

Low-temperature thermodynamics of the classical frustrated ferromagnetic chain in a magnetic field

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(Received 6 October 2011; revised manuscript received 12 December 2011; published 27 December 2011)

Low-temperature magnetization curves of the classical frustrated ferromagnetic chain in the external magnetic field near the transition point between the ferromagnetic and the helical phases is studied. It is shown that the calculation of the partition function in the scaling limit reduces to the solution of the Schrödinger equation of the special form for the quantum particle. It is proposed that the magnetization of the classical model in the ferromagnetic part of the phase diagram including the transition point defines the universal scaling function which is valid for the quantum model as well. Explicit analytical formulas for the magnetization are given in the limiting cases of low and high magnetic fields. The influence of the easy-axis anisotropy on the magnetic properties of the model is studied. It is shown that even small anisotropy essentially changes the behavior of the susceptibility in the vicinity of the transition point.

DOI: 10.1103/PhysRevB.84.214438

PACS number(s): 75.10.Hk, 75.10.Jm

I. INTRODUCTION

Strongly frustrated low-dimensional magnets have attracted much attention in recent years.¹ A very interesting class of such compounds is edge-sharing chains where CuO_4 plaquets are coupled by their edges.²⁻⁷ An important feature of the edge-sharing chains is that the nearest-neighbor (NN) interaction J_1 between Cu spins is ferromagnetic while the next-nearest-neighbor (NNN) interaction J_2 is antiferromagnetic. The competition between them leads to the frustration. A minimal model describing the magnetic properties of these cuprates is the so-called F-AF spin chain model the Hamiltonian of which has the form

$$H = J_1 \sum \mathbf{S}_n \cdot \mathbf{S}_{n+1} + J_2 \sum \mathbf{S}_n \cdot \mathbf{S}_{n+2} - h \sum S_n^z, \quad (1)$$

where \mathbf{S}_n is the spin operator on n th site, h is the external magnetic field, and the exchange integrals are $J_1 < 0$ and $J_2 > 0$.

This model is characterized by the frustration parameter $\alpha = J_2/|J_1|$. The ground-state phase diagram of the quantum $s = \frac{1}{2}$ model has been intensively studied.⁸⁻¹⁷ The ground state of model (1) at $h = 0$ is ferromagnetic for $\alpha < \frac{1}{4}$. At $\alpha = \frac{1}{4}$ the quantum phase transition to the phase with incommensurate spin correlations of the helical type takes place. Remarkably, this transition occurs at the same frustration parameter $\alpha = \frac{1}{4}$ both in the quantum and in the classical model. However, the influence of the frustration on the low-temperature thermodynamics in the vicinity of the transition point is less studied. This problem is of a special interest because the recently studied edge-sharing compound $\text{Li}_2\text{ZrCuO}_4$ is well described by the F-AF model with the frustration parameter close to $\alpha = \frac{1}{4}$.¹⁸

At present the low-temperature thermodynamics of the quantum $s = \frac{1}{2}$ model at $\alpha \neq 0$ can be studied only either by numerical calculation of finite chains or by approximate methods. On the other hand, the classical version of model (1) can be studied exactly at $T \rightarrow 0$ and the classical limit is a starting point for the study of quantum effects. Another reason to study the classical version of F-AF model comes from the following argument established for the quantum spin- s ferromagnetic chain, i.e., for model (1) at $\alpha = 0$. It was conjectured in Ref. 19 that the low-temperature magnetization of this model is

a function of the scaling variable $g_F = s^3|J_1|h/T^2$. According to this scaling hypothesis the normalized magnetization $m = \langle S^z \rangle / s$ ($\langle S^z \rangle$ is the magnetization per site) of the quantum chain is expressed as

$$m(T, h) = \phi(g_F). \quad (2)$$

This equation is valid in the scaling limit, which means that $T \rightarrow 0$ and $h \rightarrow 0$ but g_F is fixed. Then the dependence of the magnetization m on the spin magnitude s comes only via the scaling variable g_F . Generally, the calculation of the function $\phi(g_F)$ is a very complicated problem. It was proposed in Ref. 19 that this function can be obtained from the solution of the classical ferromagnetic chain and such scaling function $\phi(g_F)$ was obtained explicitly in Ref. 19,20. In particular, the zero-field susceptibility χ is

$$\chi = s \left. \frac{dm}{dh} \right|_{h=0} = \frac{2s^4|J_1|}{3T^2}. \quad (3)$$

Actually the conjecture of the universality of the function $\phi(g_F)$ is based on the following observations:^{19,21} The zero-field susceptibility of the $s = \frac{1}{2}$ Heisenberg ferromagnetic chain at $T \rightarrow 0$ coincides with that given by Eq. (3); the magnetization $m(T, h)$ obtained numerically from the thermodynamic Bethe-ansatz equations and plotted as a function of $g_F = h/8T^2$ approaches $\phi(g_F)$ at $T \rightarrow 0$; the leading terms of the spin-wave expansion for magnetization coincide with those for $\phi(g_F)$. In addition, as noted in Ref. 19, the hypothesis of the universality originates in the universal behavior of the spin-wave excitations from the ferromagnetic ground state for both quantum and classical model. For this reason it is natural to expect that such universality remains for all α corresponding to the ferromagnetic ground state, i.e., for $0 \leq \alpha \leq \frac{1}{4}$. Moreover, the function $\phi(g_F)$ for $0 \leq \alpha < \frac{1}{4}$ (but α not too close to $\frac{1}{4}$) will be the same as for $\alpha = 0$ but with g_F replaced by $g_F(1 - 4\alpha)$. Really, the zero-field susceptibility $\chi = 2s^4(1 - 4\alpha)/3T^2$ fits very well with numerical and analytical results.²² However, χT^2 vanishes at $\alpha = \frac{1}{4}$ signaling the change of the critical exponent at the transition point.

In our previous paper²³ we studied the zero-field susceptibility of the classical F-AF chain exactly at the transition point $\alpha = \frac{1}{4}$ and we have shown that $\chi \sim T^{-4/3}$ in contrast with the

low-temperature asymptotic $\chi \sim T^{-2}$ for $0 \leq \alpha < \frac{1}{4}$. As was shown in Ref. 23 the change of the critical exponent for χ is a consequence of the modification of the energy of spin-wave excitations from $\varepsilon(k) \sim k^2$ for $0 \leq \alpha < \frac{1}{4}$ to $\varepsilon(k) \sim k^4$ at $\alpha = \frac{1}{4}$. Therefore, the form of the universal magnetization curve and the scaling variable for $\alpha = \frac{1}{4}$ (if the universality is valid) differ from the case $0 \leq \alpha < \frac{1}{4}$ and require a special study.

Another interesting problem related to the F-AF model is the influence of the anisotropy of exchange interactions of the easy-axis type on the low-temperature magnetic properties of this model. This problem is actual because it is known that in the real edge-sharing compounds the exchange interactions are anisotropic and the anisotropy can be of the easy-axis type.^{24,25} Although this anisotropy is weak it can be important especially near the transition point. In particular, it essentially changes the behavior of the zero-field susceptibility.²⁶

In this paper we investigate the effect of weak anisotropy on the magnetic curves of the classical F-AF model at the transition point. In the low-temperature limit the easy-axis anisotropy of the NN and NNN interactions have the same effect (we will explain this fact below) and for simplicity we consider the anisotropy of the NN interaction only; i.e., we add to Hamiltonian (1) the term

$$-(\Delta - 1) \sum S_n^z S_{n+1}^z, \quad (4)$$

where $\Delta > 1$.

