consider the influence of the external magnetic field we add to the Hamiltonian the term

$$\Delta \mathcal{H} = -H \sum_i S_i^x. \quad (25)$$

The longitudinal magnetic field results in the appearance of nonzero $\langle S_i^x \rangle$ at any Ω/I . The influence of both transverse and external longitudinal fields is, of course, equivalent to applying one effective field which has the value $(H^2 + \Omega^2)^{1/2}$ and makes the angle $\arctan(H/\Omega)$ with the π_x axis. However, it is useful to consider these fields as two independent ones.

Performing the calculations which are similar to those of Sec. II B and Appendix B we obtain to first order in $1/S$ the equation for the angle θ of coordinate system rotation

$$\Omega - \Omega_0 r(\theta) \cos \theta - H \cot \theta = 0, \quad (26)$$

where

$$r(\theta) = 1 + \frac{1}{2S} - \frac{1}{4S} \sum_{\mathbf{q}} \frac{2(I_0+I_{\mathbf{q}})\varphi(\theta) - I_{\mathbf{q}} \cos^2 \theta}{\sqrt{I_0 \varphi(\theta) [I_0 \varphi(\theta) - I_{\mathbf{q}} \cos^2 \theta]}}, \quad (27)$$

with $\varphi(\theta) = \sin^2 \theta + (\Omega/\Omega_c) \cos \theta$. For a general Ω/Ω_c the solution of this equation is rather cumbersome. However, near the QPT (i.e., at $1 - \Omega/\Omega_c \ll 1$), where the angle θ is small, one can expand Eq. (26) in θ to obtain

$$\theta = \begin{cases} \theta_0 + H/2[I_0 S r(0) - \Omega], & \theta_H \ll \theta_0, \\ \theta_H + 2\delta r/3\theta_H, & \theta_0 \ll \theta_H \ll 1, \end{cases} \quad (28)$$

where $\theta_0 = \sqrt{2(1 - \Omega/\Omega_c)}$, $\theta_H = (2H/\Omega_c)^{1/3}$, and $\delta r = r(\theta_H) - r(0)$.

For the magnetization we derive

$$\bar{S} = \begin{cases} \bar{S}(H=0) + \chi^{xx} H, & \theta_H^2 \ll 1 - \Omega/\Omega_c, \\ \left(1 + \frac{1}{2S} - \frac{X_0+Y_0}{2}\right) \theta_H [1+B'(\theta_H^2)], & \\ 1 - \Omega/\Omega_c \ll \theta_H^2 \ll 1, & \end{cases} \quad (29)$$

where χ^{xx} is determined by Eq. (24), and

$$B'(\theta_H^2) = -\frac{1}{6S\theta_H^2} \sum_{\mathbf{q}} \left[\frac{2(I_0 + I_{\mathbf{q}})(1 + \theta_H^2/2) - I_{\mathbf{q}}(1 - \theta_H^2)}{\sqrt{I_0[I_0(1 + \theta_H^2) - I_{\mathbf{q}}(1 - \theta_H^2/2)]}} - \frac{2I_0 + I_{\mathbf{q}}}{\sqrt{I_0(I_0 - I_{\mathbf{q}})}} \right]. \quad (30)$$

The ground-state energy gap is given by

$$\Delta_-^2 = \begin{cases} \Delta_-^2(H=0), & \theta_H^2 \ll 1 - \Omega/\Omega_c, \\ \frac{3}{2} \theta_H^2 [1 + A'(\theta_H^2)], & 1 - \Omega/\Omega_c \ll \theta_H^2 \ll 1, \end{cases} \quad (31)$$

where

$$A'(\theta_H^2) = B'(\theta_H^2) - \frac{1}{12S} \sum_{\mathbf{q}} \frac{(I_0 + 2I_{\mathbf{q}})^2}{I_0^{1/2} [I_0(1 + \theta_H^2/2) - I_{\mathbf{q}}(1 - \theta_H^2)]^{3/2}}. \quad (32)$$

The longitudinal susceptibility in the presence of the magnetic field is still determined by Eq. (23), and again the first term gives main contribution near the QPT. Alternatively, the same result can be obtained by direct differentiation of \bar{S} [which is given by Eq. (29)] with respect to H .

D. Ground-state renormalizations near the QPT

The results of the $1/S$ expansion can be applied only at not too small t_{\pm} . Indeed, at $d \leq 3$ the functions A and B contain terms which are divergent at $t_{\pm} \rightarrow 0$ as $t_{\pm}^{(d-3)/2}$ (at $d=3$, logarithmic divergences are present). The same situation takes place for the functions A' and B' which are divergent as θ_H^{d-3} at $\theta_H \rightarrow 0$. Thus an $\varepsilon = 3 - d$ expansion can be developed within the RG approach to treat these divergences more correctly and to improve thereby the behavior of Δ_{\pm} and \bar{S} near the QPT. Further consideration of this section is related to the critical region $|1 - \Omega/\Omega_c| \ll 1$. However, as it will be clear below, the results can be extrapolated to arbitrary Ω , since in the limits $\Omega \ll \Omega_c$ and $\Omega \gg \Omega_c$ they are smoothly joined with the results of the $1/S$ expansion of Sec. II B.

First we pick up the nonuniversal factors from \bar{S} , Δ_{\pm} by introducing the quantities

$$\bar{S}_R(t, T) = [1 + 1/2S - (X_0 + Y_0)/2]^{-1} \bar{S}(t, T)/S, \\ \Delta_{\pm R}(t, T) = (1 - X'_0)^{-1} \Delta_{\pm}(t, T). \quad (33)$$

Consider the continuum limit of the above theory. The action $S = S_{\text{dyn}} + S_{\text{st}}$ in this limit takes the form

$$S_{\text{cont}} = \frac{1}{2} \int d^d r \int_0^{c/T} d\tau [2i \tilde{\pi}_x (\partial \tilde{\pi}_y / \partial \tau) + \tilde{\pi}_y^2 + (\nabla \tilde{\pi}_x)^2 + m^2 \tilde{\pi}_x^2] + \frac{u}{4!} \int d^d r \int_0^{c/T} d\tau \tilde{\pi}_x^4, \quad (34)$$

where the parameters u , m^2 , and c , determined in such a way, are given by

$$u_{\text{cont}} = 6d \frac{c_0}{IS^2} \zeta, \\ c_{\text{cont}} = c_0, \\ m_{\text{cont}}^2 = 2t_+ d, \quad (35)$$

$c_0 = (2d)^{1/2} IS$ being the bare spin-wave velocity, $\tilde{\pi}_x^2 = (IS^2/c_0) \pi_x^2$, $\tilde{\pi}_y^2 = (IS^2/c_0) \pi_y^2$ and the factor ζ ($\zeta = 1 - t_-$ in the ordered phase and $\zeta = 1$ in the disordered phase) is introduced to extend the region of applicability of results obtained to arbitrary t_{\pm} . Note that the coefficients for the first three terms of the quadratic part of Eq. (34) can always be chosen equal to their values in Eq. (34) by appropriate rescaling of $\pi_{x,y}$ and τ . The model (34) is completely equivalent to the quantum ϕ^4 model. Indeed, integrating out the field π_y we obtain

$$S_{\text{cont}} = \frac{1}{2} \int d^d r \int_0^{c/T} d\tau [(\partial \tilde{\pi}_x)^2 + m^2 \tilde{\pi}_x^2] + \frac{u}{4!} \int d^d r \int_0^{c/T} d\tau \tilde{\pi}_x^4. \quad (36)$$

The continuum representation (34) determines the way in which the original lattice model can be renormalized. Following the standard procedure³⁵ we introduce the renormalization factors Z_i^{\pm} for the ground-state parameters in the disordered and ordered phases by the relations

$$\pi_x = Z_x^{\pm} \pi_{xR}, \quad \pi_y = Z_y^{\pm} \pi_{yR}, \\ t_{\pm} = (Z_2^{\pm}/Z) t_{\pm R}, \quad g = (Z_4^{\pm}/Z^2) g_R, \quad (37)$$

where the indices R denote quantum-renormalized quantities,

$$g = K_{4-\varepsilon} L_{\varepsilon} \mu^{-\varepsilon} u_{\text{cont}} \quad (38)$$

is the coupling constant, μ is a parameter with the dimensionality of inverse length, $K_d = [2^{d-1} \pi^{d/2} \Gamma(d/2)]^{-1}$, and the factor $L_{\varepsilon} = \Gamma(1 + \varepsilon/2) \Gamma(1 - \varepsilon/2)$ [$\Gamma(z)$ is the Euler gamma function] ensures the applicability of the one-loop order results for not small ε .³⁶ For further treatment it is useful to represent the renormalization factors as

$$Z_i^{\pm} = Z_{Li}^{\pm}(g) Z_i^{\text{cont}}(g_R, \mu), \quad (39)$$

where Z_i^{cont} are the corresponding factors for the continuum model (34) that contain divergent terms (which are independent of lattice structure, etc.) and Z_{Li} all the others (lattice dependent) corrections. It is important that the factors Z_{Li} do not contain divergences.

The expressions for Z factors in the continuum model (34) are well known (see, e.g., Ref. 35). We use the cutoff scheme with cutting integrals over quasimomentum at Λ . Then to one-loop order we have

$$\begin{aligned}
Z_x^{\text{cont}} &= Z_y^{\text{cont}} = 1 + \mathcal{O}(g_R^2), \\
Z_2^{\text{cont}} &= 1 + \frac{g_R}{2\varepsilon} \left(1 - \frac{\mu^\varepsilon}{\Lambda^\varepsilon} \right), \\
Z_4^{\text{cont}} &= 1 + \frac{3g_R}{2\varepsilon} \left(1 - \frac{\mu^\varepsilon}{\Lambda^\varepsilon} \right).
\end{aligned} \tag{40}$$

For our purposes it is convenient to set $\Lambda = (2d)^{1/2}$ (the lattice constant is assumed to be equal to unity), rather than to pass to the limit $\Lambda \rightarrow \infty$ (as it is usual in the quantum field theory). The expressions for Z_{Li} can be deduced by comparing the above results of perturbation theory for the original lattice model (Secs. II B and II C) with the standard perturbation results for the continuum model (34), see Ref. 35. We obtain

$$\begin{aligned}
Z_{Lx} &= Z_{Ly} = 1, \\
(Z_{L2}^\pm)^{-1} &= 1 + A_\pm(t_\pm) + \frac{g}{2\varepsilon} \left(\frac{1}{t_\pm^{\varepsilon/2}} - 1 \right), \\
(Z_{L4}^-)^{-1} &= 1 + A_-(t_-) - B(t_-) + \frac{3g}{2\varepsilon} \left(\frac{1}{t_-^{\varepsilon/2}} - 1 \right).
\end{aligned} \tag{41}$$

Note that, unlike the factors Z_i^{cont} , the quantities (41) are defined only for integer ε . As follows from Eq. (39), the determination of factors Z_{Li} enables one to consider the continuum model (34) with the parameters

$$m^2 = (Z_{L2}^\pm)^{-1} m_{\text{cont}}^2, \quad u = (Z_{L4}^\pm)^{-1} u_{\text{cont}}, \tag{42}$$

and $c = c_0(1 + 1/2S - X_0)$ instead of the original lattice one. Thus the factors Z_{Li} represent the corrections owing to passing from the cutoff scheme in the original lattice model to that in the continuum model, cf. Ref. 29.

The flow functions for the coupling constant and energy gap have the standard form³⁵

$$\begin{aligned}
\beta(g_R) &= \mu \frac{\partial g_R}{\partial \mu} = -\varepsilon g_R + \frac{3}{2} g_R^2, \\
\gamma(g_R) &= \mu \frac{\partial \ln Z_2^{\text{cont}}}{\partial \mu} = -\frac{1}{2} g_R.
\end{aligned} \tag{43}$$

The effective-Hamiltonian parameters g_ρ , t_ρ at the scale $\mu' = \mu\rho$ as determined by these flow functions read

$$\begin{aligned}
g_\rho &= \left[1 + \frac{g_R}{g^*} (\rho^{-\varepsilon} - 1) \right]^{-1} \rho^{-\varepsilon} g_R, \\
t_\rho &= \left[1 + \frac{g_R}{g^*} (\rho^{-\varepsilon} - 1) \right]^{-1/3} t_{\pm R},
\end{aligned} \tag{44}$$

where $g^* = 2\varepsilon/3$ is the stable fixed point to one-loop order.

