

Universal low-temperature magnetic properties of the classical and quantum dimerized ferromagnetic spin chain

D. V. Dmitriev* and V. Ya. Krivnov

Joint Institute of Chemical Physics of RAS, Kosygin str. 4, 119334, Moscow, Russia.

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Low-temperature magnetic properties of both classical and quantum dimerized ferromagnetic spin chains are studied. It is shown that at low temperatures the classical dimerized model reduces to the classical uniform model with the effective exchange integral $J_0 = J(1 - \delta^2)$, where δ is the dimerization parameter. The partition function and spin correlation function are calculated by means of mapping to the continuum limit, which is justified at low temperatures. The quantum model is studied using the Dyson-Maleev representation of the spin operators. It is shown that in the long-wavelength limit the Hamiltonian of the quantum dimerized chain reduces to that of the uniform ferromagnetic chain with the effective exchange integral $J_0 = J(1 - \delta^2)$. This fact implies that the known equivalence of the low-temperature magnetic properties of classical and quantum ferromagnetic chains remains for the dimerized chains. The considered model is generalized to include the next-neighbor antiferromagnetic interaction.

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I. INTRODUCTION

The Peierls instability plays an important role in quasi-one-dimensional materials. The Peierls metal-dielectric transition originated from the coupling between electrons and phonons occurs, as a rule, in organic solids.¹ Such transition can take place in the quantum spin chains coupled to phonons as well [so-called the spin-Peierls transition (SP)]. In particular, the SP transition has been observed in the antiferromagnetic spin chain CuGeO_3 .² Currently there is a growing interest in the quasi-one-dimensional magnets with ferromagnetic exchange interactions,³⁻⁵ and the possibility of the Peierls instability in them is widely discussed.⁶ It is argued that the possible real system where this instability takes place is monatomic chains of Co on the Pt surface.⁷ As it is proposed,⁷ these chains have the effectively ferromagnetic spin-spin interaction and very weak elastic constants. Recently, another mechanism of the Peierls instability in spin systems has been proposed.^{8,9} It is based on the coupling of the spins with an electronic subsystem (spin-orbital mechanism). It is expected that this mechanism is relevant to the transition metal oxide YVO_3 . The properties of this compound is described by the spin-orbital model.¹⁰ The mean-field treatment of this model leads to the 1D dimerized spin model with the ferromagnetic sign of the interaction.⁶

Therefore, the study of the dimerized ferromagnetic (FM) chains is important from both theoretical and experimental points of view. The spin chains with the spin-phonon interaction are often described in the adiabatic approximation which is valid if the phonon energy is smaller than the Peierls gap. The Hamiltonian of this 1D spin model has the form

$$H = H_{\text{spin}} + E_{\text{elastic}}, \quad (1)$$

where

$$H_{\text{spin}} = J \sum_{n=1}^N (1 - (-1)^n \delta) \mathbf{S}_n \cdot \mathbf{S}_{n+1} \quad (2)$$

$$E_{\text{elastic}} = \frac{N \varkappa \delta^2}{2}, \quad (3)$$

where \mathbf{S} is the spin operator, J is the exchange integral, δ is the dimerization parameter characterizing lattice distortion, and \varkappa is the effective elastic constant.

There is an essential difference between the antiferromagnetic (AF) and ferromagnetic (FM) chains with respect to the coupling to the lattice distortions. For the AF model ($J > 0$) the ground state energy of model (2) is $\sim -N\delta^{4/3}$ (Ref. 11), and the gain in this energy exceeds the loss in E_{elastic} and the SP transition takes place. Contrary to the AF model the ground state of H_{spin} at $J < 0$ does not depend on δ , and the ground state of model (1) has the uniform lattice $\delta = 0$. However, as was shown in Ref. 6, the thermal fluctuations can activate the dimerization. It was shown in Ref. 6 that the free energy of the FM chain at $T > 0$ is $-NT^{3/2}\delta^2$, and the dimerized phase is stable at finite temperature for small enough elastic constant \varkappa . Such a situation can occur in the system Co chains on the Pt surface where the Co atoms can be easily moved on the surface.

The dimerized FM chain can not be solved by the Bethe ansatz in contrast with the uniform model with $\delta = 0$. The thermodynamics of this model has been studied in Ref. 12 using both numerical TMRG simulations and the analytical modified spin-wave theory.¹³ In particular, the phase diagram of the model has been determined and the behavior of spin correlation functions and the zero-field susceptibility are studied.

It is interesting to consider the influence of the external magnetic field on the thermodynamics of the dimerized FM chain. The aim of the present paper is to study the low-temperature magnetic properties of model (2) independent of the dimerization mechanism. Therefore, we will consider the model with the Hamiltonian having a form

$$H = -J \sum (1 - (-1)^n \delta) \mathbf{S}_n \cdot \mathbf{S}_{n+1} - h \sum S_n^z, \quad (4)$$

where h is the dimensionless magnetic field and $J > 0$.

Before we study this model it is instructive to note the remarkable fact related to the uniform FM chain, $\delta = 0$. It was claimed in Ref. 14 that the normalized magnetization $M = \langle S^z \rangle / s$ of this model at $T \rightarrow 0$ is the universal function

of the scaling variable $g = s^3 Jh/T^2$. That is, the dependence on spin value s is totally captured in the scaling variable g and the universal function $M(g)$ is valid for any s . In other words, this function is valid for both quantum and classical ferromagnetic chains.

In this paper we show that in the low-temperature limit, when the continuum approximation is valid, the classical dimerized FM chain reduces to the classical uniform FM model with the effective exchange integral. Then, we show that the spin-wave expansion for the quantum dimerized FM chain coincides with that for the uniform quantum model with the same exchange integral as in the classical case. Using the arguments of Ref. 14 we conclude that the universality holds in the scaling limit for the dimerized model as well. To support these arguments we show the equivalence of the spin-wave expansion for the quantum model with the large g expansion of the classical magnetization. We show also that the universality survives in case of the presence of the frustrated next-nearest neighbor (nnn) antiferromagnetic interaction.

We calculate the spin correlation functions for the classical dimerized FM spin chain and argue in favor of the universality of their behavior on large distances. We show that the correlation functions are generally different for the dimerized and uniform models. In particular, the even-odd asymmetry of the correlation functions takes place.