It is interesting to note that for the pure ferromagnetic case ($\alpha = 0$) the similarity in the magnetic properties of quantum and classical models remains in the case of the easy-axis anisotropy. This resemblance is based on the close relation between the classical solitons and the quantum multimagnon bound complexes. In this paper we will elucidate the question of to which extent the resemblance between the anisotropic quantum and classical models remains in the F-AF model.

The paper is organized as follows. In Sec. II the continuum version of the model is introduced and the scaling parameters are determined. The calculation of the partition function is reduced to the solution of the Schrödinger equation of a special type. In Sec. III the behavior of the magnetization curve at the transition point is studied. The asymptotics of magnetization for low and high magnetic field are presented and the relation to the quantum spin model is discussed. The numerical and analytical results for the magnetization curve in the helical phase are given in Sec. IV. In Sec. V the influence of the easy-axis anisotropy on the magnetic properties is studied. The summary of the obtained results is given in Sec. VI.

II. PARTITION FUNCTION IN THE CONTINUUM LIMIT

In Refs. 23,27 we studied the partition function and the spin correlation functions of the classical F-AF chain in the vicinity of the transition point $\alpha = \frac{1}{4}$ at zero magnetic field. This study was based on the use of a continuum approximation and the interpretation of the partition function as a path integral for the quantum particle in a potential well. However, the extension of the model to nonzero magnetic field and/or nonzero anisotropy needs the essential modification of this approach.

In the vicinity of the transition point $\alpha = \frac{1}{4}$ it is convenient to rewrite Hamiltonian (1) with the anisotropic term (4) in the form

$$\begin{aligned} H = & \frac{1}{8} \sum (\mathbf{S}_{n+1} - 2\mathbf{S}_n + \mathbf{S}_{n-1})^2 \\ & - \frac{1}{2} \left(\alpha - \frac{1}{4} \right) \sum (\mathbf{S}_{n+2} - \mathbf{S}_n)^2 \\ & - (\Delta - 1) \sum S_n^z S_{n+1}^z - h \sum S_n^z. \end{aligned} \quad (5)$$

In Eq. (5) we put $|J_1| = 1$ and omit the unessential constant.

In the classical approximation the spin operators \mathbf{S}_i are replaced by the classical vectors $\vec{S}_i = s\vec{n}_i$, where \vec{n}_i are the unit vectors. In the low-temperature limit the thermal fluctuations are weak so that neighbor spins are directed almost parallel to each other. Therefore, at $T \rightarrow 0$ we can use the continuum approximation replacing \vec{n}_i by the classical unit vector field $\vec{n}(x)$, so that

$$(\vec{S}_{i+1} - 2\vec{S}_i + \vec{S}_{i-1}) \simeq s \frac{d^2 \vec{n}(x)}{dx^2}, \quad (\vec{S}_{i+2} - \vec{S}_i) \simeq 2s \frac{d\vec{n}(x)}{dx}, \quad (6)$$

where the lattice constant is chosen as unit length.

Using Eqs. (6) Hamiltonian (5) goes over into the energy functional

$$\begin{aligned} E[\vec{n}(x)] = & \int dx \left[\frac{s^2}{8} \left(\frac{d^2 \vec{n}}{dx^2} \right)^2 - \frac{s^2(4\alpha - 1)}{2} \left(\frac{d\vec{n}}{dx} \right)^2 \right. \\ & \left. - s^2(\Delta - 1)n_z^2 - shn_z \right]. \end{aligned} \quad (7)$$

One can easily check that in the continuum approximation the easy-axis anisotropy of NNN interactions Δ_2 results in the term $\alpha s^2(\Delta_2 - 1)n_z^2$. This term merely changes the coefficient in the third term of Eq. (7), so that the results obtained below cover the case of the NNN anisotropy as well.

Energy functional (7) contains the second-order derivative $d^2 \vec{n}/dx^2$ in contrast with that for the ferromagnetic chain,¹⁹ which contains the first-order derivative $d\vec{n}/dx$ only. This fact demonstrates an essential difference between the cases $\alpha = 0$ and $\alpha = \frac{1}{4}$.

The partition function is a functional integral over all configurations of the vector field on a ring of length L :

$$Z = \int D[\vec{n}(x)] \exp \left(- \frac{E[\vec{n}(x)]}{T} \right). \quad (8)$$

It is useful to scale the spatial variable as

$$\xi = \frac{T^{1/3} x}{s^{2/3}}. \quad (9)$$

Then, the partition function takes the dimensionless form

$$\begin{aligned} Z = & \int D[\vec{n}(\xi)] \exp \left\{ - \int_0^\lambda d\xi \left[\frac{1}{8} \left(\frac{d^2 \vec{n}}{d\xi^2} \right)^2 \right. \right. \\ & \left. \left. - \frac{\gamma}{2} \left(\frac{d\vec{n}}{d\xi} \right)^2 - \delta n_z^2 - g n_z \right] \right\}, \end{aligned} \quad (10)$$

where

$$\lambda = \frac{T^{1/3} L}{s^{2/3}} \quad (11)$$

is the scaled system length and

$$\gamma = \frac{(4\alpha - 1)s^{4/3}}{T^{2/3}}, \quad \delta = \frac{(\Delta - 1)s^{8/3}}{T^{4/3}}, \quad g = \frac{hs^{5/3}}{T^{4/3}} \quad (12)$$

are the parameters of the model scaled by temperature.

As follows from Eq. (10) the partition function and with it the low-temperature thermodynamics of the F-AF model near the transition point is governed by three scaling parameters γ , δ , and g . The definition of the scaling parameters (12) implies that we consider the scaling limit when $T \rightarrow 0$, $\alpha \rightarrow \frac{1}{4}$, $\Delta \rightarrow 1$, $h \rightarrow 0$, but the values of the scaling parameters γ , δ , and g are finite.

We express the unit vector field through two scalar fields $\phi(\xi)$ and $n_z(\xi)$,

$$\vec{n}(\xi) = (\cos \phi \sqrt{1 - n_z^2}, \sin \phi \sqrt{1 - n_z^2}, n_z), \quad (13)$$

and the magnetic field is directed along the Z axis. In terms of the fields $n_z(\xi)$ and $\phi(\xi)$ the partition function takes the form of the functional integral

$$Z = \int D[n_z(\xi)] D[\phi(\xi)] \exp \left\{ - \int_0^\lambda W(n_z, \phi) d\xi \right\}, \quad (14)$$

where the energy density $W(n_z, \phi)$ has a rather cumbersome form:

$$\begin{aligned} W = & \frac{1}{8} \left[(1 - n_z^2)(\dot{\phi}^2 + \dot{\phi}^4) + \frac{\ddot{n}_z^2}{1 - n_z^2} + \frac{\dot{n}_z^4}{(1 - n_z^2)^3} \right. \\ & \left. - 4n_z \dot{n}_z \dot{\phi} \ddot{\phi} + \frac{2n_z \dot{n}_z \ddot{n}_z}{(1 - n_z^2)^2} + 2n_z \ddot{n}_z \dot{\phi}^2 + \frac{2 + 4n_z^2}{1 - n_z^2} \dot{n}_z^2 \dot{\phi}^2 \right] \\ & - \frac{\gamma}{2} \left[\frac{\dot{n}_z^2}{1 - n_z^2} + (1 - n_z^2)\dot{\phi}^2 \right] - \delta n_z^2 - g n_z. \end{aligned} \quad (15)$$

Here \dot{n}_z , \ddot{n}_z and $\dot{\phi}$, $\ddot{\phi}$ are the first- and the second-order derivatives of n_z and ϕ with respect to ξ .