We start the scaling procedure at $\mu = \Lambda$ and stop it at $\mu' = \Lambda t_\pm^{1/2}$ (thus $\rho = t_\pm^{1/2}$). For Δ_\pm and \bar{S} we obtain the results

$$\Delta_{\pm R}^2(t_\pm, 0) = \frac{1}{Z_{L2}^\pm} \frac{t_\pm}{[1 + (3g_R/2\varepsilon)(1/t_\pm^{\varepsilon/2} - 1)]^{1/3}}, \tag{45}$$

$$\bar{S}_R(t_-, 0) = t_-^{1/2} \sqrt{\frac{Z_{L4}^-}{Z_{L2}^-} \left[1 + \frac{3g_R}{2\varepsilon} \left(\frac{1}{t_-^{\varepsilon/2}} - 1 \right) \right]^{1/3}}, \tag{46}$$

where, according to Eqs. (37), (40),

$$g_R = (Z_{4L}^\pm)^{-1} (2d)^{-\varepsilon/2} K_{4-\varepsilon} L_\varepsilon. \tag{47}$$

In the 3D case

$$\frac{1}{\varepsilon} \left(\frac{1}{t^{\varepsilon/2}} - 1 \right) \rightarrow \frac{1}{2} \ln \frac{1}{t}, \tag{48}$$

so that the QPT critical exponents for the order parameter and the gap (inverse correlation length) are the Gaussian one,

$$\beta = 1/2, \quad \nu = 1/2, \tag{49}$$

and logarithmic corrections are present. At the same time, in the 2D case we obtain

$$\beta = 1/3, \quad \nu = 7/12, \tag{50}$$

which are standard one-loop results for the one-component ϕ^4 theory in $d+1=3$ dimensions.

In a strong enough longitudinal magnetic field ($-\Omega/\Omega_c \ll \theta_H^2 \ll 1$), we obtain

$$\begin{aligned}
\Delta_{\pm R}^2(\theta_H, 0) &= \frac{2}{3Z'_{L2}} \frac{1}{[1 + (3g_R/2\varepsilon)(1/\theta_H^\varepsilon - 1)]^{1/3}}, \\
\bar{S}_R(\theta_H, 0) &= \theta_H \sqrt{\frac{Z'_{L4}}{Z'_{L2}}} \left[1 + \frac{3g}{2\varepsilon} \left(\frac{1}{\theta_H^\varepsilon} - 1 \right) \right]^{1/3},
\end{aligned} \tag{51}$$

where

$$\begin{aligned}
Z'_{L2} &= 1 + A'(\theta_H^2) + \frac{g}{2\varepsilon} \left(\frac{1}{\theta_H^\varepsilon} - 1 \right), \\
Z'_{L4} &= 1 + A'(\theta_H^2) - B'(\theta_H^2) + \frac{3g}{2\varepsilon} \left(\frac{1}{\theta_H^\varepsilon} - 1 \right).
\end{aligned} \tag{52}$$

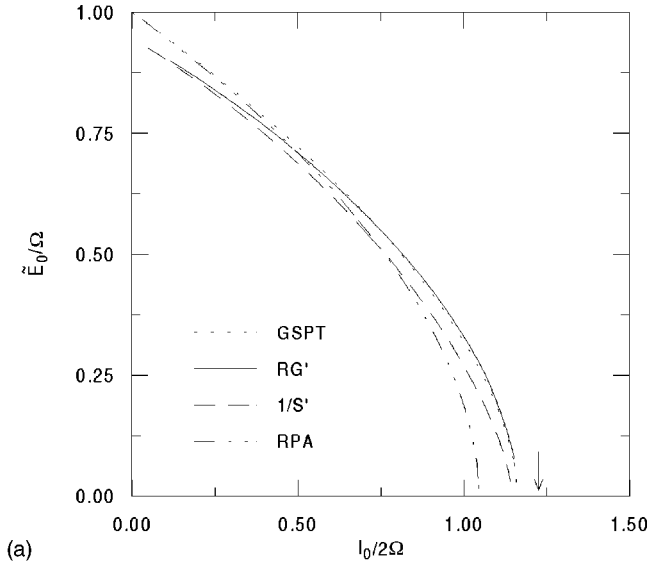
Thus, as well as for the dependences of ground-state properties on t , in the 3D case one has the mean-field value

$$\delta = 3, \tag{53}$$

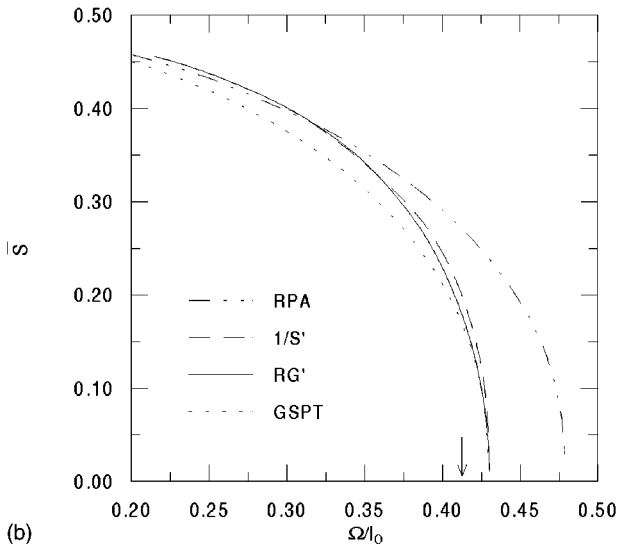
and the logarithmic corrections are present. At $d=2$ we obtain the critical exponent

$$\delta = 9/2. \tag{54}$$

Note that the scaling relations at $d=2$ are slightly violated since the corresponding value of ε is in fact not small and the ε expansion is applicable with a poor accuracy. However, this violation is not too large (the value $\delta=5$ can be calculated taking into account that the critical exponent η



(a)

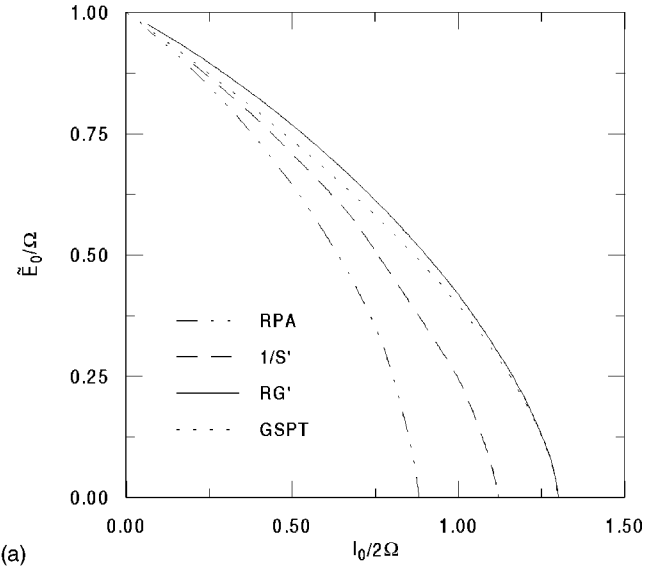


(b)

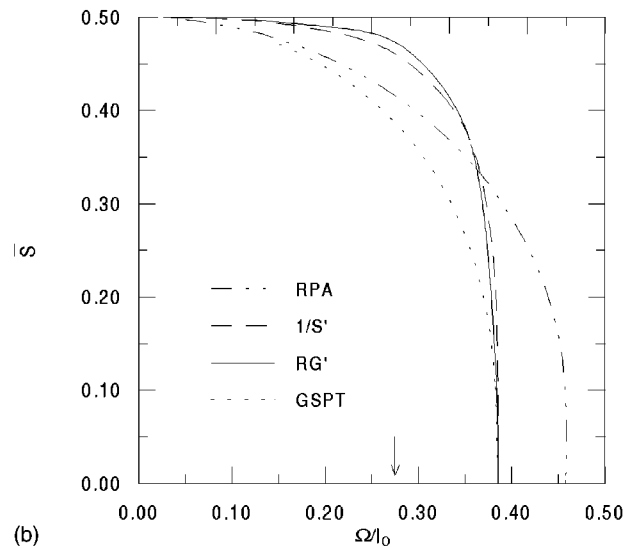
FIG. 1. Ground-state energy gap $\bar{E}_0(\Omega)$ ($\Omega > \Omega_c$, a) and order parameter $\bar{S}(\Omega)$ ($\Omega < \Omega_c$, b) for the 3D transverse-field Ising model in different approaches. The value $\Omega_c = 2.58I$ is used for calculating the $1/S'$ and RG' curves. The arrow shows the value of the critical field Ω_c , obtained by $1/S$ expansion.

=0 to one-loop order), which indicates that the one-loop approximation gives adequate results even in this case.

The ground-state parameters at zero longitudinal magnetic field are shown and compared with RPA (Ref. 11) and GSPT (Ref. 13) results in Fig. 1 for the 3D case and in Fig. 2 for the 2D case. The primes mean that corrected values of Ω_c obtained from GSPT (see above), instead of those from the first-order $1/S$ expansion, are used in the calculations. The $1/S$ results for Ω_c are marked by arrows. One can see that, unlike the results of RPA and $1/S$ expansions, RG results have a correct critical behavior with critical exponents given by Eqs. (49) and (50); besides that, they are very close to the GSPT result for $d=3$. For $d=2$ the difference between RG' and GSPT results increases, which demonstrates that the ε expansion has a poor accuracy here. Far from the quantum phase transition, the RG results coincide with those of $1/S$ perturbation theory.



(a)



(b)

FIG. 2. Ground-state energy gap $\bar{E}_0(\Omega)$ ($\Omega > \Omega_c$, a) and order parameter $\bar{S}(\Omega)$ ($\Omega < \Omega_c$, b) for the 2D transverse-field Ising model in different approaches. The notations used are the same as in Fig. 1.

E. Finite-temperature properties near the QPT

At finite temperature the situation is more complicated, since not only “spin-wave” excitations, considered in previous sections, contribute to thermodynamic properties. At $\Omega/\Omega_c \ll 1$ we have $T_c \sim IS^2$ and the phase transition occurs due to vanishing of $\langle |\boldsymbol{\pi}| \rangle$. The dominant excitations in this case are domain walls. Another situation occurs near the QPT ($1 - \Omega/\Omega_c \ll 1$) where the temperature phase transition is connected with the rotation of $\langle \boldsymbol{\pi} \rangle$ in the spin space, while its absolute value is only slightly changed with temperature. The dominant excitations here are the “spin-wave” excitations, except for a narrow critical region close to T_c . At intermediate values of Ω both effects, the rotation of $\langle \boldsymbol{\pi} \rangle$ and temperature variation of its absolute value, are important. Thus the $1/S$ expansion can be applied to describe the temperature phase transition only near the QPT.

Being rewritten through the quantum-renormalized ground-state parameters, finite-temperature properties near

the QPT are universal. The finite-temperature order parameter and energy gaps obey the scaling laws

$$\bar{S}^2(t_-, T) = \bar{S}^2(t_-, 0) f\left(\frac{T}{c\Delta_{-0}}\right), \quad (55a)$$

$$\Delta_{\pm}(t_{\pm}, T) = \Delta_{\pm}(t_{\pm}, 0) g_{\pm}\left(\frac{T}{c\Delta_{\pm 0}}\right), \quad (55b)$$

where $\Delta_{\pm 0} = \Delta_{\pm}(t, 0)$, f and g_{\pm} are universal scaling functions with $f(0) = g_{\pm}(0) = 1$. The transition temperature is determined by zero of the function $f(T/c\Delta_{-0})$ or, equivalently, of $g_{-}(T/c\Delta_{-0})$. As discussed in Ref. 28, the functions $g_{+}(x)$ and $g_{-}(x)$ are connected by the procedure of analytical continuation. Due to universality of scaling functions (55a), (55b), the continuum limit of developed theory, i.e., the action (34), can be used when treating the finite-temperature properties.