The paper is organized as follows. In Sec. II we consider the partition function of the dimerized classical ferromagnetic chain in the magnetic field. We show that the field-dependent part of the free energy coincides in the scaling limit with that for the uniform model with the renormalized scaling parameter. In Sec. III it is demonstrated that the spin-wave expansion of the dimerized quantum ferromagnetic chain reproduces the expansion of the magnetization of the classical model. In Sec. IV the effect of the frustrated nnn interaction on the magnetic properties of the dimerized model is studied. In Sec. V the summary of the results is given.

II. CLASSICAL DIMERIZED SPIN CHAIN IN THE SCALING LIMIT

In this section we show that the low-temperature magnetic properties of the classical dimerized spin model are reduced to that of the FM spin chain with the renormalized exchange integral. It is convenient to represent the Hamiltonian function of the considered classical model (4) in a form

$$H = -J_1 \sum_{i=1}^{N/2} \vec{S}_{2i-1} \cdot \vec{S}_{2i} - J_2 \sum_{i=1}^{N/2} \vec{S}_{2i} \cdot \vec{S}_{2i+1} - \sum_{i=1}^N \vec{h} \cdot \vec{S}_i, \quad (5)$$

where $J_1 = J(1 + \delta)$, $J_2 = J(1 - \delta)$, and \vec{S}_i are spin vectors of the fixed length s and the magnetic field is directed along the Z axis: $\vec{h} = (0, 0, h)$.

We represent spin vectors on odd and even sites as follows:

$$\begin{aligned} \vec{S}_{2i-1} &= s\vec{n}_i \\ \vec{S}_{2i} &= s\vec{n}_i + s\vec{m}_i, \end{aligned} \quad (6)$$

where \vec{n}_i are unit vectors and \vec{m}_i are vector differences between neighbor spins (we will assume $|\vec{m}_i|$ to be small at low temperatures).

Then, the scalar products of spins on odd and even bonds become

$$\begin{aligned} \vec{S}_{2i-1} \cdot \vec{S}_{2i} &= s^2 - \frac{1}{2}(\vec{S}_{2i-1} - \vec{S}_{2i})^2 = s^2 - \frac{s^2}{2}\vec{m}_i^2 \\ \vec{S}_{2i} \cdot \vec{S}_{2i+1} &= s^2 - \frac{s^2}{2}(\vec{n}'_i - \vec{m}_i)^2, \end{aligned} \quad (7)$$

where we denoted

$$\vec{n}'_i \equiv \vec{n}_{i+1} - \vec{n}_i. \quad (8)$$

After simple algebra the Hamiltonian function can be transformed to the form (we omit here the unimportant constant term)

$$\begin{aligned} H &= -\frac{h^2 N}{4(J_1 + J_2)} + s^2 \frac{J_1 + J_2}{2} \sum_{i=1}^{N/2} \left(\vec{m}_i - \frac{s J_2 \vec{n}'_i + \vec{h}}{s(J_1 + J_2)} \right)^2 \\ &+ \frac{s^2 J_1 J_2}{2(J_1 + J_2)} \sum_{i=1}^{N/2} \vec{n}_i^2 - 2s \sum_{i=1}^{N/2} \vec{h} \cdot \vec{n}_i. \end{aligned} \quad (9)$$

Then, the partition function of the system reads

$$Z = \int \dots \int \prod_{i=1}^{N/2} d\vec{m}_i d\vec{n}_i \exp \left(-\frac{H\{\vec{m}_i, \vec{n}_i\}}{T} \right). \quad (10)$$

We stress that up to here we did not make any assumption, and Eqs. (9) and (10) are the exact expressions. Now we notice that for low temperature $T \ll s^2 J_1$ the neighbor spin vectors \vec{S}_{2i-1} and \vec{S}_{2i} coupled by strong FM interaction J_1 are almost parallel, which means that all vectors \vec{m}_i are small and directed in plane perpendicular to the corresponding vectors \vec{n}_i . Then, we can integrate over vectors \vec{m}_i in the infinite limits. That gives

$$\begin{aligned} Z &= e^{\frac{h^2 N}{4T(J_1 + J_2)}} \left(\frac{2\pi T}{s^2(J_1 + J_2)} \right)^{N/2} \int \dots \int \prod_{i=1}^{N/2} d\vec{n}_i \exp \\ &\times \left(\frac{s^2 J_1 J_2}{T(J_1 + J_2)} \sum (\vec{n}_i \cdot \vec{n}_{i+1} - 1) + \frac{2sh}{T} \sum n_i^z \right). \end{aligned} \quad (11)$$

The first factor in Eq. (11) gives a constant contribution to the magnetic susceptibility $\sim 1/J$. As will be shown below, in the low-temperature limit the main contribution is given by the integral in Eq. (11) and it is much higher ($\sim J/T^2$). Therefore, we neglect the first factor in Eq. (11). The second factor does not influence on the magnetic properties of the system, and will be omitted. Thus, we reduced the partition function of the dimerized chain to that of the uniform ferromagnetic chain with the effective exchange integral

$$J_0 = \frac{2J_1 J_2}{J_1 + J_2} = J(1 - \delta^2). \quad (12)$$

The partition function of the classical FM chain was calculated in Ref. 14 by taking the continuum limit of the model. The continuum limit is justified when the direction of vectors \vec{n}_i changes smoothly along the chain, so that

the neighbor vectors are almost parallel to each other. This condition is satisfied in the low-temperature limit $T \ll s^2 J_0$. We will follow this method. Partition function (11) in the continuum approximation takes the form

$$Z \propto \int D[\vec{n}(x)] \exp \left(- \int_0^L dx \left[\frac{s^2 J_0 a^2}{2a} \left(\frac{d\vec{n}}{dx} \right)^2 - \frac{2hs}{T} n_z \right] \right), \quad (13)$$

where $L = Na$ and we notice that the distance between neighbor vectors \vec{n}_i and \vec{n}_{i+1} is two lattice spaces $2a$, so that the vector \vec{n}_i corresponds to the vector field $\vec{n}(x)$ at the point $x = 2ia$ in the continuum limit.

It is useful to transform Eq. (13) to dimensionless variables. We rescale the spatial coordinate $x = ys^2 a J_0 / T$ and obtain

$$Z \propto \int D[\vec{n}(y)] \exp \left(- \int_0^\lambda dy \left[\frac{1}{2} \left(\frac{d\vec{n}}{dy} \right)^2 - \gamma n_z \right] \right), \quad (14)$$

where $\lambda = LT/as^2 J_0$ is the scaled system length, which is assumed to be infinite in the thermodynamic limit $L \rightarrow \infty$, and

$$\gamma = \frac{s^3 J_0 h}{T^2} = g(1 - \delta^2). \quad (15)$$

Here γ and g are the scaling variables of the dimerized and uniform models.