If we treat ξ as an imaginary time then partition function (14) takes the form of a path integral of a quantum particle with the Euclidean Lagrangian $W(n_z, \phi)$. Here we notice that $W(n_z, \phi)$ comprises the derivatives $\dot{\phi}$ and $\ddot{\phi}$ of the field $\phi(\xi)$, but does not contain explicitly the field $\phi(\xi)$ itself. This allows us to rewrite partition function (14) in terms of a new field

$$q(\xi) = \frac{d\phi}{d\xi}, \quad \dot{q}(\xi) = \frac{d^2\phi}{d\xi^2}. \quad (16)$$

The energy density $W(n_z, \phi)$ contains explicitly the field $n_z(\xi)$ and its derivatives \dot{n}_z and \ddot{n}_z . The presence of the second-order derivative requires the use of the special methodology developed by Ostrogradski²⁸ which allows us to obtain the Hamiltonian corresponding to the higher gradient Lagrangian. In the Ostrogradski formalism²⁹ the independent generalized coordinates are n_z and $v = \dot{n}_z$. That is, we treat the derivative $\dot{n}_z = v$ as a new independent variable, so that

$$v(\xi) = \frac{dn_z}{d\xi}, \quad \dot{v}(\xi) = \frac{d^2n_z}{d\xi^2}. \quad (17)$$

According to this formalism the Lagrangian (15) is replaced by the equivalent one

$$\begin{aligned} L = & \frac{1}{8} \left[(1 - n_z^2)(\dot{q}^2 + q^4) + \frac{v^2}{(1 - n_z^2)} + \frac{v^4}{(1 - n_z^2)^3} \right. \\ & \left. - 4n_z v q \dot{q} + \frac{2n_z v^2 \dot{v}}{(1 - n_z^2)^2} + 2n_z \dot{v} q^2 + \frac{2 + 4n_z^2}{1 - n_z^2} q^2 v^2 \right] \\ & - \frac{\gamma}{2} \left[\frac{v^2}{1 - n_z^2} + (1 - n_z^2)q^2 \right] - \delta n_z^2 - g n_z - i p (\dot{n}_z - v), \end{aligned} \quad (18)$$

where the Lagrange multiplier p ensures the equality of \dot{n}_z and v . The canonical momenta are $p = i \frac{\partial L}{\partial \dot{n}_z}$, $p_v = i \frac{\partial L}{\partial \dot{v}}$, and $p_q = i \frac{\partial L}{\partial \dot{q}}$. Then, partition function (14) takes the form written in terms of three scalar fields $q(\xi)$, $v(\xi)$, and $n_z(\xi)$:

$$Z = \int D[n_z] D[v] D[q] \exp \left\{ - \int_0^\lambda L(n_z, v, q) d\xi \right\}. \quad (19)$$

The last term in Eq. (18) is a specific property of the Ostrogradski methodology and we will pay a special attention to it because it makes the following quantum Hamiltonian a non-Hermitian one.

Now we construct the Hamilton function $H = i p \dot{n}_z + i p_v \dot{v} + i p_q \dot{q} + L$, which after replacing momenta by the corresponding differential operators $\hat{p} = -i \frac{\partial}{\partial n_z}$, $\hat{p}_v = -i \frac{\partial}{\partial v}$, and $\hat{p}_q = -i \frac{\partial}{\partial q}$ results in the quantum Hamiltonian:

$$\begin{aligned} \hat{H} = & -2(1 - n_z^2) \frac{\partial^2}{\partial v^2} - \frac{2}{1 - n_z^2} \frac{\partial^2}{\partial q^2} \\ & - n_z \left(\frac{v^2}{1 - n_z^2} + (1 - n_z^2)q^2 \right) \frac{\partial}{\partial v} + \frac{2n_z v q}{1 - n_z^2} \frac{\partial}{\partial q} \\ & + v \frac{\partial}{\partial n_z} + \frac{1}{8} \left(\frac{v^2}{1 - n_z^2} + (1 - n_z^2)q^2 \right)^2 \\ & - \frac{\gamma}{2} \left(\frac{v^2}{1 - n_z^2} + (1 - n_z^2)q^2 \right) - \delta n_z^2 - g n_z. \end{aligned} \quad (20)$$

It is convenient to change variables v , q , n_z to new variables r , φ , θ connected by the relations

$$v = r \cos \varphi \sin \theta, \quad q = \frac{r \sin \varphi}{\sin \theta}, \quad n_z = \cos \theta. \quad (21)$$

Then we obtain the Schrödinger equation for the quantum particle in the form

$$\hat{H}_0 \Psi_n - \frac{\gamma}{2} r^2 \Psi_n - g \cos \theta \Psi_n - \delta \cos^2 \theta \Psi_n = \varepsilon_n \Psi_n, \quad (22)$$

where

$$\begin{aligned} \hat{H}_0 = & -2 \left(\frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \varphi^2} \right) \\ & + \frac{1}{8} r^4 + r \sin \varphi \cot \theta \frac{\partial}{\partial \varphi} - r \cos \varphi \frac{\partial}{\partial \theta} \end{aligned} \quad (23)$$

describes the model at the transition point at $h = 0$. The last two terms in Eq. (23) make the Hamiltonian to be non-

Hermitian one. Therefore, we have to consider the transposed counterpart of Eq. (22):

$$\hat{H}_0^T \Phi_n - \frac{\gamma}{2} r^2 \Phi_n - g \cos \theta \Phi_n - \delta \cos^2 \theta \Phi_n = \varepsilon_n \Phi_n. \quad (24)$$

The transposed differential operator \hat{H}_0^T has the same form as \hat{H}_0 , but the sign of the last two terms in Eq. (23) is changed. This change of sign is equivalent to the change $\theta \rightarrow -\theta$, which implies that $\Phi_n(r, \theta, \varphi) = \Psi_n(r, -\theta, \varphi)$. Then, the normalization condition for functions Ψ_n takes the form

$$\frac{1}{4\pi} \int_0^\infty r dr \int_0^\pi \sin \theta d\theta \int_0^{2\pi} d\varphi \Psi_n(r, \theta, \varphi) \Psi_m(r, -\theta, \varphi) = \delta_{nm}. \quad (25)$$

As a result of the above manipulations the partition function Z can be considered as the partition function of quantum model (22) at a “temperature” $1/\lambda$:

$$Z = \sum e^{-\lambda \varepsilon_n}. \quad (26)$$

In the thermodynamic limit $\lambda \rightarrow \infty$ ($\lambda = s^{-2/3} T^{1/3} L$) only the lowest eigenvalue of Eq. (22) gives the contribution to Z . Thus, the free energy of the classical spin model is determined by the ground-state energy ε_0 of the Schrödinger equation (22). The dependence of the lowest eigenvalue ε_0 of Eq. (22) on the scaling parameters g , γ , and δ determines the magnetic properties of the system. In particular, the normalized magnetization is given by

$$m = -\frac{\partial \varepsilon_0}{\partial g}. \quad (27)$$

Thus, Eq. (22) is the main result of this paper. In general, Eq. (22) does not admit analytical solution and should be solved numerically. However, the limiting cases of high and low magnetic fields can be studied analytically. In the following we present both numerical solutions and analytical expressions for asymptotics.

III. MAGNETIZATION CURVE AT THE TRANSITION POINT

At first, let us consider the isotropic F-AF model at the transition point when $\delta = 0$ and $\gamma = 0$. For low magnetic field ($g \ll 1$) the ground-state energy ε_0 can be found using the perturbation theory (PT) in g . The numerical solution of Eq. (22) for $g = 0$ shows that the ground-state wave function does not depend on φ and θ ; i.e., it satisfies the equation

$$-2 \frac{\partial^2 \Psi_0}{\partial r^2} - \frac{2}{r} \frac{\partial \Psi_0}{\partial r} + \frac{1}{8} r^4 \Psi_0 = \varepsilon_0 \Psi_0, \quad (28)$$

and $\varepsilon_0 = 1.861$.