Consider first the perturbation approach. We obtain

$$\Delta_{+}^2(t_{+}, T) = \Delta_{+}^2(t_{+}, 0) + \frac{u}{2d} \left(\frac{2T}{c}\right)^{d-1} F_d\left(\frac{c^2 d}{4T^2} t_{+}\right) \quad (56)$$

for the disordered phase and

$$\bar{S}_R^2(t_-, T) = \bar{S}_R^2(t_-, 0) - \frac{u}{4d} \left(\frac{2T}{c}\right)^{d-1} F_d\left(\frac{c^2 d}{2T^2} t_{-}\right), \quad (57a)$$

$$\Delta_{-}^2(t_-, T) = \bar{S}_R^2(t_-, T) \left[\frac{\Delta_{-}^2(t_-, 0)}{\bar{S}_R^2(t_-, 0)} + \frac{3u}{4} \left(\frac{2T}{c}\right)^{d-3} F_d'\left(\frac{c^2 d}{2T^2} t_{-}\right) \right], \quad (57b)$$

for the ordered phase, where

$$F_d(x) = K_d \int_0^{\infty} \frac{q^{d-1} dq}{\sqrt{q^2+x}} (\coth \sqrt{q^2+x} - 1), \quad F_3(0) = \frac{1}{24},$$

and $F_d'(x)$ is the derivative with respect to x . Thus we have for the static susceptibility in the disordered phase at $I\Delta_{+} \ll T \ll I$ (Refs. 26,28)

$$\chi^{xx} = \frac{1}{I_0} \frac{1}{\Delta_{+}^2(t_+, 0) + \gamma(2T/c)^{d-1}} \quad (58)$$

with $\gamma = 3I_0 F_d(0)/4c$.

At $T \geq I$ thermodynamic properties cannot be determined correctly from the above approach since in this temperature region higher-order terms in the $1/S$ expansion contribute to the partition function and such an expansion becomes inapplicable. However, one can expect that at $T \gg I$ the thermodynamics is the same as for the well-studied Ising model. In particular, the susceptibility obeys the Curie law

$$\chi^{xx} = \frac{S(S+1)}{3T} \quad (59)$$

on both sides of the QPT.

The equation for the transition temperature reads

$$\bar{S}^2(t_-, 0) = \frac{u}{4d} \left(\frac{2T_c}{c}\right)^{d-1} F_d\left(\frac{c^2 d}{2T_c^2} t_{-}\right). \quad (60)$$

Since at small t_{-} and $d \leq 3$ one has from Eq. (22) $\bar{S}^2(t_-, 0) \propto (t_{-})^{(d-1)/2}$, we obtain

$$T_c \propto \sqrt{t_{-}}, \quad 1 < d \leq 3, \quad (61)$$

where the coefficient of proportionality is determined by the solution of Eq. (60). For $d > 3$ we derive

$$T_c \propto (t_{-})^{1/(d-1)}, \quad d > 3. \quad (62)$$

The mean-field logarithmic behavior (5) is reproduced only for $d \rightarrow \infty$.

Consider now the renormalization of the finite-temperature properties at $d \leq 3$. To this end we use the approach of Ref. 28, which treats the renormalization of the effective classical model. The disordered phase was considered in detail in Ref. 28. Instead of the analytical continuation of these results to the ordered phase, we perform direct calculation of finite-temperature properties in the ordered phase. This gives the possibility of calculating correctly the value of T_c not too close to the QPT and also of describing finite-temperature properties at $T < T_c$. The generalization of the approach of Ref. 28 to the ordered phase is trivial. We integrate out all the modes with nonzero Matsubara frequencies from the finite-temperature partition function to obtain the effective action for the field

$$\Pi = \int_0^{c/T} d\tau \pi_x, \quad (63)$$

which corresponds to the $\omega_n = 0$ mode, in the form

$$\begin{aligned} \mathcal{S}_{\text{cl}} = & \frac{c}{2T} \int d^d r [K(\nabla \tilde{\Pi})^2 + R\tilde{\Pi}^2] + \frac{\bar{\Pi}}{3!} \frac{cU}{T} \int d^d r \tilde{\Pi}^3 \\ & + \frac{1}{4!} \frac{cU}{T} \int d^d r \tilde{\Pi}^4 + \dots \end{aligned} \quad (64)$$

Here $\tilde{\Pi} = \Pi - \bar{\Pi}$, $\bar{\Pi}$ is determined by the condition of absence in Eq. (64) of terms that are linear in $\tilde{\Pi}$. The parameters of the model (64) are given by

$$R(T) = \frac{1}{3} U(T) \bar{\Pi}^2(T) \quad (65)$$

and for $d = 3$

$$\bar{\Pi}^2(T) = \frac{18}{u} \left[\bar{S}_R^2(t_-, 0) - \frac{1}{3} \frac{8\pi^2 g_R}{1 + (3g_R/2)\ln(1/\Delta_-)} \left(\frac{T}{c}\right)^2 \bar{F}_3\left(\frac{3\Delta_-^2 c^2}{2T^2}\right) \right], \quad (66)$$

$$U(T) = \frac{8\pi^2 g_R}{1 + (3g_R/2)\ln(1/\Delta_-)} \left[1 + \frac{6\pi^2 g_R}{1 + (3g_R/2)\ln(1/\Delta_-)} \bar{F}_3\left(\frac{3\Delta_-^2 c^2}{2T^2}\right) \right], \quad (67)$$

where

$$\bar{F}_3(x) = K_3 \int_0^\infty q^2 dq \left[\frac{\coth\sqrt{q^2+x}-1}{\sqrt{q^2+x}} - \frac{1}{q^2+x} + \frac{1}{q^2} \right], \quad (68)$$

$\bar{F}'_3(x)$ means the derivative with respect to x , and we have represented Eqs. (66) and (67) in the scaling form by replacing $t_- \rightarrow \Delta_-^2$ in arguments of $F_3(x)$, $F'_3(x)$. Near the QPT (i.e., for small Δ_-) function $R(T)$ coincides with that determined by continuation from paramagnetic phase, as it should be. The value of $K(T)$ will be needed only in zeroth-loop order, $K=1$.

The critical temperature is determined by the condition $\bar{\Pi}(T_c)=0$. Closely enough to the critical point [at $\ln(1/\Delta_-) \gg 1$] we have

$$T_c = \frac{3}{2\pi} c \Delta_- \sqrt{6 \ln(1/\Delta_-)}, \quad (69)$$

in agreement with Ref. 28 [our definition of Δ_- differs $(2d)^{1/2}c$ times from that used in Ref. 28]. At the same time, the expansion in the bare splitting (magnetic field) yields

$$T_c \propto c \sqrt{t_-} \ln^{1/3}(1/t_-) \propto \bar{S}_R(t_-, 0), \quad (70)$$

where the coefficient of proportionality can be determined numerically from Eqs. (45) and (69). Thus, due to ground-state renormalizations, the dependences of T_c on the bare and renormalized splittings turn out to be different in form.

The resulting classical action (104) is renormalized in a standard way.³⁵ One can introduce the renormalization constants for finite-temperature theory by

$$R = (Z_2^T/Z^T)R_r, \quad \Pi = Z^T\Pi_r, \quad U = \frac{\mu^\epsilon}{K_{4-\epsilon}L_\epsilon} (Z_4^T/Z^{T^2})U_r, \quad (71)$$

where the index ‘‘r’’ stands for the quantities renormalized by temperature fluctuations, and $\epsilon=1+\varepsilon$. The expressions for Z factors are the same as for the ground-state renormalization factors (40) with the replacement $\varepsilon \rightarrow \epsilon$. Formulas of RG transformation also have the same form (44) as for the ground-state properties with $t \rightarrow R$, $g \rightarrow U$, etc. However, now already at $d=3$ ($\varepsilon=0$), we have $\epsilon=1$ and thus the ϵ expansion can be used only approximately.

For the energy gap we obtain in this way the expression

$$\Delta_-^2(t_-, T) = \frac{R(T)}{6} \left[1 + \frac{3TK_3L_1U(T)}{2cR^{1/2}(T)} \right]^{-1/3}, \quad (72)$$

where we have set $\epsilon=1$. For the temperature-dependent magnetization we obtain

$$\bar{S}_R^2(t_-, T) = \frac{uR(T)}{6U(T)} \left[1 + \frac{3TK_3L_1U(T)}{2cR^{1/2}(T)} \right]^{2/3}. \quad (73)$$

The values of the temperature-transition critical exponents,

$$\beta_T = 1/3, \quad \nu_T = 7/12, \quad (74)$$

coincide with those of 2D quantum phase transition (50).

The calculated dependence $T_c(\Omega)$ is shown and compared with the mean-field and HTSE results¹² in Fig. 3. One can see that near the QPT the dependence $T_c(\Omega)$ calculated from Eq. (66) is in excellent agreement with HTSE data. At the same time, far from the QPT our approach gives much larger values of T_c , as discussed in the beginning of the present section. The inflection point of the curve $T_c(\Omega)$, $\Omega^* = 0.35I_0$, may be approximately related to the transverse-field value where the ‘‘non-spin-wave’’ excitations become important for description of finite-temperature properties.

For $d=2$ the system is far from its upper critical dimensionality ($\epsilon=2$) and ϵ expansion becomes inapplicable. Therefore we can perform only ground-state renormalizations in the results of perturbation theory (57a) and (57b). In this case the critical exponents of the temperature phase transition still have their Gaussian values. However, universality hypothesis predicts that the temperature phase-transition critical exponents coincide with those for the 2D Ising model,

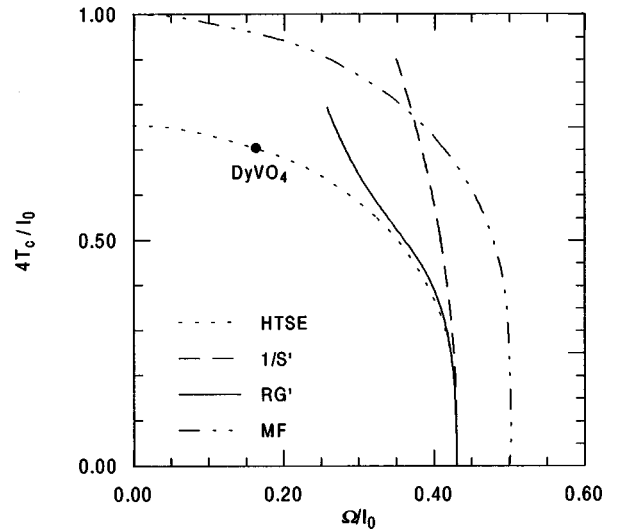


FIG. 3. Transition temperature as a function of Ω/I_0 for the 3D transverse-field Ising model in different approaches.

$$\beta_T = 1/8, \quad \nu_T = 1. \quad (75)$$

With account of the ground-state renormalizations, the result (61) for the critical temperature near the quantum phase transition ($1/\Delta_{-0} \gg 1$) takes the form

$$T_c \propto \Delta_{-0}, \quad (76)$$

while

$$T_c \propto (t_-)^{5/12} \quad (77)$$

in terms of bare splitting (or external transverse magnetic field). The correct description of thermodynamics below T_c in the 2D case is still an open problem.

III. THE HEISENBERG MODEL WITH STRONG EASY-PLANE ANISOTROPY

A. Ground-state properties

We start from the general Hamiltonian of a spin system in crystal field which induces the single-site anisotropy,

$$\mathcal{H} = V_{\text{cf}} - \frac{\mathcal{I}}{2} \sum_{\langle ij \rangle} \mathbf{J}_i \mathbf{J}_j, \quad (78)$$

where V_{cf} is the crystal-field potential, \mathbf{J} are momentum operators, \mathcal{I} is the exchange integral, and the direction of spin alignment will be supposed along the z axis. In this section we consider the single-site easy-plane anisotropy which corresponds to

$$V_{\text{cf}} = D \sum_i (J_i^x)^2, \quad (79)$$

where $D > 0$ is the anisotropy parameter. For integer values of J the lowest level is singlet. In this case with increasing D the model (79) demonstrates at some value D_c a second-order phase transition from the phase with collinear ferromagnetic order $\langle J^z \rangle \neq 0$ to the disordered phase. At the same time, the quadrupole order parameter

$$Q \equiv 3 \langle (J^x)^2 \rangle - J(J+1) \quad (80)$$

is nonzero in both the phases. For half-integer values of J , such a transition is absent since the lowest state is twofold degenerate. In the classical limit $J \rightarrow \infty$ with J being the integer, we have $D_c \sim J(J+1)\mathcal{I} \rightarrow \infty$, so that integer and half-integer values of J become indistinguishable.