Taking advantage of the well-known equivalence of the one-dimensional statistical field theory with the quantum mechanics, the calculation of the partition function (14) reduces to the eigenvalue problem of the quantum rotator in the ‘‘gravitational’’ field.¹⁴ The corresponding Schrödinger equation in the spherical coordinates has the form

$$\left(-\frac{1}{2} \frac{d^2}{d\theta^2} - \frac{\cot \theta}{2} \frac{d}{d\theta} - \frac{m^2}{2 \sin^2 \theta} - \gamma \cos \theta \right) \psi_{nm} = \varepsilon_{nm} \psi_{nm}, \quad (16)$$

where we used an axial symmetry of the model and introduced the azimuthal quantum number m .

Then, the partition function is expressed through the ground state energy of Eq. (16) as $Z \propto \exp(-\lambda \varepsilon_{00})$ and the normalized magnetization $M = \langle n^z \rangle$ is

$$M = -\frac{\partial \varepsilon_{00}(\gamma)}{\partial \gamma}. \quad (17)$$

The solution of the Schrödinger equation (16) has been found analytically for small and large scaling parameter in Ref. 14. On the other hand, this equation can be solved numerically for all values of γ and the magnetization curve can be found. It is shown in Fig. 1. To demonstrate δ -dependence of the magnetization we represent it as a function of the scaled magnetic field g rather than γ . As follows from Fig. 1 the increase of the dimerization leads to the decrease of the magnetization for all values of the magnetic field.

We notice that for reduction of the dimerized FM chain to the uniform one [Eq. (11)] it is sufficient to satisfy only the condition $T \ll s^2 J_1$ so that the temperature can be higher than the weak bond interaction $s^2 J_2$. However, the following continuum approximation requires $T \ll s^2 J_0$, which implies that the partition function in the form of Eq. (13)

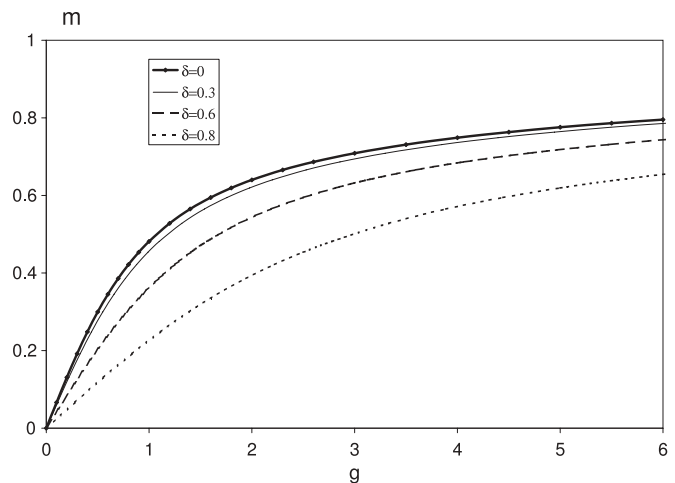


FIG. 1. Dependence of the normalized magnetization M on the scaled magnetic field $g = s^3 J h / T^2$ for several values of the dimerization parameter δ .

is valid when the temperature is lower than both exchange couplings $T \ll s^2 J_1$ and $T \ll s^2 J_2$. These conditions impose the corresponding restrictions on the value of dimerization: $T \ll s^2 J(1 - \delta)$. Therefore, in the limit of strong dimerization $\delta \rightarrow 1$, when the system reduces to decoupled dimers, the reduction to the uniform lattice model (11) is valid for $T \ll s^2 J$, but the continuum approximation is restricted to very low temperatures $T \ll s^2 J(1 - \delta)$. In the case $\delta = 0$ the original model becomes uniform one and effective exchange integral (12) correctly reduces to $J_0 = J$.

A. Spin correlation functions

The low-temperature magnetization of the dimerized FM chain coincides with that for the uniform model and only the scaling parameter γ is renormalized. But the spin correlation functions of the dimerized and uniform models are different. The dimerized spin chain in contrast with the uniform one contains alternating ‘‘strong’’ J_1 and ‘‘weak’’ J_2 bonds. Obviously, the nearest-neighbor correlation functions are different for strong and weak bonds at $T > 0$: $\langle \vec{S}_{2i-1} \cdot \vec{S}_{2i} \rangle = \partial F / \partial J_1$ and $\langle \vec{S}_{2i} \cdot \vec{S}_{2i+1} \rangle = \partial F / \partial J_2$. Their ratio depends on the dimerization parameter as

$$\frac{\langle \vec{S}_{2i-1} \cdot \vec{S}_{2i} \rangle}{\langle \vec{S}_{2i} \cdot \vec{S}_{2i+1} \rangle} = \frac{(1 - \delta)^2}{(1 + \delta)^2}. \quad (18)$$

Similarly, the behavior of the spin correlation function $\langle \vec{S}_i \cdot \vec{S}_j \rangle$ depends on the number of strong and weak bonds between the sites i and j . When the distance between the sites i and j is an odd number of the lattice spacing, $2r + 1$, then the numbers of strong and weak bonds differ by one and which number is greater depends on whether the site i is even or odd. As a consequence, in this case the correlation function depends on i . When the distance between the sites i and j is an even number of the lattice spacing $2r$, then the number of strong and weak bonds are equal and there is no such even-odd difference.

The longitudinal and transverse correlators are different for the nonzero magnetic field, and we will consider both types of correlators. At first we consider the correlators $\langle S_i^z S_{i+2r}^z \rangle$ and

$\langle S_i^x S_{i+2r}^x \rangle = \langle S_i^y S_{i+2r}^y \rangle$ for distances of even number of lattice spacing $2r$. As explained above the correlation functions in this case do not depend on i and are defined by the reduced uniform model (11):

$$\langle S_i^\alpha S_{i+2r}^\alpha \rangle = s^2 \langle n_0^\alpha n_r^\alpha \rangle. \quad (19)$$

The correlator $\langle n_0^\alpha n_r^\alpha \rangle$ can be expressed through the eigenvalues and the eigenfunctions of the Schrödinger equation:¹⁵

$$\langle n_0^\alpha n_r^\alpha \rangle = \sum_{nm} |\langle \psi_{00} | \hat{n}_\alpha | \psi_{nm} \rangle|^2 \exp\left(-\frac{T(\varepsilon_{nm} - \varepsilon_{00})}{s^2 J(1 - \delta^2)} 2r\right). \quad (20)$$