The eigenfunctions of Eq. (22) giving the contribution to the second order in g have the form

$$\Psi_n = f_{1n}(r) \cos \varphi \sin \theta + f_{2n}(r) \cos \theta, \quad (29)$$

where the functions $f_{1n}(r)$ and $f_{2n}(r)$ satisfy the following system of equations:

$$\begin{aligned} -2 \frac{\partial^2 f_{1n}}{\partial r^2} - \frac{2}{r} \frac{\partial f_{1n}}{\partial r} + \frac{2}{r^2} f_{1n} + \frac{1}{8} r^4 f_{1n} - r f_{2n} &= \varepsilon_n f_{1n}, \\ -2 \frac{\partial^2 f_{2n}}{\partial r^2} - \frac{2}{r} \frac{\partial f_{2n}}{\partial r} + \frac{1}{8} r^4 f_{2n} + r f_{1n} &= \varepsilon_n f_{2n}. \end{aligned} \quad (30)$$

Normalization condition (25) transforms for the functions $f_{1n}(r)$ and $f_{2n}(r)$ to equation

$$\frac{1}{3} \int_0^\infty r dr (f_{2n} f_{2m} - f_{1n} f_{1m}) = \delta_{nm}. \quad (31)$$

Further, we calculate the second-order correction to the ground-state energy in g :

$$\varepsilon = \varepsilon_0 + \frac{g^2}{9} \sum_n \frac{M_{0n}^2}{\varepsilon_0 - \varepsilon_n}, \quad (32)$$

where M_{0n} is the following matrix element:

$$M_{0n} = \int_0^\infty \Psi_0(r) f_{2n}(r) r dr. \quad (33)$$

The numerical solution of Eq. (30) and the calculation of the sum in Eq. (32) gives

$$\varepsilon = \varepsilon_0 - 0.534 g^2. \quad (34)$$

Then, the magnetization m at $g \rightarrow 0$ is

$$m = 1.07 g + O(g^3) \quad (35)$$

and the zero-field susceptibility is

$$\chi = \frac{1.07 s^{8/3}}{T^{4/3}}. \quad (36)$$

Expression (36) naturally reproduces the result found in Ref. 23 obtained by another method and confirmed by Monte Carlo simulations.³⁰ As follows from Eq. (36) the critical exponent of χ is changed from 2 to $\frac{4}{3}$ when $\alpha \rightarrow \frac{1}{4}$ from the ferromagnetic side.

If we assume that the hypothesis of the universality is valid, then the susceptibility χ at the transition point for the $s = \frac{1}{2}$ F-AF chain at $T \rightarrow 0$ is

$$\chi = \frac{0.1681}{T^{4/3}}. \quad (37)$$

Unfortunately, the exact low-temperature asymptotic of χ for the $s = \frac{1}{2}$ F-AF model at $\alpha = \frac{1}{4}$ is unknown. However, we can compare Eq. (37) with the susceptibility obtained for this model by the approximate modified spin-wave method (MSWT) proposed by Takahashi.³¹ The MSWT gives $\chi = 0.099 T^{-4/3}$.^{26,30} The comparison of MSWT result with Eq. (37) shows that the critical exponents of both expressions are the same although the prefactors are different. In Ref. 30 the transfer-matrix renormalization group (TMRG) algorithm was used for the calculation of the low-temperature asymptotic of χ . The obtained numerical results are not fully consistent with Eq. (37) and show that the exponent might actually be smaller than $4/3$. However, as pointed out in Ref. 30 the possible reason of the deviation of the TMRG results from Eq. (37) is that the obtainable temperatures in the TMRG calculations are

just not low enough to observe the $T^{-4/3}$ power law predicted by Eq. (37).

Now we consider the limit of large g when the magnetization is close to saturation. In this limit we expand $\cos \theta$ near $\theta = 0$ and scale the variables r and θ as

$$r = zg^{-1/8}, \quad \theta = xg^{-3/8}. \quad (38)$$

Keeping in Eq. (22) the terms proportional to $g^{1/4}$ we arrive at the Schrödinger equation in a form

$$\begin{aligned} -2 \left(\frac{\partial^2 \Psi}{\partial z^2} + \frac{1}{z} \frac{\partial \Psi}{\partial z} + \frac{1}{z^2} \frac{\partial^2 \Psi}{\partial \varphi^2} \right) - \frac{z \sin \varphi}{x} \frac{\partial \Psi}{\partial \varphi} \\ + z \cos \varphi \frac{\partial \Psi}{\partial x} + \frac{x^2}{2} \Psi = \frac{\varepsilon + g}{g^{1/4}} \Psi. \end{aligned} \quad (39)$$

Fortunately, the ground-state wave function and the ground-state energy of Eq. (39) can be found exactly:

$$\Psi_0(x, z, \varphi) = C \exp \left(-\frac{z^2}{4} + \frac{zx \cos \varphi}{2} - \frac{x^2}{2} \right), \quad (40)$$

$$\varepsilon_0 = -g + 2g^{1/4}, \quad (41)$$

where C is unessential normalization constant.

One can also calculate the next-order correction to the ground-state energy (41). For this aim we estimate the effect of the next-order term which was omitted in Eq. (39) and has the form

$$g^{-3/4} \left(\frac{3z^4 - x^4}{24} + \frac{xz}{3} \sin \varphi \frac{\partial}{\partial \varphi} \right). \quad (42)$$

The calculation of the first order in perturbation (42) gives for $\varepsilon_0(g)$ the correction proportional to $g^{-1/2}$:

$$\varepsilon_0 = -g + 2g^{1/4} + \frac{3}{4g^{1/2}}. \quad (43)$$

Then, the asymptotics for the magnetization and the susceptibility for $h \gg T^{4/3}$ are

$$m = 1 - \frac{1}{2g^{3/4}} + \frac{3}{8g^{3/2}} + O(g^{-9/4}), \quad (44)$$

$$\chi(h) = \frac{3T}{8h^{7/4}s^{1/4}} \left[1 - \frac{3}{2} \frac{T}{h^{3/4}s^{5/4}} + O\left(\frac{T^2}{h^{3/2}s^{5/2}}\right) \right]. \quad (45)$$

It is interesting to compare the leading terms of this expansion with the spin-wave expansion of the magnetization for the spin- s quantum F-AF chain at $\alpha = \frac{1}{4}$. We have checked that this expansion reproduces Eq. (44). The second term in Eq. (44) corresponds to the result of the linear spin-wave theory, but the third one includes the spin-wave interaction effect and, therefore, the coincidence is not trivial. Certainly, we cannot prove that both expansions coincide in all orders in small parameter $g^{-3/4}$. Nevertheless, the coincidence of the leading terms of $m(g)$ for the quantum and the classical model gives a promise that the universality is valid at the transition point of the F-AF model.