For integer J the ground state is $|A\rangle = |\bar{0}\rangle$, and first excited state is doublet $|B_1\rangle = |\bar{1}\rangle$, $|B_2\rangle = |-\bar{1}\rangle$ where $|\bar{M}\rangle$ are the eigenstates of J^x . For $J=1$ passing to the eigenstates $|M\rangle$ of J^z yields

$$\begin{aligned} |A\rangle &= \frac{1}{\sqrt{2}}(|1\rangle - |-1\rangle), \\ |B_1\rangle &= |0\rangle, \quad |B_2\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |-1\rangle). \end{aligned} \quad (81)$$

To consider the vicinity of the QPT, we have to generalize the theory developed in the previous section on the singlet-doublet case. Further we restrict ourselves to the case

$J=1$. In the initial spin space, the QPT in the model (78) with Eq. (79) is not of orientational character: the spins always lie in the easy plane. Thus the spin-wave theory in its standard form cannot properly describe the model (78) near such a transition (see, e.g., Ref. 40). However, as discussed in Refs. 22,23, this transition can be viewed as an orientational one in the complete $SU(3)$ space which includes the $SU(2)$ spin subspace. The most convenient way to consider the rotations in the extended $SU(3)$ space is to rewrite the Hamiltonian (78) with the crystal field (79) in terms of the Hubbard operators $X_i^{mn} = |m_i\rangle\langle n_i|$,

$$\begin{aligned} \mathcal{H} = & \frac{D}{2} \sum_i (X_i^{00} + X_i^{1,-1} + X_i^{-1,1}) - \frac{\mathcal{I}}{2} \sum_{\langle ij \rangle} [(X_i^{10} + X_i^{0,-1}) \\ & \times (X_j^{01} + X_j^{-10}) + (X_i^{11} - X_i^{-1,-1})(X_i^{11} - X_j^{-1,-1})]. \end{aligned} \quad (82)$$

The rotation through ‘‘angle’’ θ in $SU(3)$ space is performed by the unitary transformation operator $U(\theta)$ (see Appendix C).

Following the strategy described in Sec. II, we define the ground-state critical value of D_c from the condition $\sin \theta = 1$ which yields

$$\frac{D_c}{2\mathcal{I}_0} = 1 + \frac{3\lambda}{2} - \lambda \sum_{\mathbf{k}} \frac{6\mathcal{I}_0 + \mathcal{I}_{\mathbf{k}} + \mathcal{I}_{\mathbf{k}}^2/\mathcal{I}_0}{2E_{\mathbf{k}}^0}, \quad (83)$$

where $E_{\mathbf{k}}^0 = 2\sqrt{\mathcal{I}_0(\mathcal{I}_0 - \mathcal{I}_{\mathbf{k}})}$, $\lambda (=1)$ is the formal expansion parameter. The critical value obtained from Eq. (83) in the 3D case is $D_c/2\mathcal{I}_0 = 0.73$, which turns out to coincide with the result of HTSE.²¹ For the ground-state magnetization we obtain

$$\langle J^z \rangle_{T=0}^2 = t_- [1 + B(t_-)], \quad (84)$$

$$\begin{aligned} B(t_-) = & -\frac{\lambda}{t_-} \sum_{\mathbf{k}} \left[\frac{2\mathcal{I}_0 + (2 - \eta^2)\mathcal{I}_{\mathbf{k}}}{E_{\mathbf{k}\alpha}} \right. \\ & \left. + \frac{(1 + \eta)\mathcal{I}_0 - \mathcal{I}_{\mathbf{k}} + \eta\mathcal{I}_{\mathbf{k}}^2/\mathcal{I}_0}{E_{\mathbf{k}\beta}} - \frac{6\mathcal{I}_0 + \mathcal{I}_{\mathbf{k}} + \mathcal{I}_{\mathbf{k}}^2/\mathcal{I}_0}{E_{\mathbf{k}}^0} \right], \end{aligned} \quad (85)$$

where the excitation spectrum $E_{\mathbf{k}\alpha,\beta}$ is given by Eqs. (C12), (C13), and $t_- = 1 - (D/D_c)^2$, $\eta = (1 - t_-)^{1/2}$. The excitations of α type have a gap; they are analogous to the excitations in the transverse-field Ising model, considered in the previous section. The excitations of β type are gapless due to spontaneous breaking of rotational symmetry in the y - z plane of spin space; these excitations are specific for $n \geq 2$ systems. Near the QPT we have $E_{\mathbf{k}\beta} \approx E_{\mathbf{k}}^0$ and we return to the perturbation result (B19) for the transverse-field Ising model with $E_{\mathbf{k}} = E_{\mathbf{k}\alpha}$ being the critical mode. However, the renormalization of Eq. (85) is performed in a different way in comparison with the transverse-field Ising model because of another symmetry of the model (see below). The energy for the critical mode α to first order in λ has the form

$$\tilde{E}_{\mathbf{k}\alpha} = 2\sqrt{\mathcal{I}_0(1 + B_0 + B_1)(\mathcal{I}_0 - \mathcal{I}_{\mathbf{k}} + \mathcal{I}_0\Delta_-^2)}, \quad (86)$$

where Δ_- in the ordered phase is given by

$$\Delta_-^2(t_-,0) = t_-[1 + A(t_-)],$$

$$A(t_-) = A_0 + A_1, \quad (87)$$

and $A_{0,1}$, $B_{0,1}$ are determined by (C17a)–(C17d).

In the presence of the longitudinal magnetic field, i.e., of the field H , directed along the z axis, both modes α and β become gapped, since this field breaks the rotational symmetry. As well as for the transverse-field Ising model, we can expect that at the intermediate magnetic field values $1 - D/D_c \ll (H/D_c)^{2/3} \ll 1$ the ground-state properties near the QPT will be determined by the magnetic field rather than by t_{\pm} . In this region we obtain the energy spectra

$$E_{\mathbf{k}\alpha}^2 = 4\mathcal{I}_0[\mathcal{I}_0(1 + \theta_H^2) - \mathcal{I}_{\mathbf{k}}(1 - \theta_H^2)],$$

$$E_{\mathbf{k}\beta}^2 = [2(\mathcal{I}_0 - \mathcal{I}_{\mathbf{k}}) + \theta_H^2(\mathcal{I}_0 + \mathcal{I}_{\mathbf{k}})/2][2\mathcal{I}_0 + \theta_H^2(\mathcal{I}_0 - \mathcal{I}_{\mathbf{k}})/2], \quad (88)$$

where $\theta_H = (4H/D_c)^{1/3}$. Performing the calculations which are similar to those for the transverse-field Ising model, we obtain the result

$$\bar{S} = \theta_H[1 + B'(\theta_H^2)], \quad (89)$$

where

$$B'(\theta_H^2) = -\frac{\lambda}{3\theta_H^2} \sum_{\mathbf{k}} \left[2 \frac{2(\mathcal{I}_0 + \mathcal{I}_{\mathbf{k}})(1 + \theta_H^2/2) - \mathcal{I}_{\mathbf{k}}(1 - \theta_H^2)}{E_{\mathbf{k}\alpha}} \right. \\ \left. + \frac{(2 + \theta_H^2/2)\mathcal{I}_0 - \mathcal{I}_{\mathbf{k}} + (1 - \theta_H^2/2)\mathcal{I}_{\mathbf{k}}^2/\mathcal{I}_0}{E_{\mathbf{k}\beta}} \right. \\ \left. - \frac{6\mathcal{I}_0 + \mathcal{I}_{\mathbf{k}} + \mathcal{I}_{\mathbf{k}}^2/\mathcal{I}_0}{E_{\mathbf{k}}^0} \right]. \quad (90)$$

A more complicated situation takes place in the case of the transverse field directed along the x axis.^{22,40} This field induces a deviation of spins from easy plane. With increasing the field value there occurs a cascade of J second-order phase transitions from ferromagnetically ordered phases with $\langle J^z \rangle \neq 0$, $\langle J^x \rangle \neq 0$ to phases which are ordered only along the x axis ($\langle J^z \rangle = 0$, $\langle J^x \rangle \neq 0$) and vice versa. The reason for this is the modification of the level scheme in the magnetic field directed along the hard axis: in the case where lowest state is doublet the long-range order along the z axis is present, while in the case of singlet ground state it is evidently absent. We do not consider these transitions here (see discussion of such transitions in Refs. 22,40,37).

B. Ground-state renormalizations

The above theory can be easily reformulated in the path-integral formalism. The partition function has the form

$$\mathcal{Z} = \int D[a, a^\dagger, b, b^\dagger] \exp \left\{ a^\dagger \frac{\partial a}{\partial \tau} + b^\dagger \frac{\partial b}{\partial \tau} - \mathcal{H}(a, a^\dagger, b, b^\dagger) \right\}, \quad (91)$$

where $\mathcal{H}(a, a^\dagger, b, b^\dagger)$ is the average of the boson Hamiltonian over the coherent states $|a, b\rangle$ (Ref. 34) (see also Ref.

41). The continuum limit of the theory can be obtained if we introduce real variables $\pi_{x,y}$ and $Q_{x,y}$ instead of the complex ones a, b by the relations

$$a = \pi_x + iQ_x, \\ b = Q_y + i\pi_y. \quad (92)$$

[Note that π_x and π_y correspond to S^z and S^y in the original spin space, and two additional variables $Q_{x,y}$ arise due to passing from SU(2) to SU(3) space]. We obtain

$$\mathcal{S}_{\text{cont}} = \frac{1}{2} \int_0^{c/T} d\tau \int d^d r [-2i\bar{Q}_x(\partial\tilde{\pi}_x/\partial\tau) + 2i\bar{Q}_y(\partial\tilde{\pi}_y/\partial\tau) \\ + \bar{Q}^2 + (\nabla\tilde{\pi})^2 + m^2\tilde{\pi}^2] + \frac{u}{4!} \int_0^{c/T} d\tau \int d^d r \tilde{\pi}^4 \\ + h \int_0^{c/T} d\tau \int d^d r \tilde{\pi}_x, \quad (93)$$

where we have introduced the notations $\tilde{\pi}^2 = (\mathcal{I}/c_0)\pi^2$, $\bar{Q}^2 = (\mathcal{I}_0/c_0)Q^2$, $h = H/(\mathcal{I}c_0)^{1/2}$, the bare spin-wave velocity is given by $c_0 = 2\sqrt{2d}\mathcal{I}$, and we have included in Eq. (93) the term connected with the external magnetic field H along the S^z axis. The parameters of this model, determined by the continuum limit, read

$$m_{\text{cont}}^2 = -t_-d, \\ u_{\text{cont}} = 6d(c_0/\mathcal{I})\lambda\zeta, \\ c_{\text{cont}} = c_0, \quad (94)$$

with $\zeta = 1 - t_-$ in the ordered phase under consideration. Proceeding in the same way as in the previous section we integrate over $Q_{x,y}$. Then we obtain the action of the standard two-component quantum ϕ^4 theory in an external field,

$$\mathcal{S}_{\text{cont}} = \frac{1}{2} \int_0^{c/T} d\tau \int d^d r [(\partial\tilde{\pi})^2 + m^2\tilde{\pi}^2] + \frac{u}{4!} \int_0^{c/T} d\tau \int d^d r \tilde{\pi}^4 \\ + h \int_0^{c/T} d\tau \int d^d r \tilde{\pi}_x. \quad (95)$$

There is a crucial difference from the one-component model of the previous section, which is due to existence in the ordered phase of the gapless Goldstone mode at $H=0$. This mode changes the renormalization conditions since it leads to infrared divergences.³⁹ To treat these divergences, we take the value of magnetic field H finite, but small enough to satisfy $(H/D_c)^{2/3} \ll 1 - D/D_c$. The renormalization of the action (95) is considered in Appendix D. We obtain for effective Hamiltonian parameters at the scale $\Lambda\rho$, $\Lambda = (2d)^{1/2}$ the results ($d=3$)

$$g_\rho^{-1} = g_R^{-1} [1 + (3g_R/4)\ln(1/t_-) + (g_R/6)\ln(1/\rho)], \\ t_\rho^{-1} = t_R^{-1} [1 + (3g_R/4)\ln(1/t_-) + (g_R/6)\ln(1/\rho)] \\ \times [1 + (5g_R/6)\ln(1/t_-)]^{-3/5} \Phi_0(g_R, t_-), \quad (96)$$

where the function $\Phi_0(g, x)$ is given by Eq. (D6), and

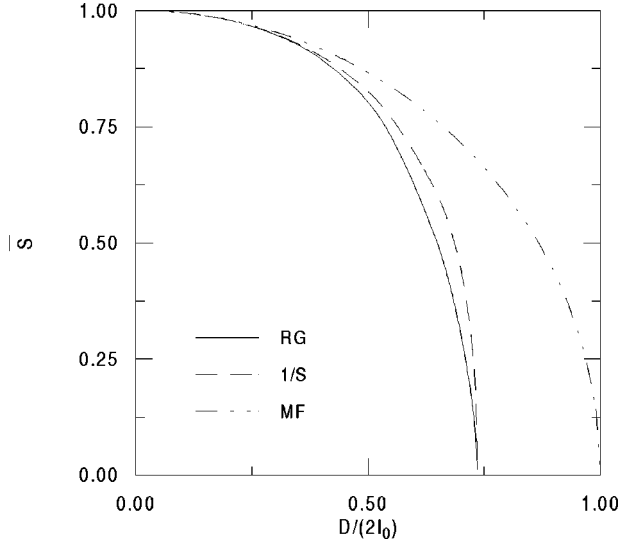


FIG. 4. The order parameter $\bar{S}(\Omega)$ ($\Omega < \Omega_c$) for the 3D easy-plane ferromagnet in mean-field theory, 1/S expansion, and the RG approach.

$$g_R = K_4^{-1} Z_{L4}^- u_{\text{cont}} \quad (97)$$

is the renormalized coupling constant. For the nonuniversal Z factors we have

$$Z_L = 1,$$

$$(Z_{L2}^-)^{-1} = 1 + \tilde{A}(t_-) + \frac{g}{4} \ln \frac{1}{t_-}, \quad (98)$$

$$(Z_{L4}^-)^{-1} = 1 + \tilde{A}(t_-) - B(t_-) + \frac{3g}{4} \ln \frac{1}{t_-},$$

where $A(t_-)$, $B(t_-)$ are given by Eqs. (85), (87), the tilde sign means that the contributions of the Goldstone mode β should be excluded from $A(t_-)$.