We expect that the universality in the long distance behavior of the correlation functions holds, so we are interested in the asymptotic of the correlation function $r \gg 1$. In this limit only the lowest level(s) having nonzero matrix element makes a contribution to Eq. (20). The operator n_z has nonzero expectation value over the ground state $\langle \psi_{00} | \hat{n}_z | \psi_{00} \rangle$, which is the normalized magnetization of the system M . Therefore, the main contribution to sum (20) is given by $n = m = 0$ term and equals M^2 . The decaying correction to this main term is given by the lowest excited state with the same azimuthal number $m = 0$, ε_{10} . Thus, the long-distance asymptotic for the correlation function $\langle n_0^z n_r^z \rangle$ is

$$\langle n_0^z n_r^z \rangle = M^2 + |\langle \psi_{00} | n_z | \psi_{10} \rangle|^2 \exp\left(-\frac{2r}{\xi_{\parallel}}\right), \quad (21)$$

with the correlation length defined by the energy of the lowest excited states as

$$\xi_{\parallel} = \frac{s^2 J(1 - \delta^2)}{T(\varepsilon_{10} - \varepsilon_{00})}. \quad (22)$$

The operator n_x changes the azimuthal number m , therefore the lowest level for correlator $\langle n_0^x n_r^x \rangle$ is ε_{01} . This implies that the transverse correlation function does not show the long range order and exponentially decays on large distances:

$$\langle n_0^x n_r^x \rangle = |\langle \psi_{00} | n_x | \psi_{01} \rangle|^2 \exp\left(-\frac{2r}{\xi_{\perp}}\right) \quad (23)$$

$$\xi_{\perp} = \frac{s^2 J(1 - \delta^2)}{T(\varepsilon_{01} - \varepsilon_{00})}.$$

The correlation lengths ξ_{\parallel} and ξ_{\perp} and the pre-exponential factors can be found analytically in the limits $\gamma \rightarrow 0$ and $\gamma \rightarrow \infty$. At $\gamma = 0$ the Schrödinger equation (16) reduces to the equation for the operator of angular momentum with well-known spherical eigenfunctions and the spectrum $l(l+1)/2$. So the correlation functions for large r are

$$\langle S_i^z S_{i+2r}^z \rangle = \langle S_i^x S_{i+2r}^x \rangle = \frac{s^2}{3} \exp(-2r/\xi), \quad (24)$$

where $\xi_{\parallel} = \xi_{\perp} = \xi$ and

$$\xi = \frac{s^2 J(1 - \delta^2)}{T}. \quad (25)$$

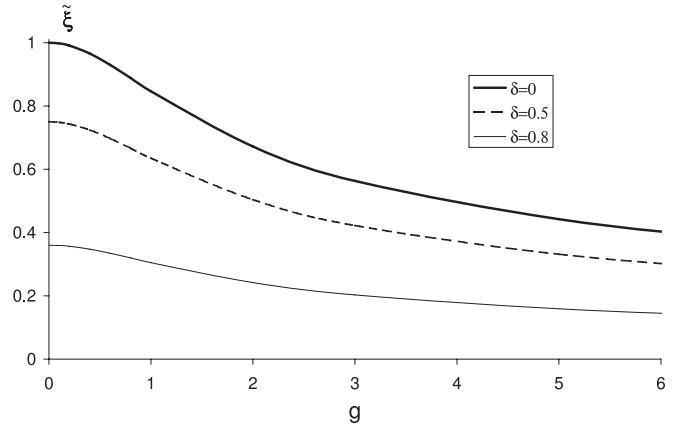


FIG. 2. Dependencies of $\bar{\xi} = \xi_{\perp} T / s^2 J$ on the scaled magnetic field $g = s^3 J h / T^2$ for dimerization parameters $\delta = 0, 0.5, 0.8$.

In the limit of high magnetic field ($\gamma \gg 1$) the correlation functions are

$$\langle S_i^z S_{i+2r}^z \rangle = s^2 M^2 + \frac{s^2}{4\gamma} \exp(-2r/\xi_{\parallel}), \quad \xi_{\parallel} = \frac{1}{2} \sqrt{\frac{sJ(1 - \delta^2)}{h}}$$

$$\langle S_i^x S_{i+2r}^x \rangle = \frac{s^2}{\sqrt{\gamma}} \exp(-2r/\xi_{\perp}), \quad \xi_{\perp} = \sqrt{\frac{sJ(1 - \delta^2)}{h}}. \quad (26)$$

According to Eqs. (24) and (26) the correlation lengths are changed from $\xi \sim 1/T$ at $\gamma = 0$ to $\xi \sim h^{-1/2}$ for $\gamma \rightarrow \infty$. The crossover between two types of the behavior of ξ occurs at $\gamma \simeq 1$. The dependencies of ξ_{\perp} on g for some values of δ are shown in Fig. 2.

Now we study the spin correlation function on “odd” distances. In this case the correlation function $\langle S_i^\alpha S_{i+2r+1}^\alpha \rangle$ is different for odd and even i . Therefore, we distinguish two types of “odd” correlators: $\langle S_{2j-1}^\alpha S_{2j+2r}^\alpha \rangle$ and $\langle S_{2j}^\alpha S_{2j+2r+1}^\alpha \rangle$. The longitudinal correlators $\langle S_i^z S_{i+2r+1}^z \rangle$ has nonzero asymptotic M^2 at $r \rightarrow \infty$ and the calculation of the small corrections caused by the dimerization to this value is not important. On the contrary, the transverse correlator $\langle S_i^x S_{i+2r+1}^x \rangle$ decays exponentially and it is a more interesting object for the calculation of subtle effects like difference on odd and even distances.