We complete this subsection with the results for the spin correlation function. It can be shown²³ that the spin correlation function $\langle S_z(0)S_z(l) \rangle$ has the form

$$\langle S_z(0)S_z(l) \rangle = \sum (\Psi_0 | \Psi_n)^2 \exp[-T^{1/3}(\varepsilon_n - \varepsilon_0)l]. \quad (46)$$

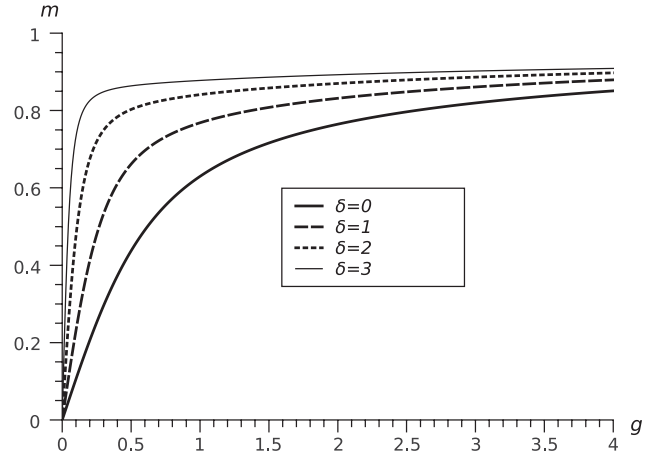


FIG. 1. Magnetization curves $m(g)$ at $\gamma = 0$ for some values of scaled anisotropy δ . The case $\delta = 0$ corresponds to the transition point.

As follows from Eq. (46) the spin correlation function exponentially decays on long distances $l \gg T^{-1/3}$, and the correlation length is governed by the lowest eigenstates of Eq. (22). In the case of absence of the magnetic field ($g = 0$) all the eigenvalues ε_n are real and several lowest levels were calculated in Ref. 23, which gives the asymptotic for the correlation length $l_0 = 1.04T^{-1/3}$ at $g \rightarrow 0$.

In the high-field limit ($g \gg 1$) there are three lowest excited states having equal real parts of their eigenvalues:

$$\varepsilon_1 = -g + 4g^{1/4} + O(g^{-1/2}), \quad (47)$$

$$\varepsilon_{2,3} = -g + 2g^{1/4}(2 \pm i) + O(g^{-1/2}).$$

According to Eq. (46) the presence of the imaginary part in eigenvalues (47) causes the oscillations on the background of the exponential decay of the correlation function. The imaginary part of the eigenvalues determines the period of the oscillations while the real part determines the correlation length. According to Eqs. (43) and (47) the asymptotic of the correlation length in the high-field limit is

$$l_0 = \frac{1}{2s^{5/12}h^{1/4}}. \quad (48)$$

So we see that the correlation length is defined by the temperature for $h \ll T^{4/3}$ and by the magnetic field when $h \gg T^{4/3}$. We note that the ratio of the correlation lengths in these limits is proportional to $g^{1/4}$. The crossover between these two regimes occurs at $g \approx 1$.

In general, the solution of Eq. (22) and the computation of $\varepsilon_0(g)$ and $m(g)$ has been obtained numerically. The dependence $m(g)$ at the transition point is shown by the thick solid line in Fig. 1.

IV. MAGNETIZATION CURVE IN THE HELICAL PHASE

In this section we consider the behavior of the magnetization in the helical phase in the vicinity of the transition point, when $\alpha > \frac{1}{4}$, but the anisotropy is zero $\delta = 0$. For $\alpha > \frac{1}{4}$ the ground state has the helical type of long-range order (LRO) with the wave number $k_h = \cos^{-1}(1/4\alpha)$. The saturation field h_s at α close to $\frac{1}{4}$ is $h_s = s(4\alpha - 1)^2$. The ground-state

magnetization is given by $m = h/h_s$ for $h \leq h_s$ and $m = 1$ for $h > h_s$. At finite temperature the helical LRO is destroyed by thermal fluctuations and thermodynamic quantities have singular behavior at $T \rightarrow 0$.

The behavior of the system in the case of absence of the magnetic field was studied in detail in Ref. 27. It was shown that with the increase of the temperature the gapless excitations over the helical ground states (spin waves) smear the δ peaks of the static structure factor at $k = \pm k_h$ and shift the peaks to $k = 0$. Finally, at $T_c = 0.925\gamma^{3/2}$ the maximum of the spin structure factor reaches $k = 0$ defining the Lifshitz boundary, so that the helical type of the spin correlations for $T > T_c$ disappears.

Most likely, the hypothesis of the universality of the function $m(g)$ breaks down for $\alpha > \frac{1}{4}$ because the excitations above the ground state are different in the quantum and in the classical F-AF chain. Nevertheless, as was shown in Ref. 23 some peculiarities of the low-temperature behavior of the classical model at $\alpha > \frac{1}{4}$ is qualitatively similar to that for the quantum $s = \frac{1}{2}$ chain. For example, the temperature dependence of the zero-field susceptibility is in a qualitative agreement with the numerical data for the quantum $s = \frac{1}{2}$ model and is in accord with the experimental data for the real edge-sharing compounds.

The finding of the magnetization in the helical phase reduces to the solution of Eq. (22) for $\gamma > 0$ and can be analyzed in full analogy with the case $\gamma = 0$. For low magnetic field ($g \rightarrow 0$) the magnetization is $m \sim g$ and can be represented as

$$m = \frac{h}{h_s} G(\gamma). \quad (49)$$

The function $G(\gamma)$ is found from the solution of Eq. (30) where the terms $-\frac{1}{2}\gamma r^2 f_{1(2)m}$ are added to the first (the second) equation of (30). In fact, $G(\gamma)$ coincides with the normalized zero-field susceptibility obtained before in Ref. 23. Therefore, we do not present this function here. We note only that $G(\gamma)$ vanishes at $\gamma \rightarrow \infty$, tends to finite value at $\gamma \rightarrow 0$, and has a maximum at $\gamma \simeq 2.2$.

In the high magnetic field limit we use rescaling (38) for Eq. (22) and keep the leading terms. The obtained equation repeats Eq. (39) with the additional term $-\frac{1}{2}\sqrt{h_s/h}z^2\Psi$. The ground-state wave function of this equation has a form similar to Eq. (40),

$$\Psi = C \exp\left(-az^2 + \frac{1}{2}zx \cos \varphi - 2ax^2\right), \quad (50)$$

and the ground-state energy is

$$\varepsilon_0 = -g + 8ag^{1/4}, \quad (51)$$

where

$$a = \frac{1}{4}\sqrt{1 - \sqrt{h_s/h}}. \quad (52)$$

Equation (50) is valid for high fields when $h > h_s$. The asymptotic of the magnetization curve in this limit has the form

$$m = 1 - \frac{(h_s/h)^{3/4}}{2\gamma^{3/2}\sqrt{1 - \sqrt{h_s/h}}}. \quad (53)$$

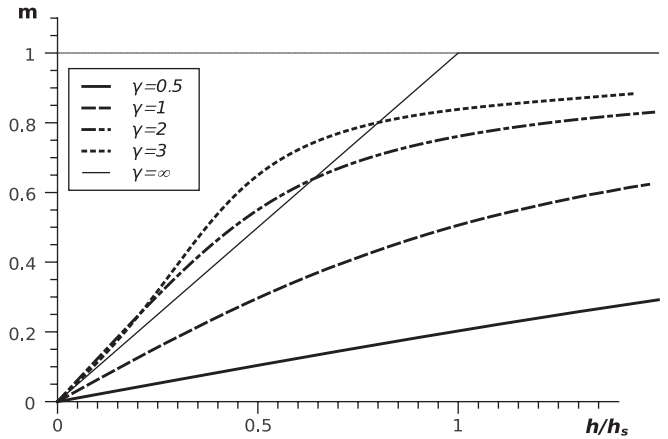


FIG. 2. Magnetization as a function of h/h_s for several values of parameter γ for isotropic case ($\delta = 0$).

As follows from Eq. (53) the temperature-dependent correction to $m = 1$ at $h \gg h_s$ is proportional to $\gamma^{-3/2}$.