Putting in the above expressions $\rho = \tilde{h}^{1/2}$, where $\tilde{h} = H/[\mathcal{I}_0 \bar{J}_R(H=0)]$, we have for the magnetization at $d=3$ the result

$$\bar{J}_R(t_-, 0) = \sqrt{\frac{Z_{L4}^- t_-}{Z_{L2}^-}} \left[1 + \frac{5g_R}{6} \ln \frac{1}{t_-} \right]^{3/10} \Phi_0^{1/2}(g_R, t_-) \quad (99)$$

(the terms divergent in H are canceled in \bar{J}_R). The RG result for the ground-state parameter at zero magnetic field in the 3D case is shown and compared with mean-field and first-order 1/S expansion results in Fig. 4. One can see a consid-

erable difference in the 1/S-expansion and RG results near the quantum phase transition.

The gap for α -type excitations, which determines the longitudinal susceptibility, reads

$$\Delta_-^2(t_-, 0) = 12\Theta_0^2 / \ln(1/\tilde{h}), \quad (100)$$

$$\Theta_0^2 = \frac{t_-}{Z_{L2}^-} \left[1 + \frac{5g_R}{6} \ln \frac{1}{t_-} \right]^{3/5} \frac{\Phi_0(g_R, t_-^2)}{g_R} = Z_{L4}^- \frac{\bar{J}_R^2(t_-, 0)}{g_R}.$$

Up to some nonuniversal factor Z_ρ we have in the one-loop order $\Theta_0 = Z_\rho (\rho_s/6dc)^{1/2}$ with ρ_s being the ground-state spin stiffness. At $H \rightarrow 0$ the gap vanishes as $\ln^{-1}(\mathcal{I}_0/H)$, which is a consequence of degeneracy of the system.

For intermediate values of the external magnetic field, i.e., at $1 - D/D_c \ll (H/D_c)^{2/3} \ll 1$, a characteristic scale for both types of excitations is $1/\theta_H$, and the expressions for renormalization factors Z_i^{cont} have the form, which is standard in the two-component ϕ^4 model.³⁵ Then we obtain for the magnetization

$$\bar{J}_R(\theta_H, 0) = \theta_H \sqrt{\frac{Z_{L4}'}{Z_{L2}'}} \left[1 + (5g_R/6) \ln(1/\theta_H^2) \right]^{3/10} \quad (101)$$

with

$$Z_{L4}'/Z_{L2}' = 1 - B'(\theta_H^2) + g \ln \frac{1}{\theta_H}. \quad (102)$$

C. Finite-temperature properties

Using perturbation theory we obtain for the finite-temperature magnetization the result (see Appendix C)

$$\langle J^z \rangle^2 = \langle J^z \rangle_{T=0}^2 - \frac{\mathcal{I}_0 \lambda}{2c_0} \left(\frac{2T}{c_0} \right)^{d-1} \left[3F_d \left(\frac{c_0^2 d}{2T^2} t_- \right) + F_d(0) \right], \quad (103)$$

where $t_- = 1 - (D/D_c)^2$. The first and second terms in the square brackets correspond to contributions of α - and β -type excitations, respectively. At extremely low temperatures $T \ll \mathcal{I}_0 t_-$ the contribution of the α excitations is exponentially small and the temperature-dependent part of the magnetization is determined entirely by the first term in the square brackets of Eq. (103). At temperatures $T \gg \mathcal{I}_0 t_-$ the situation changes and both types of excitations give the same temperature dependence, the contribution of the mode α being three times larger.

Consider now the renormalization of the finite-temperature theory. Integrating out the field $\pi(q, \omega_n)$ with $\omega_n \neq 0$ from action (95) we obtain the action of the effective classical model

$$\begin{aligned} \mathcal{S}_{\text{cl}} = & \frac{c}{2T} \sum_{\mathbf{q}} \left\{ q^2 \tilde{\Pi}_{\mathbf{q}} \tilde{\Pi}_{-\mathbf{q}} + \left[R(T) + \frac{3h}{\tilde{\Pi}(T)} \right] \tilde{\Pi}_{x\mathbf{q}} \tilde{\Pi}_{x,-\mathbf{q}} + \frac{h}{\tilde{\Pi}(T)} \tilde{\Pi}_{y\mathbf{q}} \tilde{\Pi}_{y,-\mathbf{q}} \right\} + \frac{\tilde{\Pi}}{3!} \frac{cU}{T} \sum_{\mathbf{q}_1 \mathbf{q}_2 \mathbf{q}_3} (\tilde{\Pi}_{\mathbf{q}_1} \tilde{\Pi}_{\mathbf{q}_2}) \tilde{\Pi}_{x, \mathbf{q}_3} \delta(\mathbf{q}_1 + \mathbf{q}_2 + \mathbf{q}_3) \\ & + \dots + \frac{1}{4!} \frac{cU}{T} \sum_{\mathbf{q}_1 \mathbf{q}_2 \mathbf{q}_3 \mathbf{q}_4} (\tilde{\Pi}_{\mathbf{q}_1} \tilde{\Pi}_{\mathbf{q}_2}) (\tilde{\Pi}_{\mathbf{q}_3} \tilde{\Pi}_{\mathbf{q}_4}) \delta(\mathbf{q}_1 + \mathbf{q}_2 + \mathbf{q}_3 + \mathbf{q}_4) + \dots, \end{aligned} \quad (104)$$

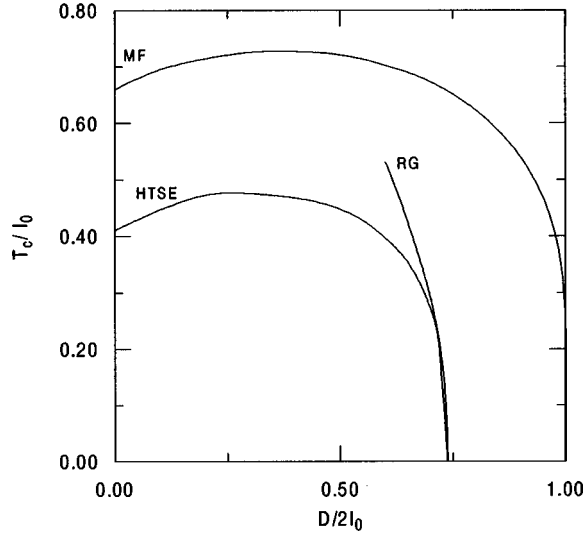


FIG. 5. Transition temperature as a function of $D/2I_0$ for the 3D easy-plane ferromagnet in different approaches.

where the field $\tilde{\mathbf{\Pi}} = \mathbf{\Pi} + (\bar{\Pi}, 0)$ is now a two-component one, and the dots stand for higher-order terms. For the parameters of the model (104) we have

$$R(T) = \frac{1}{3} \bar{\Pi}^2(T) U(T) \quad (105)$$

and for $d=3$

$$\bar{\Pi}^2(T) = \frac{18g_R}{u} \left[\Theta_0^2 - \frac{32\pi^2}{9} \left(\frac{T}{c} \right)^2 \tilde{F}_3(0) \right],$$

$$U(T) = \frac{8\pi^2 g_R}{\ln(1/\hbar)} \left[1 + \frac{20\pi^2 g_R}{3\ln(1/\hbar)} \tilde{F}_3' \left(\frac{\hbar^2 c^2}{4T^2} \right) \right]. \quad (106)$$

Note that both $R(T)$ and $U(T)$ vanish at $H \rightarrow 0$ as $\ln^{-1}(\mathcal{I}_0/H)$ due to quantum fluctuations, while $\bar{\Pi}(T)$ is finite in this limit. The value of T_c , as determined by the condition $\bar{\Pi}(T_c) = 0$, reads

$$T_c = \frac{3\sqrt{3}}{2\pi} c \Theta_0, \quad (107)$$

where Θ_0 is given by Eq. (87). Thus the result (107) coincides with that obtained in Ref. 28 up to the nonuniversal factor Z_ρ . As well as for the 3D transverse-field Ising model, in one-loop order the transition temperature turns out to be proportional to the ground-state magnetization.

It should be noted that, owing to the presence of the gapless Goldstone mode, the model (104) is applicable at $T = T_c$ only very close to the QPT, unlike the corresponding model (64) for the one-component case. Thus one can set $Z_{L2} = Z_{L4} = 1$. The calculated dependence $T_c(D)$ is shown and compared with HTSE data²¹ in Fig. 5. Note that, unlike the transverse-field Ising model, no replacement of Ω_c is required since, as discussed above, its values from $1/S$ expansion and HTSE coincide. As well as for the one-

component case, the result (107) agrees well with HTSE data closely enough to the QPT. A more complete treatment can be performed by considering quasi-momentum-dependent vertices in Eq. (104). This is a complicated task which is not considered in the present paper.

For the same reason, model (104) cannot be used for determining magnetization below T_c . However, one can expect from scaling relations that the standard value of the two-component three-dimensional ϕ^4 theory critical exponent takes place

$$\beta_T = \frac{1}{2} - \frac{3\epsilon}{2(n+8)} = 7/20, \quad (108)$$

which is practically the same as in the one-component case ($\beta_T = 1/3$). Unlike the one-component case, the logarithmic correction to $\bar{S}(t_-, T)$ is expected near the temperature phase transition due to the gapless Goldstone mode.

For $d=2$ the contribution of the gapless mode is logarithmically divergent and therefore the long-range order at finite temperatures is absent, unlike the case of the transverse-field Ising model.

IV. CONCLUSIONS

In the present paper we have considered systems that demonstrate in the ground state a quantum phase transition (QPT). Near the QPT the saturation moment \bar{S}_0 is small, but the Curie constant in Eq. (59) is not suppressed. We have $T_c \propto \bar{S}_0$ which is determined by the value of the dynamical critical exponent, $z=1$. The susceptibility (58) in the intermediate-temperature region $\Delta_0 \ll T/I \ll 1$ is governed by the small ground-state energy gap Δ_0 and demonstrates a $1/T^{d-1}$ behavior. In the strong enough longitudinal magnetic field $\Delta_0 \ll (H/IS)^{1/3} \ll 1$ the ground-state parameters are determined by magnetic-field value rather than by closeness to the QPT. The corresponding dependences have been obtained. Our approach gives the possibility of investigating both nonuniversal and universal renormalizations of the ground-state parameters. The ground-state renormalizations turn out to be important in the vicinity of the QPT. Thus the results for thermodynamic quantities (e.g., transition temperature) have different forms as functions of renormalized splitting and bare transverse (external magnetic) field, see Eqs. (69),(70) and (76),(77). This should be taken into account when treating experimental data.