According to Eq. (6), the transverse correlator on odd distances is represented as

$$\langle S_{2j-1}^x S_{2j+2r}^x \rangle = s^2 \langle n_0^x (n_r^x + m_r^x) \rangle. \quad (27)$$

The correlator $\langle n_0^x n_r^x \rangle$ was found above in Eq. (23). For the correlator $\langle n_0^x m_r^x \rangle$ we use the following identity:

$$\int_{-\infty}^{\infty} x e^{-\alpha(x-y)^2} dx = y \int_{-\infty}^{\infty} e^{-\alpha(x-y)^2} dx. \quad (28)$$

Therefore, the integration over \vec{m}_r in the multiple integral

$$\langle n_0^x m_r^x \rangle = \int \dots \int \prod d\vec{m}_i d\vec{n}_i n_0^x m_r^x \exp\left(-\frac{H\{\vec{m}_i, \vec{n}_i\}}{T}\right) \quad (29)$$

can be transformed as

$$\begin{aligned} & \int m_r^x \exp \left[-\frac{J_1 + J_2}{2T} \left(\vec{m}_r - \frac{sJ_2 \vec{n}'_r + \vec{h}}{s(J_1 + J_2)} \right)^2 \right] d\vec{m}_r \\ &= \frac{J_2 n_r'^x}{J_1 + J_2} \int \exp \left[-\frac{J_1 + J_2}{2T} \left(\vec{m}_r - \frac{sJ_2 \vec{n}'_r + \vec{h}}{s(J_1 + J_2)} \right)^2 \right] d\vec{m}_r \end{aligned} \quad (30)$$

so that

$$\langle n_0^x m_r^x \rangle = \frac{J_2}{J_1 + J_2} \langle n_0^x n_r'^x \rangle. \quad (31)$$

Using the definition $n_r'^x = n_{r+1}^x - n_r^x$ and Eq. (23) we obtain

$$\begin{aligned} & \langle S_{2j-1}^x S_{2j+2r}^x \rangle \\ &= s^2 |\langle \psi_{00} | n_x | \psi_{01} \rangle|^2 e^{-2r/\xi_\perp} \left(1 - \frac{J_2(1 - e^{-2/\xi_\perp})}{J_1 + J_2} \right). \end{aligned} \quad (32)$$

Here we note that for $\xi_\perp \gg 1$, which is always assumed for low-temperature limit, the last factor in Eq. (32) can be expanded and the correlator takes the form

$$\langle S_{2j-1}^x S_{2j+2r}^x \rangle = s^2 |\langle \psi_{00} | n_x | \psi_{01} \rangle|^2 e^{-(2r+1)/\xi_\perp} \left(1 - \frac{\delta}{\xi_\perp} \right). \quad (33)$$

Similarly, for the correlator $\langle S_{2j}^x S_{2j+2r+1}^x \rangle$ we need merely to exchange $J_2 \longleftrightarrow J_1$, which gives

$$\langle S_{2j}^x S_{2j+2r+1}^x \rangle = s^2 |\langle \psi_{00} | n_x | \psi_{01} \rangle|^2 e^{-(2r+1)/\xi_\perp} \left(1 + \frac{\delta}{\xi_\perp} \right). \quad (34)$$

Let us consider an alternation correlation function:¹²

$$\Delta_\perp(r) = |\langle S_n^x S_{n+r}^x \rangle - \langle S_n^x S_{n-r}^x \rangle|. \quad (35)$$

It equals zero for even r . But for large odd r it becomes

$$\Delta_\perp = s^2 |\langle \psi_{00} | n_x | \psi_{01} \rangle|^2 \frac{2|\delta|}{\xi_\perp} e^{-r/\xi_\perp}. \quad (36)$$

For the small and large γ we obtain

$$\begin{aligned} \Delta_\perp &= \frac{2T|\delta|}{3J(1-\delta^2)} e^{-r/\xi_\perp}, \quad \gamma \ll 1 \\ \Delta_\perp &= \frac{2T|\delta|}{J(1-\delta^2)} e^{-r/\xi_\perp}, \quad \gamma \gg 1. \end{aligned} \quad (37)$$

The comparison of correlation functions (24) and (37) for $\gamma = 0$ with those for the quantum dimerized FM model obtained in Ref. 12 shows that they coincide in the leading terms in T . Therefore, we claim that these correlation functions for $r \gg 1$ obtained for the classical model are valid in the scaling limit for the quantum model as well.

Comparing Eqs. (33) and (34) one can see that the corrections δ/ξ_\perp annihilate each other and give no contribution to the spin structure factor

$$S_\perp(q) = \frac{1}{N} \sum_{j,r} \langle S_j^x S_{j+r}^x \rangle e^{iqr}, \quad (38)$$

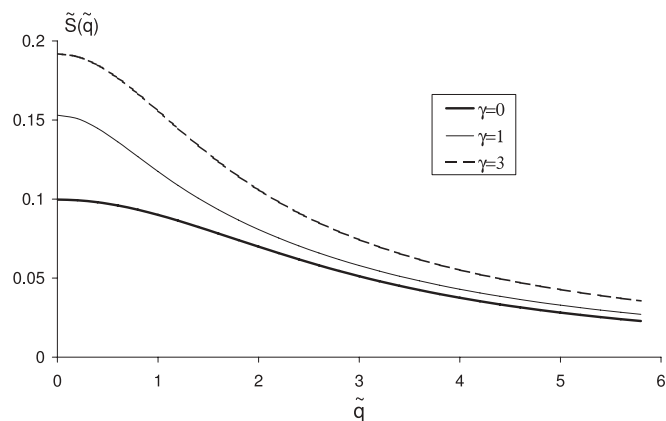


FIG. 3. Dependencies of the normalized spin structure factor $\tilde{S}(q) = S_\perp(q)T/s^4 J_0$ on the scaled wave vector $\tilde{q} = qs^2 J_0/T$ for $\gamma = 0, 1, 3$.

which is the sum of these equations. This is valid in the linear in δ/ξ_\perp terms in the low-temperature limit. The terms $\sim(\delta/\xi_\perp)^2$ can introduce this dimerization effect into $S_\perp(q)$, but this effect is out of the scope of the used continuum approximation. Thus, in the leading term in $\delta T/J$ the spin structure factor for the dimerized model coincides with that of the FM model with the renormalized exchange coupling. Using Eq. (20) for the correlator $\langle S_j^x S_{j+r}^x \rangle$ we obtain the spin structure factor in the form

$$S_\perp(q) = \frac{s^4 J(1-\delta^2)}{T} \sum_n \frac{|\langle \psi_{00} | n_x | \psi_{n1} \rangle|^2 (\varepsilon_{n1} - \varepsilon_{00})}{(\varepsilon_{n1} - \varepsilon_{00})^2 + \tilde{q}^2}, \quad (39)$$

with $\tilde{q} = qs^2 J_0/T$. The dependencies of the normalized spin structure factor $\tilde{S}(q) = S_\perp(q)T/s^4 J_0$ on \tilde{q} for several values of γ is demonstrated in Fig. 3.