The magnetization curves for several values of γ as a function of h/h_s are shown in Fig. 2 together with the ground-state magnetization ($\gamma \rightarrow \infty$). The zero-field susceptibility defines the slopes of the magnetization curves for small h/h_s and as follows from Fig. 2 this slope can be both larger and smaller than the ground-state value. Such behavior of the magnetization follows from the nonmonotonic dependence of G on γ .

V. EASY-AXIS ANISOTROPY

Up to now we have considered the isotropic F-AF chain. At the same time it is important to study the influence of the anisotropy of exchange interactions on the low-temperature thermodynamics. In this subsection we pay attention mainly to the dependence of the zero-field susceptibility on the anisotropy at $\alpha = \frac{1}{4}$.

At first, we briefly review the effect of the anisotropy on the susceptibility for the classical and quantum ferromagnetic model ($\alpha = 0$). At $T \rightarrow 0$ and in the scaling limit the magnetization of the classical ferromagnetic chain is given by Eq. (27), where ε_0 is the lowest eigenvalue of the equation:^{19,20}

$$-\frac{1}{2} \frac{d^2\Psi}{d\theta^2} - \frac{1}{2} \cot \theta \frac{d\Psi}{d\theta} - \delta_F \cos^2 \theta \Psi - g_F \cos \theta \Psi = \varepsilon \Psi. \quad (54)$$

In this equation $\delta_F = (\Delta - 1)s^4/T^2$ and $g_F = s^3h/T^2$ are the scaling parameters.

To find the susceptibility in the limit $\delta_F \ll 1$ and $g_F \ll 1$ we can use the PT in $V = -\delta_F \cos^2 \theta - g_F \cos \theta$. At $V = 0$ the eigenfunctions of Eq. (54) are the Legendre polynomials $P_l(\cos \theta)$ with the eigenvalues $\varepsilon_l = l(l+1)/2$. The PT in the lowest orders in V gives

$$\varepsilon_0 = -\frac{\delta_F}{3} - \frac{g_F^2}{3} - \frac{44g_F^2\delta_F}{135}. \quad (55)$$

Then, according to Eq. (27) the zero-field susceptibility in the limit of weak anisotropy $\delta_F \rightarrow 0$ ($\Delta - 1 \ll T^2$) is

$$\chi = \frac{2s^4}{3T^2} \left(1 + \frac{44s^4(\Delta - 1)}{45T^2} \right). \quad (56)$$

In the opposed limit $\delta_F \rightarrow \infty$ and $g_F = 0$ Eq. (54) has two almost degenerated lowest eigenvalues corresponding to the states with even and odd parity with respect to exchange $\theta \leftrightarrow (\pi - \theta)$. The tunnel splitting between these states can be found with the exponential accuracy in the WKB approximation.³² $\Delta E \sim \exp(-2\sqrt{2\delta_F})$. The term $(-g_F \cos \theta)$ in Eq. (54) has a nonzero matrix element between the states with even and odd parities, so that the contribution to the second-order PT in g_F is given by

$$\varepsilon_0 \sim -g_F^2 \exp(2\sqrt{2\delta_F}) \quad (57)$$

and the zero-field susceptibility is

$$\chi \sim \frac{1}{T^2} \exp\left(\frac{\Delta E}{T}\right), \quad (58)$$

where $\Delta E = 2s^2\sqrt{2(\Delta - 1)}$.

As follows from Eq. (58) the susceptibility diverges exponentially at $T \rightarrow 0$ and the value of the thermal gap ΔE is equal to the kink energy (or one-half of the energy of the large soliton) of the weakly anisotropic ferromagnetic chain. As is known³³ the soliton energy coincides with the energy of the multimagnon bound states of the quantum anisotropic ferromagnetic chain. It is interesting to note that the susceptibility of the easy-axis anisotropic $s = \frac{1}{2}$ ferromagnetic chain found on the basis of the Gaudin formalism in Ref. 34 behaves at $T \rightarrow 0$ as $\chi \sim \exp(\Delta E/T)/T$ and ΔE is the same as given in Eq. (58). This fact manifests the close relation between the magnetic properties of the quantum and the classical anisotropic ferromagnetic chains.

We will show that this resemblance remains in the F-AF model at the critical point $\alpha = \frac{1}{4}$. For example, it was shown by us in Refs. 26,36 that the energies of multimagnon bound states in the quantum model and the energy of large classical solitons at $\alpha = \frac{1}{4}$ are both proportional to $(\Delta - 1)^{3/4}$ although the numerical coefficients are different. We have also shown²⁶ that the susceptibility of the quantum $s = \frac{1}{2}$ F-AF model diverges at $T \rightarrow 0$ exponentially; i.e., $\chi \sim \exp(\Delta E/T)$ and the thermal gap ΔE equals one-half of the energy of the multimagnon complexes. We will show below that the susceptibility of the classical model at $\delta \gg 1$ has similar exponential behavior and the corresponding thermal gap is the classical kink energy.

Similar to the pure ferromagnetic chain the calculation of the zero-field susceptibility reduces to the computation of the ground-state energy of Eq. (22) in the second order in $V = -g \cos \theta$. Then the susceptibility can be represented as $\chi = 2(s^2/T)^{4/3} f(\delta)$ where

$$f(\delta) = \sum_{n \neq 0} \frac{\langle \Psi_0 | \cos \theta | \Psi_n \rangle^2}{\varepsilon_n - \varepsilon_0} \quad (59)$$

and Ψ_n and ε_n are the eigenfunctions and the eigenvalues of Eq. (22) at $g = 0$.

It is convenient to introduce the normalized susceptibility $\tilde{\chi} = (\Delta - 1)\chi$ and the normalized temperature

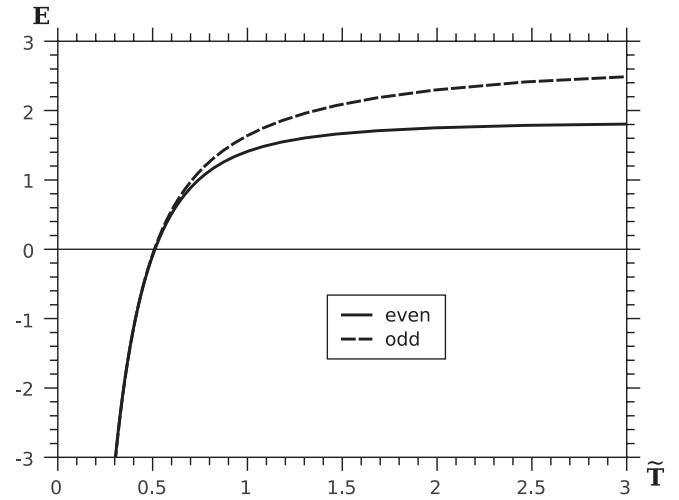


FIG. 3. Dependence of two lowest eigenvalues of Eq. (22) on the normalized temperature $\tilde{T} = T/s^2(\Delta - 1)^{3/4}$ at $\gamma = g = 0$.