The discussed class of magnets is similar in some respects to weak itinerant magnets. Note that for weak itinerant ferromagnets we have $T_c \propto \bar{S}_0^{3/2}$ (see, e.g., Ref. 24), which is due to the fact that the main contribution to thermodynamics comes from paramagnons ($z=3$). As well as for the considered localized-moment systems, calculation of nonuniversal ground-state parameters for itinerant magnets is of interest, in particular for different forms of bare electron density of states.

Now we discuss the experimental situation for some systems exhibiting magnetic and structural transitions. The compound DyVO_4 demonstrates a structural phase transition at $T_D = 14$ K. The low-lying energy levels in the spectrum of this system are two Kramers doublets with the splitting $\Delta_1 = 27 \text{ cm}^{-1}$ at $T=0$ and $\Delta_2 = 9 \text{ cm}^{-1}$ at $T > T_D$. Neglecting

the Kramers degeneracy one can describe this system by the transverse-field Ising model with $\Omega/I=1/3$ (see Ref. 7). The corresponding point in $\Omega/I-T_c$ coordinates is marked in Fig. 3. This point lies exactly on the HTSE curve and therefore HTSE results are applicable in this region of Ω/I . One can see that DyVO_4 lies far from the QPT, so that the above-developed theory is not applicable for this system.

Other systems, which are well described by the transverse-field Ising model, are the ferroelectric quantum crystals like KH_2PO_4 (see, e.g., Ref. 5). However, to our knowledge, corresponding detailed data on the ground-state order parameters are absent. To fit experimental data on the T_c of Ref. 5, we need explicit dependence of the tunneling parameter Ω on pressure.

There are very few experimental data on singlet-singlet systems demonstrating magnetic phase transitions. The system $\text{LiTb}_x\text{Y}_{1-x}\text{F}_4$ (Ref. 42) is usually assumed to be characterized by long-range exchange interactions and therefore well described by the mean-field theory. The singlet-doublet case is represented by the system NiSi_2F_6 which is a $J=1$ easy-plane Heisenberg magnet. The anisotropy constant is changed under pressure and thus the value of D/D_c can be varied near unity in the experiment. The pressure dependence of the anisotropy constant was measured experimentally.² However, to our knowledge, the data on the pressure dependence of exchange parameters are absent, although it is supposed to be considerable.²¹ There are also few experimental data on the ground-state magnetization near QPT. At $p=8.6$ Kbar, one has the experimental values $\bar{J}(T=0)=0.3$ and $T_c=110$ mK.⁴³ The calculation according to Eq. (107) yields $\mathcal{I}=90$ mK which is nearly twice larger than the $p=0$ value, $\mathcal{I}=40$ mK.⁴⁴ Praseodymium in the dhcp phase contains both ‘‘cubic’’ and ‘‘hexagonal’’ sites,^{1,45} so that separation of different contributions makes an additional problem. Generalization of our approach to the singlet-triplet case in connection with the Pr ions in the cubic crystal field will be presented elsewhere.

Generally, the $1/S$ perturbation theory combined with field-theoretical scaling analysis enables one to obtain a description of the ground-state properties of the transverse-field Ising model, which is in a good agreement with the results of the fourth-order ground-state perturbation theory¹³ for all the values of Ω . The only fitting parameter used is the critical field value Ω_c . The finite-temperature properties are considered with the use of the approach of Ref. 28. The same analysis for the $S=1$ easy-plane Heisenberg model is performed within the expansion in the formal parameter λ ($=1$) which plays the role of $1/S$. In this case, besides the critical mode, there is a gapless Goldstone mode, which considerably modifies the conditions of renormalizations. The consideration of the QPT in degenerate systems induced by the external magnetic field within the approach used is of interest. In particular, in the case of single-site anisotropy, oscillations of the effective moment with increasing magnetic field or temperature are expected in such systems with $S>1$.

It is of interest to apply the approach used to various 3D and 2D systems demonstrating orientational and metamagnetic phase transition with changing the external magnetic field or anisotropy, e.g., for yttrium garnets⁴ and magnetic

films.⁴⁶ Depending on a concrete physical situation, such systems can be described by the strongly anisotropic transverse-field Ising model or Heisenberg model with small anisotropy.

APPENDIX A: MAPPING OF THE ANISOTROPIC HEISENBERG MODEL ONTO THE TRANSVERSE-FIELD ISING MODEL

In this appendix we discuss the possibility of a mapping procedure of the anisotropic Heisenberg model (78) onto the transverse-field Ising model. We consider only one important case where the lowest level of V_{cf} is a singlet and there is a QPT to the disordered phase at strong enough V_{cf} . Provided that the first excited state is also a singlet, neglecting all energy levels except lowest and first excited states, we can introduce the pseudospin-1/2 operators \mathbf{S} , to obtain^{1,10}

$$V_{\text{cf}} = -\Delta \sum_i S_i^z, \quad J_i^z = 2\alpha S_i^x, \quad (\text{A1})$$

where $\alpha = \langle A | J^z | B \rangle$ is the matrix element of \mathbf{J} , $|A\rangle$, and $|B\rangle$ are the lowest and first excited states, Δ is the energy gap between these states. [It should be noted that the left-hand sides of Eqs. (A1) act in real-spin space, while right-hand sides in pseudospin space. Thus the equality signs are used only in the sense of identity of averages.] Then we obtain the transverse-field Ising model with $I=4\alpha^2\mathcal{I}$ and $\Omega=\Delta$. The order parameter of the Heisenberg model $\langle J^z \rangle$ is connected with the order parameter in the transverse-field Ising model by

$$\langle J^z \rangle = 2\alpha \langle S^x \rangle. \quad (\text{A2})$$

Consider now the case where the excited state is a multiplet with the states $|B_m\rangle$, $m=1 \dots N-1$. Neglecting the degeneracy of the upper energy level, one can use the same mapping (A1) if we choose $\alpha^2 = \sum_{m=1}^{N-1} \langle A | J^z | B_m \rangle^2$. However, in this case the original $\text{SU}(N)$ spin space is projected onto $\text{SU}(2)$ pseudospin space, and thus $N-2$ degrees of freedom are neglected. Thus this approach does not give the possibility of taking into account properly the symmetry of the original model and therefore can be applied only outside the critical region. To obtain a correct description of such systems in the critical region one should consider the transition in the complete $\text{SU}(N)$ space. The above consideration shows that, in principle, the transverse-field Ising model (1) can qualitatively describe singlet magnets even in the case where the exchange interactions in the true momentum space are isotropic, as in model (78).

APPENDIX B: CALCULATION OF SPIN GREEN'S FUNCTION AND ORDER PARAMETER OF THE TRANSVERSE-FIELD ISING MODEL WITHIN THE $1/S$ EXPANSION

Consider first the disordered phase where $\langle \pi_x \rangle = 0$. Representing $\pi_{zi} = (1 + 1/S - \pi_{xi}^2 - \pi_{yi}^2)^{1/2}$ and assuming $\langle \pi_{x,y}^2 \rangle \sim 1/S$ (the validity of this statement will be checked below), we expand square root to second order in $1/S$ to obtain

$$\mathcal{S}_{\text{dyn}} = \frac{iS w_S}{2} \sum_i \int_0^{1/T} d\tau \left(\pi_{xi} \frac{\partial \pi_{yi}}{\partial \tau} - \pi_{yi} \frac{\partial \pi_{xi}}{\partial \tau} \right) + \frac{iS}{8} \sum_i \int_0^{1/T} d\tau (\pi_{xi}^2 + \pi_{yi}^2) \left(\pi_{xi} \frac{\partial \pi_{yi}}{\partial \tau} - \pi_{yi} \frac{\partial \pi_{xi}}{\partial \tau} \right), \quad (\text{B1})$$

$$\mathcal{S}_{\text{st}} = -\frac{1}{2} \int_0^{1/T} d\tau \left[I S^2 \sum_{\langle ij \rangle} \pi_{xi} \pi_{xj} + (T\mathcal{P} - \Omega S w_S) \sum_i (\pi_{xi}^2 + \pi_{yi}^2) - \frac{\Omega S}{4} \sum_i (\pi_{xi}^2 + \pi_{yi}^2)^2 \right], \quad (\text{B2})$$

where $w_S = (1 + 1/2S)^{-1}$ and $\mathcal{P} = \sum_{\omega_n} 1$ (ω_n being the Matsubara frequencies) is a formally divergent quantity which comes from the measure of integration, this divergence will be canceled in final results.⁴⁷ To first order in $1/S$ (we suppose that $\Omega \sim \Omega_c \sim I_0 S$), we obtain by standard perturbation theory methods the matrix two-point vertex function of π_x , π_y fields in the form

$$\Gamma(\mathbf{q}, \omega_n) = \begin{pmatrix} \Omega S \left(w_S + \frac{3X+Y}{2} \right) + SY - T\mathcal{P} - I_q S^2 & iS \omega_n \left(w_S + \frac{X+Y}{2} \right) \\ iS \omega_n \left(w_S + \frac{Y+X}{2} \right) & \Omega S \left(w_S + \frac{3Y+X}{2} \right) + SY - T\mathcal{P} \end{pmatrix}, \quad (\text{B3})$$

where

$$X = \langle \pi_{xi}^2 \rangle = T \sum_{\mathbf{q}, \omega_n} \frac{\Omega/S}{\omega_n^2 + E_{\mathbf{q}}^2},$$

$$Y = \langle \pi_{yi}^2 \rangle = T \sum_{\mathbf{q}, \omega_n} \frac{\Omega/S - I_{\mathbf{q}}}{\omega_n^2 + E_{\mathbf{q}}^2}, \quad (\text{B4})$$

and

$$Y = i \langle \pi_{xi} (\partial \pi_{yi} / \partial \tau) \rangle = \frac{T}{S} \sum_{\mathbf{q}, \omega_n} \frac{\omega_n^2}{\omega_n^2 + E_{\mathbf{q}}^2}, \quad (\text{B5})$$

with $E_{\mathbf{q}} = \sqrt{\Omega(\Omega - SI_{\mathbf{q}})}$ being the bare ‘‘spin-wave’’ spectrum in the disordered phase. (One can easily verify that X, Y are of the order of $1/S$, as it was supposed in the beginning). Using the identity

$$\Omega SX + SY - T\mathcal{P} = I_0 S^2 X', \quad (\text{B6})$$

where

$$X' = \langle \pi_{xi} \pi_{xj} \rangle = \frac{T\Omega}{I_0 S} \sum_{\mathbf{q}, \omega_n} \frac{I_{\mathbf{q}}}{\omega_n^2 + E_{\mathbf{q}}^2} \quad (\text{B7})$$

to eliminate the divergences, we derive

$$\Gamma(\mathbf{q}, \omega_n) = \begin{pmatrix} \Omega S \left(w_S + \frac{X+Y}{2} \right) + I_0 S^2 X' - I_q S^2 & iS \omega_n \left(w_S + \frac{X+Y}{2} \right) \\ iS \omega_n \left(w_S + \frac{Y+X}{2} \right) & \Omega S \left(w_S + \frac{3Y-X}{2} \right) + I_0 S^2 X' \end{pmatrix}. \quad (\text{B8})$$

The value of Ω_c is determined by the condition $\Gamma_{xx}(0,0) = 0$. However, the averages (B4) and (B7) which determine $1/S$ corrections to $\Gamma(\mathbf{q}, \omega_n)$ are Ω dependent themselves. For consistency, we have to calculate these averages with the zeroth-order value $\Omega_c = I_0 S$. Then we obtain the result for Ω_c Eq. (15) of the main text. At an arbitrary Ω we perform the replacement $\Omega \rightarrow I_0 S (\Omega / \Omega_c)$ in Eqs. (B4) and (B7), which changes $\Gamma(\mathbf{q}, \omega_n)$ in the order of $1/S^2$ only and gives the possibility of taking into account consistently the shift of Ω_c owing to quantum fluctuations. Substituting the result for Ω_c into Eq. (B8), we obtain the results (11), (16), and (17).