III. SPIN-WAVE EXPANSION OF THE QUANTUM MODEL

According to the results of Sec. II the magnetization of the classical dimerized model in the scaling limit $M(\gamma)$ coincides with that found in Ref. 14. In Ref. 14 a method of the computation of the expansion of $M(\gamma)$ for small and large values of γ was developed and several leading terms were presented. However, it is not clear whether the function $M(\gamma)$ is universal in the sense that it is valid for both the classical and the quantum dimerized FM chains. Below we will produce arguments in favor that such universality is the case.

The first argument is that the zero-field susceptibility calculated from the leading term of expansion of $M(\gamma)$ for small γ found in Ref. 14 coincides with the asymptotic of $\chi(0)$ at $T \rightarrow 0$ obtained in Ref. 12 for the quantum dimerized FM chain:

$$\chi(0) = \frac{2s^4 J(1-\delta^2)}{3T^2}. \quad (40)$$

Thus, the function $M(\gamma)$ correctly describes the limit $\gamma \rightarrow 0$ for the magnetization of the quantum model. In connection with Eq. (40) we note that it is not applicable for the case of full dimerization, $\delta = 1$. In this case the system consists of decoupled dimers and the susceptibility follows the Curie law $\chi(0) \sim 1/T$. Thus, our approach is valid when $J(1 -$

$\delta^2 \gg T$. Another check of the hypothesis of the universality is the comparison of the spin-wave expansion for the quantum model with the expansion of $M(\gamma)$ for large γ (strong effective magnetic field).

In order to apply the spin-wave expansion we use the Bose representation of the quantum Hamiltonian (4). It is usually carried out by expressing the spin operators using either the Holstein-Primakoff or the Dyson-Maleev transformations. Here we use the latter which is

$$\begin{aligned} S_n^+ &= \sqrt{2s} \left(1 - \frac{1}{2s} a_n^+ a_n \right) a_n \\ S_n^- &= \sqrt{2s} a_n^+ \\ S_n^z &= s - a_n^+ a_n, \end{aligned} \quad (41)$$

where a_n^+ and a_n are the Bose operators.

Using Eq. (41) we can write Hamiltonian (4) in terms of the Bose operators. The Bose analog of the spin Hamiltonian (4) contains terms which are quadratic and quartic in the Bose operators. The Fourier transform to the momentum space operators leads to the Hamiltonian in the form

$$H = H_0 + H_{\text{int}} - Ns^2 J - Nsh, \quad (42)$$

where

$$H_0 = \sum_k [2sJ(1 - \cos k) + h] a_k^+ a_k + 2i\delta s J \sum_k \sin k a_k^+ a_{k+\pi} \quad (43)$$

$$\begin{aligned} H_{\text{int}} &= \sum V(k'_1, k'_2, k_2, k_1) a_{k'_1}^+ a_{k'_2}^+ a_{k_2} a_{k_1} \delta(k'_1 + k'_2 - k_2 - k_1) \\ &\quad - i\delta \sum W(k'_1, k'_2, k_2, k_1) a_{k'_1}^+ a_{k'_2}^+ a_{k_2} a_{k_1} \\ &\quad \times \delta(k'_1 + k'_2 - k_2 - k_1 - \pi) \end{aligned} \quad (44)$$

$$\begin{aligned} V(k'_1, k'_2, k_2, k_1) &= -\frac{J}{4} [\cos(k_1 - k'_1) + \cos(k_2 - k'_1) \\ &\quad + \cos(k_1 - k'_2) + \cos(k_2 - k'_2) \\ &\quad - 2\cos(k'_1) - 2\cos(k'_2)] \end{aligned} \quad (45)$$

$$\begin{aligned} W(k'_1, k'_2, k_2, k_1) &= -\frac{J}{4} [\sin(k_1 - k'_1) + \sin(k_2 - k'_1) \\ &\quad + \sin(k_1 - k'_2) + \sin(k_2 - k'_2) \\ &\quad + 2\sin(k'_1) + 2\sin(k'_2)]. \end{aligned} \quad (46)$$

Hamiltonian (43) can be diagonalized by a standard way. Let us rewrite the Hamiltonian H_0 using the transformation of k sums to those over the reduced Brillouin zone and introducing the new Bose operators α_k and β_k by the relation

$$\begin{aligned} a_k^+ &= u_k \alpha_k^+ + v_k \beta_k^+ \\ a_{k+\pi}^+ &= -iv_k \alpha_k^+ + iu_k \beta_k^+, \end{aligned} \quad (47)$$

where $|k| < \pi/2$ and

$$\begin{aligned} u_k^2 &= \frac{1}{2} + \frac{\cos k}{2\varepsilon(k)} \\ v_k^2 &= \frac{1}{2} - \frac{\cos k}{2\varepsilon(k)} \\ \varepsilon(k) &= \sqrt{1 - (1 - \delta^2) \sin^2 k}. \end{aligned} \quad (48)$$

Then, the Hamiltonian H_0 takes the form

$$H_0 = \sum_{|k| < \pi/2} [E_\alpha(k) \alpha_k^+ \alpha_k + E_\beta(k) \beta_k^+ \beta_k], \quad (49)$$

where

$$\begin{aligned} E_\alpha(k) &= 2Js[1 - \varepsilon(k)] + h \\ E_\beta(k) &= 2Js[1 + \varepsilon(k)] + h. \end{aligned} \quad (50)$$

Hamiltonian (49) describes the noninteracting bosons. At $T \rightarrow 0$ the main contribution to the free energy from H_0 is given by the small k region. The expansion for $k \rightarrow 0$ results in

$$\begin{aligned} E_\alpha(k) &\simeq sJ(1 - \delta^2)k^2 + h \\ E_\beta(k) &\simeq 4sJ \end{aligned} \quad (51)$$

so that the thermal occupation numbers of α and β particles are

$$\begin{aligned} n_\alpha(k) &= \frac{1}{e^{E_\alpha(k)/T} - 1} \simeq \frac{T}{E_\alpha(k)} \\ n_\beta(k) &\simeq \exp\left(-\frac{4sJ}{T}\right) \rightarrow 0. \end{aligned} \quad (52)$$

According to Eq. (52) we can omit in Eq. (49) the β terms giving the exponentially small contribution to the thermodynamics at $T \rightarrow 0$. Then the Hamiltonian H_0 takes the form

$$H_0 = \sum [sJ(1 - \delta^2)k^2 + h] \alpha_k^+ \alpha_k. \quad (53)$$

Equation (53) has a standard form of the Hamiltonian H_0 obtained in the frame of linear spin-wave theory for the uniform FM model with the renormalized exchange integral $J_0 = J(1 - \delta^2)$.^{6,12}