$\tilde{T} = T/s^2(\Delta - 1)^{3/4}$ ($\tilde{T} = \delta^{-3/4}$), so that $\tilde{\chi}$ is a function of \tilde{T} only. The function $\tilde{\chi}(\tilde{T})$ can be found explicitly in the limits of large and small values of \tilde{T} (at small and large δ correspondingly). For high temperatures $\tilde{T} \gg 1$ the states giving the contributions to the sum in Eq. (59) are separated from the ground state by finite gap and the numerical calculation of this sum gives

$$\tilde{\chi} = 1.07\tilde{T}^{-4/3} + 0.87\tilde{T}^{-8/3}. \quad (60)$$

The calculation $\tilde{\chi}(\tilde{T})$ for small \tilde{T} is more complicated. At $\tilde{T} \rightarrow 0$ ($\delta \rightarrow \infty$) we can expand the term $\delta \cos^2 \theta$ up to θ^2 in the Schrödinger equation (22). Then the ground-state wave function has a form similar to Eq. (40) and the energy $\varepsilon_0 = -\tilde{T}^{-4/3} + 2^{5/4}\tilde{T}^{-1/3}$. Further, we can compute perturbative corrections to ε_0 from omitted anharmonic terms to obtain the ground-state energy in a form

$$E_0 = \varepsilon_0 + \sum a_n \tilde{T}^{n+2/3}. \quad (61)$$

If we expand the term $\delta \cos^2 \theta$ near the second minimum $\theta = \pi$ we would obtain a result identical to Eq. (61), so that we have two degenerated states. But there is a nonperturbative tunnel splitting which is not captured by the PT. The splitting is exponentially small at $\tilde{T} \rightarrow 0$ as demonstrated in Fig. 3. On the other hand, these quasidegenerated states have a nonzero matrix element in Eq. (59) and, therefore, the splitting between them determines the behavior of $\tilde{\chi}$ at $\tilde{T} \rightarrow 0$.

The most convenient way to evaluate this splitting is the calculation of the original functional integral (14). Certainly, the exact calculation of this integral is impossible and, therefore, we use a semiclassical approximation. In this approximation the functional integral (14) is represented as the sum of the contributions of the classical paths in Z minimizing the Euclidean action and the paths which are close to the classical ones. The minimization of the energy functional $W(\theta, \varphi)$ [Eq. (15)] gives $\varphi = 0$ and the following Euler equation for $\theta(\xi)$:

$$\frac{1}{4}\theta'''' - \frac{3}{2}\theta''\theta'^2 + \frac{1}{\tilde{T}^{4/3}}\sin(2\theta) = 0. \quad (62)$$

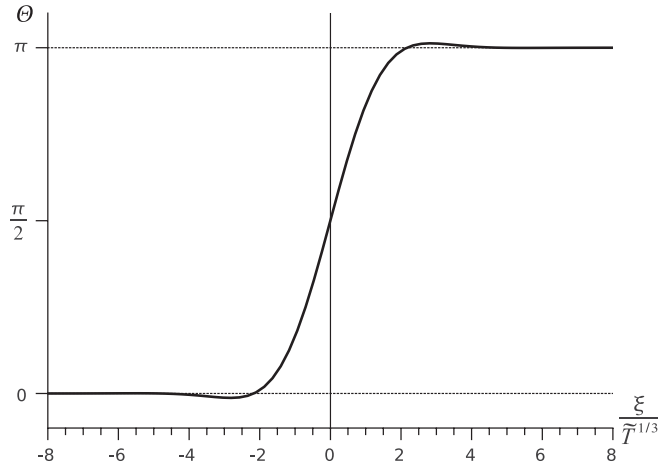


FIG. 4. Instanton solution of Eq. (62) with boundary conditions: $\theta(-\infty) = 0$, $\theta(\infty) = \pi$.

We note that there are a few classical solutions of this Euler equation. Two of them $\theta = 0$ and $\theta = \pi$ correspond to trivial ferromagnetic configurations. A systematic expansion around these saddle points is equivalent to a purely perturbation expansion of the eigenvalues of the Schrödinger equation (22). The corresponding contribution to the partition function is $Z^{(0)} = \exp(-\lambda E_0)$ where E_0 is given by Eq. (61) and λ is the scaled system length (11). The tunnel splitting is given by an instanton contribution to the functional integral (14).³⁵ The classical solution of the Euler equation corresponding to the instanton satisfies the boundary condition: $\theta(-\infty) = 0$, $\theta(\infty) = \pi$ or $\theta(-\infty) = \pi$, $\theta(\infty) = 0$. This solution of the Euler equation can be found numerically. Actually, it coincides with the solution for the kink excitation in the F-AF chain found by us in Ref. 36. The dependence $\theta(\xi)$ in this solution is shown in Fig. 4. According to the result of Ref. 36, the classical action corresponding to the instanton is $S_0 = 2/\tilde{T}$. The summation of the contributions to Z using the semiclassical approximation can be performed in the standard way.³⁵ As a result, the partition function is represented in a form

$$Z = Z^{(0)} + Z^{(2)} + Z^{(4)} + \dots, \quad (63)$$

where $Z^{(0)}$ is defined above, $Z^{(2)}$ is the instanton–anti-instanton contribution (IA), $Z^{(4)}$ is the IAIA contribution, and so on.

Using the usual approximation of the semiclassical method (in particular, neglecting instanton–instanton interactions) we have

$$Z^{(2)} = \frac{\lambda^2 e^{-2S_0}}{2} e^{-\lambda E_0}, \quad Z^{(4)} = \frac{\lambda^4 e^{-4S_0}}{4!} e^{-\lambda E_0}, \quad (64)$$

and so on [here λ is the scaled system length (11)].

Summing (63) we arrive at

$$Z = e^{-\lambda E_0} \cosh(\lambda e^{-S_0}). \quad (65)$$

On the other hand, the partition function at $\lambda \rightarrow \infty$ can be represented as

$$Z = e^{-\lambda E_s} + e^{-\lambda E_a}, \quad (66)$$

where E_s and E_a are the energies of the lowest states with even and odd parity with respect to exchange $(r, \theta) \leftrightarrow (-r, \pi - \theta)$. Then, $E_s = E_0 - e^{-S_0}$ and $E_a = E_0 + e^{-S_0}$. The tunnel splitting is

$$\Delta E = E_s - E_a = 2 \exp(-2/\tilde{T}). \quad (67)$$

Then the susceptibility at $\tilde{T} \rightarrow 0$ to the exponential accuracy is given by

$$\tilde{\chi} \sim \exp\left[\frac{2s^2(\Delta - 1)^{3/4}}{T}\right]. \quad (68)$$

The thermal gap in Eq. (68) is the kink energy of the weakly anisotropic classical F-AF chain. It is interesting to compare $\tilde{\chi}$ [Eq. (68)] with the susceptibility of the quantum F-AF model at $\alpha = \frac{1}{4}$.²⁶ The susceptibility for both models shows the exponential dependence with the thermal gap proportional to $(\Delta - 1)^{3/4}$. If we use Eq. (68) for the $s = \frac{1}{2}$ case we find that the thermal gap is $\frac{1}{2}(\Delta - 1)^{3/4}$ while in fact it is $0.35(\Delta - 1)^{3/4}$,²⁶ i.e., the numerical coefficients at $(\Delta - 1)^{3/4}$ are slightly different.

Equations (60) and (68) give asymptotics of $\tilde{\chi}(\tilde{T})$ for small and large values of \tilde{T} . In the general case the function $\tilde{\chi}(\tilde{T})$ has been calculated numerically and the dependence $\tilde{\chi}(\tilde{T})$ is shown in Fig. 5 together with asymptotics of $\tilde{\chi}$ for small and large \tilde{T} . As can be seen from Fig. 5 the dependence $\tilde{\chi}$ on \tilde{T} is characterized by two types of behavior: $\tilde{\chi}$ is proportional to $\tilde{T}^{-4/3}$ at $\tilde{T} \gg 1$ and grows exponentially at $\tilde{T} \rightarrow 0$. The crossover between the two regimes occurs at $\tilde{T} \sim 1$.