In the ordered phase we rotate the coordinate system through the angle θ around the π_y axis and again, in new coordinates, expand $\tilde{\pi}_z$ in powers of $\tilde{\pi}_x, \tilde{\pi}_y$ ($\tilde{\pi}_y = \pi_y$). Then we obtain to fourth order

$$\begin{aligned}
\mathcal{S}_{\text{st}} = & -\frac{IS^2}{2} \sum_{\langle ij \rangle} \int_0^{1/T} d\tau \left[-\tilde{\pi}_{xi} w_S^{-1} \sin 2\theta + \tilde{\pi}_{xi} \tilde{\pi}_{xj} \cos^2 \theta - (\tilde{\pi}_{xi}^2 + \tilde{\pi}_{xj}^2) \sin^2 \theta + \frac{1}{2} \tilde{\pi}_{xj} (\tilde{\pi}_{xi}^2 + \tilde{\pi}_{yj}^2) \sin 2\theta \right. \\
& + \left. \frac{(\tilde{\pi}_{xi}^2 + \tilde{\pi}_{yj}^2)(\tilde{\pi}_{xj}^2 + \tilde{\pi}_{yj}^2) - (\tilde{\pi}_{xi}^2 + \tilde{\pi}_{yj}^2)^2}{4} \sin^2 \theta \right] - \Omega S \sum_i \int_0^{1/T} d\tau \left[\tilde{\pi}_{xi} \sin \theta - \frac{\tilde{\pi}_{xi}^2 + \tilde{\pi}_{yi}^2}{2} w_S \cos \theta - \frac{(\tilde{\pi}_{xi}^2 + \tilde{\pi}_{yi}^2)^2}{8} \cos \theta \right] \\
& + \frac{TP}{2} \sum_i \int_0^{1/T} d\tau (\tilde{\pi}_{xi}^2 + \tilde{\pi}_{yi}^2), \tag{B9}
\end{aligned}$$

\mathcal{S}_{dyn} having the same form (B1) as in the disordered phase with the replacement $\pi \rightarrow \tilde{\pi}$. Determining the angle θ from the condition $\langle \tilde{\pi}_x \rangle = 0$ we obtain

$$\cos \theta = \frac{\Omega}{I_0 S} \left[1 + \frac{1}{2S} - \frac{X + 2X' + Y}{2} \right]^{-1}, \tag{B10}$$

where

$$\begin{aligned}
X = \langle \tilde{\pi}_{xi}^2 \rangle &= T \sum_{\mathbf{q}, \omega_n} \frac{I_0}{\omega_n^2 + E_{\mathbf{q}}^2}, \\
X' = \langle \tilde{\pi}_{xi} \tilde{\pi}_{xj} \rangle &= T \sum_{\mathbf{q}, \omega_n} \frac{I_{\mathbf{q}}}{\omega_n^2 + E_{\mathbf{q}}^2}, \\
Y = \langle \tilde{\pi}_{yi}^2 \rangle &= T \sum_{\mathbf{q}, \omega_n} \frac{I_0 - \eta I_{\mathbf{q}}}{\omega_n^2 + E_{\mathbf{q}}^2}. \tag{B11}
\end{aligned}$$

$E_{\mathbf{q}} = S \sqrt{I_0(I_0 - \eta I_{\mathbf{q}})}$ and $\eta = (\Omega/I_0 S)^2$. Besides the averages Eq. (B11), we introduce the quantity

$$Y = i \langle \tilde{\pi}_{xi} (\partial \tilde{\pi}_{yi} / \partial \tau) \rangle = \frac{T}{S} \sum_{\mathbf{q}, \omega_n} \frac{\omega_n^2}{\omega_n^2 + E_{\mathbf{q}}^2}. \tag{B12}$$

For the two-point vertex function of the fields $\tilde{\pi}_x, \tilde{\pi}_y$ we have

$$\Gamma(\mathbf{q}, \omega_n) = \begin{pmatrix} I_0 S^2 (1 + X - \eta X') - I_{\mathbf{q}} S^2 W + F_{\mathbf{q}n} + SY - TP & iS\omega_n \left(w_S + \frac{X+Y}{2} \right) \\ iS\omega_n \left(w_S + \frac{Y+X}{2} \right) & I_0 S^2 (1 + Y - \eta X') + SY - TP \end{pmatrix}, \tag{B13}$$

where

$$W = \eta(w_S + X + 2X' + Y) + (1 - \eta)X'. \tag{B14}$$

The term with

$$\begin{aligned}
F_{\mathbf{q}n} = & -\frac{S^4}{2T} \eta(1 - \eta) \sum_{\mathbf{k}, \omega_m} [(2I_{\mathbf{k}} I_{\mathbf{k}+\mathbf{q}} + 4I_{\mathbf{q}} I_{\mathbf{k}} \\
& + 2I_{\mathbf{k}+\mathbf{q}}^2 + I_{\mathbf{q}}^2) M_{xxxx}(k, q) + I_{\mathbf{q}}^2 M_{yyyy}(k, q) \\
& + 2I_{\mathbf{q}}(I_{\mathbf{q}} + 2I_{\mathbf{k}}) M_{xyxy}(k, q)], \tag{B15}
\end{aligned}$$

where $k = (\mathbf{k}, \omega_m)$, $q = (\mathbf{q}, \omega_n)$ and

$$M_{\alpha\beta\gamma\delta}(k, q) = \langle \tilde{\pi}_{\alpha}(k) \tilde{\pi}_{\beta}(-k) \tilde{\pi}_{\gamma}(k+q) \tilde{\pi}_{\delta}(-k-q) \rangle, \tag{B16}$$

($\alpha, \beta, \gamma, \delta = x, y$) arises due to the contribution of the cubic term in Eq. (B9) in the second order of perturbation theory.

This term has the same order in $1/S$ as other terms and should be retained. Using the identity

$$I_0 S^2 X + SY - TP = I_0 S^2 \eta X', \tag{B17}$$

which is an analog of Eq. (B6) for the ordered phase, we obtain

$$\begin{aligned}
\Gamma(\mathbf{q}, \omega_n) &= \begin{pmatrix} S^2(I_0 - WI_{\mathbf{q}}) + F_{\mathbf{q}n} & iS\omega_n(w_S + X/2 + Y/2) \\ iS\omega_n(w_S + X/2 + Y/2) & I_0 S^2(1 + Y - X) \end{pmatrix}. \tag{B18}
\end{aligned}$$

Performing again the replacement $\Omega \rightarrow I_0 S(\Omega/\Omega_c)$ in Eq. (B11) and reexpressing Eq. (B18) in terms of Ω_c , we obtain the results (11), (19), and (20) of the main text. For the temperature-dependent order parameter we obtain

$$\begin{aligned} \bar{S} &\equiv S \langle \pi_x \rangle = S \sin \theta \langle \tilde{\pi}_x \rangle & \tilde{X}_i^{pq} &= U^\dagger(\theta) X_i^{pq} U(\theta) \quad (C1) \\ &= S \left\{ 1 - \eta - \frac{\eta}{2S} \sum_{\mathbf{q}} \frac{2I_0 + \eta I_{\mathbf{q}}}{\sqrt{I_0(I_0 - \eta I_{\mathbf{q}})}} \coth \frac{S \sqrt{I_0(I_0 - \eta I_{\mathbf{q}})}}{2T} \right. & \text{with} & \\ &\quad \left. + \frac{\eta}{2S} \sum_{\mathbf{q}} \frac{2I_0 + I_{\mathbf{q}}}{\sqrt{I_0(I_0 - I_{\mathbf{q}})}} \right\}^{1/2} \left(1 + \frac{1}{2S} - \frac{X_0 + Y_0}{2} \right). \quad (B19) & U(\theta) &= \exp[\theta(X^{-1,1} - X^{1,-1})/2] \\ & & &= 1 + [\cos(\theta/2) - 1](X^{-1,-1} + X^{1,1}) \\ & & &\quad + \sin(\theta/2)(X^{-1,1} - X^{1,-1}). \quad (C2) \end{aligned}$$

Note that near the QPT the last multiplier in this expression is close to unity and only slightly temperature dependent. Thus it can be replaced by its zero-temperature value.

Then the Hamiltonian takes the form

APPENDIX C: ROTATION IN SU(3) SPACE FOR THE EASY-PLANE HEISENBERG MODEL

$$\mathcal{H} = \mathcal{H}^{(1)} + \mathcal{H}^{(2)} \quad (C3)$$

Following Refs. 20,22,23 we perform in the Hamiltonian (82) the unitary transformation

with

$$\begin{aligned} \mathcal{H}^{(1)} &= \frac{1}{2} \sum_i [(D \sin \theta + 2\mathcal{I}_0 \cos^2 \theta)(2X_i^{11} + X_i^{00}) + DX_i^{00} + (D - 2\mathcal{I}_0 \sin \theta) \cos \theta (X_i^{1,-1} + X_i^{-1,1})], \\ \mathcal{H}^{(2)} &= -\frac{\mathcal{I}}{2} \sum_{\langle ij \rangle} [\cos \theta (2X_i^{11} + X_i^{00}) - \sin \theta (X_i^{1,-1} + X_i^{-1,1})][\cos \theta (2X_j^{11} + X_j^{00}) - \sin \theta (X_j^{1,-1} + X_j^{-1,1})] \\ &\quad - \frac{\mathcal{I}}{2} \sum_{\langle ij \rangle} \sum_{\sigma=\pm 1} [2X_i^{0\sigma} X_j^{\sigma 0} + \sigma \sin \theta (X_i^{0\sigma} X_j^{0\sigma} + X_i^{\sigma 0} X_j^{\sigma 0}) + \cos \theta (X^{-\sigma 0} X^{\sigma 0} + X^{0,-\sigma} X^{0\sigma})], \quad (C4) \end{aligned}$$

where $\mathcal{I}_0 = 2d\mathcal{I}$ and we have dropped the tilde sign at the X operators. Further we represent Hubbard operators via boson ones^{22,23}

$$\begin{aligned} X^{1,-1} &= a^\dagger (1 - \lambda a^\dagger a - \lambda b^\dagger b)^{1/2}, \\ X^{0,-1} &= b^\dagger (1 - \lambda a^\dagger a - \lambda b^\dagger b)^{1/2}, \quad (C5) \\ X^{10} &= a^\dagger b, \quad X^{00} = b^\dagger b, \quad X^{11} = a^\dagger a, \end{aligned}$$

where $\lambda (= 1)$ is the parameter introduced to construct perturbation theory (cf. the Holstein-Primakoff expansion in the case of a Heisenberg magnet). Then we obtain the Hamiltonian of the bosons

$$\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_2 + \mathcal{H}_3 + \mathcal{H}_4 + \dots, \quad (C6)$$

where

$$\mathcal{H}_1 = \frac{1}{2} \cos \theta (D - 2\mathcal{I}_0 \sin \theta) \sum_i (a_i^\dagger + a_i) \quad (C7)$$

$$\begin{aligned} \mathcal{H}_2 &= (D \sin \theta + 2\mathcal{I}_0 \cos^2 \theta) \sum_i a_i^\dagger a_i + [D(1 + \sin \theta)/2 + \mathcal{I}_0 \cos^2 \theta] \sum_i b_i^\dagger b_i \\ &\quad - \frac{\mathcal{I}}{2} \sum_{\langle ij \rangle} [\sin^2 \theta (a_i^\dagger + a_i)(a_j^\dagger + a_j) + 2b_i^\dagger b_j - \sin \theta (b_i^\dagger b_j^\dagger + b_i b_j)] \quad (C8) \end{aligned}$$

$$\begin{aligned} \mathcal{H}_3 &= -\frac{1}{2} \cos \theta (D - 2\mathcal{I}_0 \sin \theta) \sum_i [a_i^\dagger (a_i^\dagger a_i + b_i^\dagger b_i) + (a_i^\dagger a_i + b_i^\dagger b_i) a_i] \\ &\quad + \mathcal{I} \cos \theta \sum_{\langle ij \rangle} [\sin \theta (2a_i^\dagger a_i + b_i^\dagger b_i)(a_j^\dagger + a_j) - (b_i a_j^\dagger b_j + b_i^\dagger b_j^\dagger a_j)] \quad (C9) \end{aligned}$$

$$\begin{aligned} \mathcal{H}_4 = & -\frac{\mathcal{I}}{2} \sum_{\langle ij \rangle} [\sin^2 \theta (a_i^\dagger a_i + 2b_i^\dagger b_i)(a_j^\dagger a_j + 2b_j^\dagger b_j) + 2a_i^\dagger a_j b_j^\dagger b_i - \cos^2 \theta (b_i^\dagger + b_i)(a_j^\dagger a_j b_j^\dagger + b_j^\dagger b_j^\dagger b_j + \text{H.c.}) + \cos 2\theta (a_i a_j b_i^\dagger b_j^\dagger \\ & + \text{H.c.}) - (a_i^\dagger a_j^\dagger a_j a_j + a_i^\dagger b_j^\dagger b_j a_j + \text{H.c.}) + \cos 2\theta (a_i^\dagger a_i^\dagger a_i a_j^\dagger + a_i^\dagger b_i^\dagger b_i a_j^\dagger + \text{H.c.})], \end{aligned} \quad (\text{C10})$$

and we have omitted terms containing more than four Bose operators. Diagonalizing the quadratic part \mathcal{H}_2 of the Hamiltonian (C6) we obtain

$$\mathcal{H}_2 = \sum_{\mathbf{k}} (E_{\mathbf{k}\alpha} \alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}} + E_{\mathbf{k}\beta} \beta_{\mathbf{k}}^\dagger \beta_{\mathbf{k}}), \quad (\text{C11})$$

where the spectra of excitations are given by

$$E_{\mathbf{k}\alpha} = 2\sqrt{\mathcal{I}_0(\mathcal{I}_0 - \eta^2 \mathcal{I}_{\mathbf{k}})}, \quad (\text{C12})$$

$$E_{\mathbf{k}\beta} = \sqrt{(1 + \eta)(\mathcal{I}_0 - \mathcal{I}_{\mathbf{k}})[\mathcal{I}_0 - \mathcal{I}_{\mathbf{k}} + \eta(\mathcal{I}_0 + \mathcal{I}_{\mathbf{k}})]}, \quad (\text{C13})$$