Now, let us consider the Hamiltonian H_{int} , which is more complicated. First of all, we need to express the operators a_k in Eq. (44) by the operators α_k and β_k using Eq. (47). As was noted above, for sufficiently low temperatures we can neglect the terms in H_{int} containing β_k^+ and β_k operators. Besides, we can replace the Dyson-Maleev vertices V and W by their long-wavelength limits. Carrying out some algebra for both terms in Eq. (44) we obtain H_{int} in the form

$$\begin{aligned} H_{\text{int}} &= -\frac{1}{2} J(1 - \delta^2) \sum k_1 k_2 \alpha_{k'_1}^+ \alpha_{k'_2}^+ \alpha_{k_2} \alpha_{k_1} \\ &\quad \times \delta(k'_1 + k'_2 - k_2 - k_1). \end{aligned} \quad (54)$$

A remarkable fact is that Eq. (54) is nothing but the quartic in the Bose operators part of the Hamiltonian of the uniform FM chain with the renormalized exchange integral $J_0 = J(1 - \delta^2)$. In other words, the Dyson-Maleev vertex of the dimerized chain is the renormalized one of the uniform model.

Thus, we established that in the long-wavelength limit, which is justified at low temperatures, the Hamiltonian of the quantum dimerized chain (42) reduces to that of the uniform FM chain with the effective exchange integral $J_0 = J(1 - \delta^2)$. That is exactly as was found in Sec. II for the classical spin chains. This fact implies that the known equivalence of the low-temperature magnetic properties of classical and quantum FM chains remains for the dimerized chains. It means that if the universality relative to the spin value holds for the uniform

model then this property remains valid for the dimerized FM chain as well. Nevertheless, it is interesting to compare the large γ expansion for the quantum and the classical models.

The calculation of the spin wave expansion for the free energy and the magnetization in all orders in $1/\gamma$ is a complicated problem. But the leading terms can be found analytically. In the zeroth order in H_{int} , which corresponds to the linear spin-wave approximation, the magnetization in the scaling limit is

$$M^{(0)} = -\frac{1}{2\sqrt{\gamma}}. \quad (55)$$

It is easy to check that the contribution of the first order $M^{(1)}$ vanishes by a symmetry. The two-loop correction $M^{(2)}$ was calculated in Ref. 16 and it is given by

$$M^{(2)} = -\frac{1}{128\gamma^{3/2}}. \quad (56)$$

Thus, the spin-wave expansion of the quantum dimerized FM chain is

$$M = 1 - \frac{1}{2\sqrt{\gamma}} - \frac{1}{128\gamma^{3/2}} + O(\gamma^{-2}). \quad (57)$$

Equation (57) exactly reproduces three leading terms of the expansion of $M(\gamma)$ in large γ limit for the classical model.¹⁴ Though we can not calculate the spin-wave expansion in all orders, coincidence of the nontrivial terms in Eq. (57) with those for $M(\gamma)$ is a strong argument that the function $M(\gamma)$ gives the low-temperature magnetization of both the classical and the quantum dimerized FM chains.

It is worth making the following remarks concerning the accuracy of the obtained spin-wave results. We used the long wavelength limit for derivation of the spin-wave expansion of magnetization (57). In fact, taking into account next terms in small- k expansion in Eq. (51) leads to the correction terms to magnetization (57) of the form $\sqrt{T/J_0}f(\gamma)$ [$f(\gamma)$ is some function of γ] and higher orders in small parameter T/J_0 . These terms are small in the scaling limit and can be omitted.

IV. FRUSTRATED DIMERIZED SPIN CHAIN

The considered dimerized ferromagnetic model can be generalized by including in Hamiltonian (4) the next-nearest-neighbor (nnn) antiferromagnetic exchange interaction

$$H = -J_1 \sum \mathbf{S}_{2i-1} \cdot \mathbf{S}_{2i} - J_2 \sum \mathbf{S}_{2i} \cdot \mathbf{S}_{2i+1} + J_{13} \sum \mathbf{S}_i \cdot \mathbf{S}_{i+2} - h \sum S_i^z. \quad (58)$$

This term leads to the frustration. It is known¹⁷ that the ground state of the quantum uniform chain with nnn interaction (so-called zigzag spin chain) has the ferromagnetic ground state for $\alpha = J_{13}/J < \frac{1}{4}$ (α is the frustration parameter) and the singlet ground state with the helical spin correlations for $\alpha > \frac{1}{4}$. For the classical model the transition from the ferromagnetic to the helical phase occurs at the same value $\alpha = \frac{1}{4}$. In this section we study the influence of the nnn interaction on the dimerized FM chain.

The classical dimerized FM chain with the frustration can be studied in a similar way as presented in Sec. II, though with the following modification. Direct use of representation

(6) for spin vectors results in appearing of terms $\vec{m}_i \cdot \vec{m}_{i+1}$ in the resulting Hamiltonian function $H(\{\vec{n}_i, \vec{m}_i\})$, which substantially complicates the subsequent calculations. Therefore, it is convenient to modify the representation of spin vectors on odd and even sites as follows:

$$\begin{aligned} \vec{S}_{2i-1} &= s\vec{n}_i - \mu s\vec{m}_i \\ \vec{S}_{2i} &= s\vec{n}_i + s\vec{m}_i. \end{aligned} \quad (59)$$

The parameter μ is chosen so to remove terms $\vec{m}_i \cdot \vec{m}_{i+1}$ from the resulting Hamiltonian function $H(\{\vec{n}_i, \vec{m}_i\})$:

$$\mu = \frac{\sqrt{J_2^2 - 4J_{13}^2} - J_2}{2J_{13}}. \quad (60)$$

Then, assuming low-temperature limit $T \ll s^2 J_1$ and following the steps made in Sec. II, we integrate over vectors \vec{m}_i in the infinite limits. That yields

$$Z \propto \int \dots \int \prod_{i=1}^{N/2} d\vec{n}_i e^{-H_{\text{eff}}(\{\vec{n}_i\})/T}, \quad (61)$$

where the reduced Hamiltonian function (up to unimportant constant) has a form:

$$\begin{aligned} H_{\text{eff}} &= -\frac{1}{2}s^2 J_{nn} \sum \vec{n}_i \cdot \vec{n}_{i+1} + \frac{1}{2}s^2 J_{nnn} \sum \vec{n}_i \cdot \vec{n}_{i+2} \\ &\quad - 2sh \sum n_i^z \end{aligned} \quad (62)$$

with the effective exchange couplings

$$\begin{aligned} J_{nn} &= J(1 - \delta^2 - 4\alpha + 4\alpha^2) \\ J_{nnn} &= J\alpha^2. \end{aligned} \quad (63)$$

As follows from Eq. (62) the Hamiltonian function of the dimerized frustrated FM model reduces to that of uniform model with the nnn interaction. This model describes well-known zigzag spin chain. According to results of Ref. 18 the transition point of uniform model (62) $J_{nn} = 4J_{nnn}$ is translated to the equation $4\alpha = 1 - \delta^2$ for original dimerized zigzag spin chain. Thus, we stated that the classical dimerized spin chain with frustrated nnn term has the ferromagnetic ground state for $4J_{13} < J(1 - \delta^2)$ and the helical phase for $4J_{13} > J(1 - \delta^2)$. The low-temperature magnetic properties of model (62) in the vicinity of the transition point was studied in Ref. 19.