The calculation of the susceptibility of the anisotropic F-AF model can be expanded to the case $\gamma > 0$. We do not dwell on details of these calculations. We note only that $\tilde{\chi}$ becomes a function of \tilde{T} and of a parameter $\mu = (4\alpha - 1)/\sqrt{\Delta - 1}$. $\tilde{\chi}(\mu, \tilde{T})$ as a function of \tilde{T} has a minimum for $\mu > \mu_0 \simeq 1$ and is finite at $\tilde{T} \rightarrow 0$. The normalized susceptibility $\tilde{\chi}$ diverges at $\tilde{T} \rightarrow 0$ for $\mu < \mu_0$. The line $(4\alpha - 1) = \mu_0 \sqrt{\Delta - 1}$ can be identified with the boundary between the ferromagnetic and the helical phase.

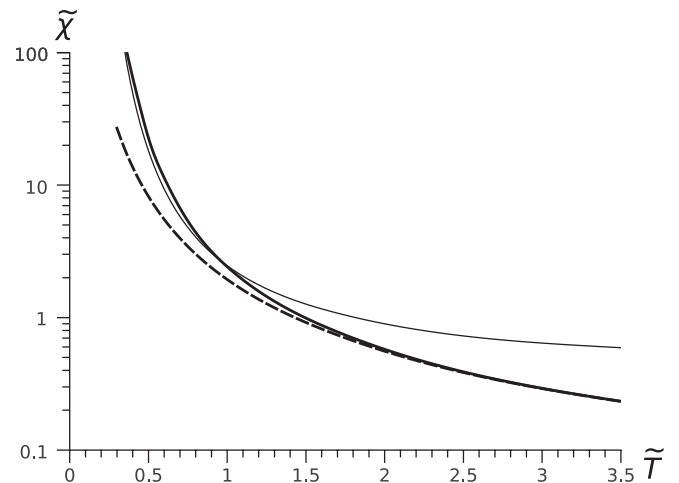


FIG. 5. Dependence of the normalized magnetic susceptibility $\tilde{\chi} = (\Delta - 1)\chi$ on the normalized temperature $\tilde{T} = T/s^2(\Delta - 1)^{3/4}$ (thick solid line). Dashed and thin solid lines are asymptotics of $\tilde{\chi}$ at $\tilde{T} \rightarrow \infty$ and $\tilde{T} \rightarrow 0$ given by Eqs. (60) and (68), correspondingly.

Finally we give the results for the magnetization of the anisotropic F-AF model at $\alpha = \frac{1}{4}$. According to Eqs. (60) and (68) $m(g)$ at $g \rightarrow 0$ is

$$\begin{aligned} m(g) &= 1.07g(1 + 0.81\delta), & \delta \ll 1, \\ m(g) &\sim g \exp(2\delta^{3/4}), & \delta \gg 1. \end{aligned} \quad (69)$$

The behavior of the magnetization in the high magnetic field limit is obtained by analogy with that for the isotropic case [see Eq. (44)]. Then $m(g)$ at $g \gg 1$ is

$$m = 1 - \frac{1}{2(g + 2\delta)^{3/4}} + O((g + \delta)^{-3/2}). \quad (70)$$

The magnetization curves $m(g)$ for several values of δ obtained by the numerical solution of Eq. (22) is shown in Fig. 1. Its behavior in the limits $g \ll 1$ and $g \gg 1$ agrees with Eqs. (69) and (70).

VI. CONCLUSIONS

We have studied the low-temperature magnetic properties of the classical anisotropic F-AF chain in the vicinity of the transition point from the ferromagnetic to the helical ground state. This means that the frustration parameter $\alpha = J_2/|J_1|$ is close to its critical value $\alpha = \frac{1}{4}$ and the anisotropy of the exchange interaction $(\Delta - 1)$ is weak. In the vicinity of the transition point the nearest spins in the ground state are directed almost (or even exactly) parallel to each other. Therefore, in the low-temperature limit when the thermal fluctuations are weak, we can use the continuum approximation and represent the partition function as a functional integral over the spin vector field. In the obtained energy functional the model parameters $(\alpha - \frac{1}{4})$, $(\Delta - 1)$ and the magnetic field h are scaled by the temperature and form three independent scaling parameters γ , δ , and g defined in Eq. (12). This implies that we considered the scaling limit when $\alpha \rightarrow \frac{1}{4}$, $\Delta \rightarrow 1$, $h \rightarrow 0$, and $T \rightarrow 0$, but the values of the scaling parameters γ , δ , and g are finite and govern the low-temperature thermodynamics of the F-AF model near the transition point.

The derived functional integral for the partition function was treated as a path integral of the quantum mechanics. The peculiarity of this path integral is that the Lagrangian contains the second-order derivative. To handle this problem we used the special Ostrogradski prescription, which allowed us to obtain the quantum Hamiltonian corresponding to such path integral in a special unusual form. Then the dependence of the lowest eigenvalue of the Hamiltonian on the scaling parameters determines the magnetization curves of the system. The eigenvalue problem has been solved numerically and explicit expressions for the magnetization were obtained in the limits of low and high magnetic fields.

It is known¹⁹ that the magnetization curve for the pure ferromagnetic chain has a universal form when plotted against the scaled magnetic field $g_F = s^3 h / T^2$, and this curve is valid for any value of spin s including the classical limit $s \rightarrow \infty$. We suppose that such universality remains for the F-AF model at the transition point against the scaling parameter $g = h s^{5/3} / T^{4/3}$. If this is the case the obtained magnetization curves for the classical model can be easily recalculated to the quantum spin case. To validate this hypothesis one needs to compare the obtained classical results with the magnetization of the $s = \frac{1}{2}$ F-AF model. Unfortunately, the exact thermodynamics of the latter model is unknown. Nevertheless, there are two indirect arguments supporting this conjecture. The first is that the obtained critical exponent $\frac{4}{3}$ in the temperature dependence of susceptibility at the transition point coincides with that obtained in the MSWT method. The second argument is that three leading terms of the spin-wave expansion of the magnetization of the quantum model coincide with those for the classical model. Certainly these two facts do not prove the proposed hypothesis and the question about its validity remains open.³⁰ In this respect the numerical calculations of the magnetization as a function of the magnetic field at $T \rightarrow 0$ for $s = \frac{1}{2}$ and $s = 1$ are very desirable.

Probably, the hypothesis of the universality of the function $m(g)$ (if any) breaks down for $\alpha > \frac{1}{4}$ because the excitations above the ground state are different in the quantum and in the classical F-AF chain. Nevertheless, as was shown in Ref. 23 some peculiarities of the low-temperature behavior of the classical model at $\alpha > \frac{1}{4}$ is qualitatively similar to that for the quantum $s = \frac{1}{2}$ chain. For example, the temperature dependence of the zero-field susceptibility is in qualitative agreement with the numerical data for the quantum $s = \frac{1}{2}$ model and is in accord with the experimental data for the real edge-sharing compounds.

We have studied the influence of the easy-axis anisotropy on the behavior of the susceptibility at the transition point. It is shown that even weak anisotropy essentially changes χ . In the low-temperature limit the susceptibility diverges exponentially in contrast with the isotropic case where the divergence is of a power-like type. We note that such behavior of the susceptibility takes place in the quantum $s = \frac{1}{2}$ F-AF chain²⁶ and the corresponding thermal gap has the same functional form as the classical one. This fact confirms the close relation between the low-temperature magnetic properties of the quantum and classical F-AF model in the ferromagnetic part of the phase diagram.

ACKNOWLEDGMENTS

We would like to thank S.-L. Drechsler and J. Sirker for valuable comments related to this work.

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