$\eta = \sin \theta = D/D_c$. The angle θ is determined by the condition $\langle a_i \rangle = 0$. To first order in the formal parameter λ we have

$$\sin \theta = \frac{D}{2I_0} [1 - \lambda(R_1 + R_2)]^{-1}, \quad (\text{C14})$$

$$R_1(T) = 2 \sum_{\mathbf{k}} \frac{2I_0 + (2 - \eta^2)I_{\mathbf{k}}}{2E_{\mathbf{k}\alpha}} (1 + 2N_{\mathbf{k}\beta}) - 1,$$

$$R_2(T) = \sum_{\mathbf{k}} \frac{(1 + \eta)I_0 - I_{\mathbf{k}} + \eta I_{\mathbf{k}}^2 / I_0}{2E_{\mathbf{k}\beta}} (1 + 2N_{\mathbf{k}\alpha}) - \frac{1}{2}. \quad (\text{C15})$$

The excitation spectrum for mode α to first order in λ is given by

$$\tilde{E}_{\mathbf{k},\alpha} = 2\sqrt{\mathcal{I}_0(1 + B_0 + B_1)(\mathcal{I}_0 - \mathcal{I}_{\mathbf{k}} + \mathcal{I}_0 \Delta_-^2)}, \quad (\text{C16})$$

where

$$\Delta_-^2 = (1 + A_0 + A_1)(1 - \eta^2)$$

and

$$A_0 = \lambda \sum_{\mathbf{k}} \left[\frac{\eta^2 \gamma_{\mathbf{k}} - 4\gamma_{\mathbf{k}} - 4}{E_{\mathbf{k}\alpha}} + \frac{\gamma_{\mathbf{k}}(1 + \eta + \eta^2)/(1 + \eta) - (\eta + 1)}{E_{\mathbf{k}\beta}} \right], \quad (\text{C17a})$$

$$B_0 = -\frac{\lambda}{2} \sum_{\mathbf{k}} \left[\frac{8(1 + \gamma_{\mathbf{k}}) - 20\eta^2 \gamma_{\mathbf{k}} + 11\eta^4 \gamma_{\mathbf{k}}}{E_{\mathbf{k}\alpha}} + \frac{2(1 + \eta) - 2\gamma_{\mathbf{k}} + 2\eta^3 \gamma_{\mathbf{k}}^2}{E_{\mathbf{k}\beta}} \right], \quad (\text{C17b})$$

$$\begin{aligned} A_1 = & 2\eta^2 \lambda \sum_{\mathbf{k}} \frac{(5/2)(2 - \eta^2 \gamma_{\mathbf{k}})^2 + 4(2 - \eta^2 \gamma_{\mathbf{k}}) \eta^2 \gamma_{\mathbf{k}} + (5/2)(\eta^2 \gamma_{\mathbf{k}})^2}{E_{\mathbf{k}\alpha}^3} \\ & + \frac{\lambda}{2} \sum_{\mathbf{k}} \frac{(\eta^2 + 1)(1 + \eta - \gamma_{\mathbf{k}})^2 + (\eta^2 + 1)(\eta \gamma_{\mathbf{k}})^2 + 4\eta(1 + \eta - \gamma_{\mathbf{k}})(\eta \gamma_{\mathbf{k}})}{E_{\mathbf{k}\beta}^3} \end{aligned} \quad (\text{C17c})$$

$$B_1 = \frac{\lambda}{2} (1 - \eta^2) \sum_{\mathbf{k}} \left[\frac{4\eta^2(2 - \eta^2 \gamma_{\mathbf{k}})}{E_{\mathbf{k}\alpha}^3} + \frac{(1 + \eta - \gamma_{\mathbf{k}})^2 - (\eta \gamma_{\mathbf{k}})^2}{E_{\mathbf{k}\beta}^3} \right]. \quad (\text{C17d})$$

The mode β is a Goldstone type and is gapless to arbitrary order in λ . Therefore we do not consider the renormalization of its energy.

APPENDIX D: RENORMALIZATION OF THE TWO-COMPONENT ϕ^4 MODEL WITH SPONTANEOUSLY BROKEN SYMMETRY

In this appendix we consider the renormalization of the action (95) in the ordered phase, $m^2 < 0$. Introducing the quantity $\kappa^2 = -2m^2 > 0$ and performing the shift $\pi_x \rightarrow \pi_x + \pi_0$ we obtain

$$\begin{aligned} \mathcal{S} = & \frac{1}{2} \int_0^{c/T} d\tau \int d^d r [(\partial \boldsymbol{\pi})^2 + (\kappa^2 + 3\tilde{h}) \pi_x^2 + \tilde{h} \pi_y^2] \\ & + \frac{u}{4!} \int_0^{c/T} d\tau \int d^d r (4\pi_x + \boldsymbol{\pi}^2) \boldsymbol{\pi}^2, \end{aligned} \quad (\text{D1})$$

where $\tilde{h} = h/\bar{\pi}_0$, $\bar{\pi}_0 = (3\kappa^2/u)^{1/2}$, and $\pi_0 = \bar{\pi}_0(1 + \tilde{h}/\kappa^2)$ is determined by the requirement of absence in the action of terms that are linear in π_x . In these notations the condition of smallness of the magnetic field is $\tilde{h}^{1/2} \ll \kappa$ (the condition of closeness to the QPT $\kappa \ll \Lambda$ is also assumed). Under these conditions, the action (D1) has two characteristic lengths, $1/\tilde{h}^{1/2}$ and $1/\kappa$. This situation is the same as in the theory of crossover phenomena.³⁸ Further we follow Ref. 38 to include exactly the smaller characteristic length into the Z factors. Then we obtain to one-loop order

$$\begin{aligned} Z^{\text{cont}} &= 1 + \mathcal{O}(g^2), \\ Z_2^{\text{cont}} &= 1 + \frac{g}{2\varepsilon} \frac{1}{(1 + \kappa^2/\mu^2)^{\varepsilon/2}} + \frac{g}{6\varepsilon} - \frac{2g}{3\varepsilon} \frac{\mu^\varepsilon}{\Lambda^\varepsilon}, \quad (\text{D2}) \\ Z_4^{\text{cont}} &= 1 + \frac{3g}{2\varepsilon} \frac{1}{(1 + \kappa^2/\mu^2)^{\varepsilon/2}} + \frac{g}{6\varepsilon} - \frac{5g}{3\varepsilon} \frac{\mu^\varepsilon}{\Lambda^\varepsilon}. \end{aligned}$$

(note that the Ward identities guarantee that the structure of the interaction term is preserved by renormalizations, and one renormalization constant is sufficient to renormalize all four-particle vertex functions, see, e.g., Ref. 35). The flow functions for the effective-Hamiltonian parameters are

$$\begin{aligned} \beta(g, \kappa/\mu) &= -\varepsilon g + \frac{3g^2}{2} \frac{1}{1 + \kappa^2/\mu^2} + \frac{g^2}{6}, \\ \gamma(g, \kappa/\mu) &= -\frac{g}{2} \frac{1}{1 + \kappa^2/\mu^2} - \frac{g}{6}. \end{aligned} \quad (\text{D3})$$

Setting in these expressions $\varepsilon = 0$, performing the integration, and supposing that scaling starts at $\mu \gg \kappa$, we obtain the effective-Hamiltonian parameters at the scale $\mu\rho$

$$\frac{1}{g_\rho} = \frac{1}{g} - \frac{3}{4} \ln(\rho^2 + \kappa^2/\mu^2) - \frac{1}{6} \ln \rho,$$

$$\begin{aligned} \kappa_\rho^2 &= \kappa^2 \exp \left[\frac{g}{2} \int_1^\rho d\rho' \left(\frac{\rho'}{\rho'^2 + \kappa^2/\mu^2} + \frac{1}{3\rho'} \right) \right. \\ & \left. \times \frac{1}{1 - (g/6) \ln \rho' - (3g/4) \ln(\rho'^2 + \kappa^2/\mu^2)} \right]. \end{aligned} \quad (\text{D4})$$

Our plan now is to use these scaling formulas to reach the scale $\mu\rho \sim \tilde{h}^{1/2} \ll \kappa$. For these values of ρ formulas (D4) are simplified:

$$\begin{aligned} g_\rho^{-1} &= g^{-1} [1 - (3g/2) \ln(\kappa/\mu) - (g/6) \ln \rho], \\ \kappa_\rho^{-2} &= \kappa^{-2} [1 - (3g/2) \ln(\kappa/\mu) - (g/6) \ln \rho] \\ & \times [1 - (5g/3) \ln(\kappa/\mu)]^{-3/5} \Phi_0(g, \kappa^2/\mu^2), \end{aligned} \quad (\text{D5})$$

where $\Phi_0(g, x)$ is given by

$$\begin{aligned} \ln \Phi_0(g, x) &= \frac{g}{12} \int_0^1 \frac{dy}{y} \left[\frac{4y+x}{y+x} \right. \\ & \times \frac{1}{1 - (g/12) \ln y - (3g/4) \ln(x+y)} \\ & - \frac{\theta(x-y)}{1 - (g/12) \ln y - (3g/4) \ln x} \\ & \left. - \frac{4\theta(y-x)}{1 - (5g/6) \ln y} \right], \end{aligned} \quad (\text{D6})$$

and $\theta(x)$ is the step function. At extremely small x we have $\Phi(g, x) \approx \exp(1/\ln^2 x) \approx 1$. The result (D5) with $\Phi(g, \kappa^2/\mu^2) = 1$ can be obtained more directly if we perform the scaling procedure in two steps: at the first step $\rho \gg \kappa/\mu$ and the flow functions are the same as for the two-component isotropic ϕ^4 model, while at the second step $\rho \ll \kappa/\mu$ and the flow functions include only contributions of the Goldstone modes. The scaling formulas are joined at $\rho = \kappa/\mu$. However, this procedure does not give the possibility of describing correctly the contribution of the crossover region $\rho \sim \kappa/\mu$. At finite but small ε we obtain in a similar way

$$\begin{aligned} g_\rho^{-1} &= g^{-1} [1 + (3g/2\varepsilon)(\kappa^{-\varepsilon}/\mu^{-\varepsilon} - 1) + (g/6\varepsilon)(\rho^{-\varepsilon} - 1)], \\ \kappa_\rho^{-2} &= \kappa^{-2} [1 + (3g/2\varepsilon)(\kappa^{-\varepsilon}/\mu^{-\varepsilon} - 1) + (g/6\varepsilon)(\rho^{-\varepsilon} - 1)] \\ & \times [1 - (5g/3\varepsilon)(\kappa^{-\varepsilon}/\mu^{-\varepsilon} - 1)]^{-3/5} \Phi_\varepsilon(g, \kappa^2/\mu^2) \end{aligned} \quad (\text{D8})$$

with some function $\Phi_\varepsilon(g, x) \approx 1$. Putting in the above results $\mu = \Lambda = (2d)^{1/2}$, we obtain the result (96) of the main text.

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