Taking the continuum limit of the reduced model (62) we obtain the same expression for partition function (13) with the effective exchange integral

$$J_0 = J(1 - \delta^2 - 4\alpha). \quad (64)$$

Thus, the low-temperature magnetic properties of the frustrated dimerized model (58) for $4J_{13} < J(1 - \delta^2)$ are described by the uniform ferromagnetic chain with the scaling parameter

$$\gamma = g(1 - \delta^2 - 4\alpha). \quad (65)$$

The spin-wave expansion for the quantum frustrated model (58) is carried out similar to Sec. IV. The nnn interaction added some terms into bosonic Hamiltonian (42). In particular,

Eqs. (50) and (45) are modified as

$$\begin{aligned}
 E_\sigma(k) &\rightarrow E_\sigma(k) - 2s\alpha J(1 - \cos(2k)) \\
 V(k'_1, k'_2, k_2, k_1) &\rightarrow V(k'_1, k'_2, k_2, k_1) \\
 &\quad + \frac{\alpha J}{4} [\cos(2k_1 - 2k'_1) + \cos(2k_2 - 2k'_1) \\
 &\quad + \cos(2k_1 - 2k'_2) + \cos(2k_2 - 2k'_2) \\
 &\quad - 2\cos(2k'_1) - 2\cos(2k'_2)]. \quad (66)
 \end{aligned}$$

In the long wavelength limit the bosonic Hamiltonian of the dimerized frustrated FM chain reduces to Eqs. (53) and (54) with renormalized exchange coupling $J(1 - \delta^2) \rightarrow J(1 - \delta^2 - 4\alpha)$.

Therefore, we believe that the magnetization of frustrated dimerized spin chain (58) is described by the universal function, which is valid for both classical and quantum model if the frustration parameter α is not too close to $\frac{1-\delta^2}{4}$. The behavior of the magnetization and the susceptibility near the transition point $\alpha = \frac{1-\delta^2}{4}$ is radically different.^{15,20} For example, the zero-field susceptibility $\chi(0) \sim T^{-4/3}$ in contrast with T^{-2} behavior for $\alpha < \frac{1-\delta^2}{4}$.

V. SUMMARY

We studied the low-temperature magnetic properties of the classical and quantum dimerized ferromagnetic spin chain. It is shown that at low temperatures the classical dimerized model reduces to the classical uniform model with the effective exchange integral $J_0 = J(1 - \delta^2)$, where δ is the dimerization parameter. The partition function and spin correlation function of the classical model are calculated with use of the mapping to the continuum limit, which is justified at low temperatures. In the continuum limit the field-dependent thermodynamics depends on one scaling parameter $\gamma = hs^3 J(1 - \delta^2)/T^2$. The calculation of the partition function and spin correlation function reduces to the solution of the Schrödinger equation for the quantum rotator in the “gravitational” field γ .

We have studied the influence of the dimerization on the magnetic properties of the classical spin model. In particular, we have shown that the magnetization decreases with the increase of the dimerization. We found the dependence of the spin correlation functions on both the magnetic field and the dimerization parameter. In contrast with the uniform model the correlation functions as a function of the distance r are different for the even and odd r . Though the correlation lengths of the spin correlations are the same for even and odd r , the pre-exponential factors are different.

It was argued in Ref. 14 that the magnetization M of the uniform classical FM chain at $T \rightarrow 0$ is the universal function of the scaling variable $g = s^3 Jh/T^2$, i.e., the universal function $M(g)$ is valid for any spin value s and the dependence on spin s is captured in the scaling variable g only. It implies that the magnetization curve $M(g)$ is valid for both quantum and classical FM chains and can be determined by the computation of the magnetization of the classical FM chain in the so-called scaling limit, when $T \rightarrow 0$ and $h \rightarrow 0$ but the value of g is finite.

We have shown that this universality holds for the dimerized chain as well. To confirm this fact we studied the quantum dimerized spin model with the use of the Dyson-Maleev representation of spin operators. It is shown that in the long-wavelength limit, which is justified at low temperatures, the Hamiltonian of the quantum dimerized chain reduces to that of the uniform quantum FM chain with the effective exchange integral $J_0 = J(1 - \delta^2)$. That is exactly the same renormalization of the exchange coupling as was found for the classical dimerized spin chains. This fact implies that the known equivalence of the low-temperature magnetic properties of classical and quantum FM chains remains valid for the dimerized chains.

The physical reason of the equivalence of the low-temperature magnetic properties of quantum and classical models is that the de Broglie wavelength of spin waves λ_B is less than the ferromagnetic correlation length ξ .¹⁴ Indeed, for the spectrum Jk^2 the de Broglie wavelength $\lambda_B \sim 1/k \sim \sqrt{J/T}$, while $\xi \sim J/T$. This implies that the physical properties defined by the long-distance asymptotics like magnetization are equal for quantum and classical models. But on the short distances the equivalence failed. For example, the short-distance correlation function behaves as $\langle S_i^z S_{i+r}^z \rangle \sim s^2 - ar^2$ in the quantum case,¹² while the classical model has $\langle S_i^z S_{i+r}^z \rangle \sim s^2 - br$.

The considered dimerized ferromagnetic model was generalized by including in Hamiltonian (4) the next-nearest-neighbor antiferromagnetic exchange interaction. It was shown that the free energy and the magnetization are equal to those for the uniform FM chain with the renormalized exchange integral $J_0 = J(1 - \delta^2 - 4\alpha)$. Therefore, we believe that the magnetization is described by the universal function, which is valid for both the classical and quantum model if the frustration parameter α is not too close to the transition point $\alpha = \frac{1-\delta^2}{4}$.

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*dmitriev@deom.chph.ras.ru

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