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Zigzag spin-*S* chain near the ferromagnet-antiferromagnet transition point

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The properties of the ferromagnetic frustrated spin-*S* one-dimensional Heisenberg model in the vicinity of the transition point from the ferromagnetic to the singlet ground state are studied using the perturbation theory (PT) in small parameter characterizing the deviation from the transition point. The critical exponents defining the behavior of the ground-state energy and spin correlation functions are determined using scaling estimates of infrared divergencies of the PT. It is shown that the quantum fluctuations for $s=1/2$ are sufficiently strong to change the classical critical exponents, while for spin systems with $s \geqslant 1$ the critical exponents remain classical. The dimerization in the singlet phase near the transition point is discussed.

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I. INTRODUCTION

The quantum spin chains with nearest-neighbor (NN) J_1 and next-nearest-neighbor (NNN) J_2 interactions have been subject of numerous studies.[1] The model with both antiferromagnetic interactions $J_1, J_2 > 0$ (AF-AF model) is well studied.[2–7] There is a critical value $J_{2c}=0.2411J_1$, which separates doubly degenerated dimer phase (at $J_2 > J_{2c}$) characterized by the excitation gap and the gapless spin-fluid phase (at $J_2 < J_{2c}$). Relatively less is known about the F-AF model with the ferromagnetic NN and the antiferromagnetic NNN interactions ($J_1 < 0, J_2 > 0$). Although the latter model has been subject of many studies,[8–13] the complete picture of the phases of this model as a function of the frustration parameter J_2/J_1 is unclear up to now. An additional motivation to study this model is related to the fact that a class of recently synthesized compounds containing CuO chains with edge-sharing CuO_4 units is described by the F-AF zigzag model.[14–17] The Cu-O-Cu angle in these compounds is close to 90° and usual antiferromagnetic NN exchange between Cu ions is suppressed. This means that the sign of J_1 can be negative, while the NNN exchange is antiferromagnetic.

It is well known that there is a critical value $J_2/J_1 = -1/4$, where the transition from the ferromagnetic ground state to the incommensurate singlet state occurs.[18,19] The study of the character of this quantum transition is one of the interesting problem related to the F-AF model. In this paper, we focus on the behavior of the model in the vicinity of the transition point. We hope that this analysis will be useful for the study of the properties of the edge-shared copper oxides where the frustration ratio is close to the critical point. In particular, for edge-shared cuprate Li_2ZrCuO_4, the ratio is $J_2/J_1 \sim -0.28$ and for $Rb_2Cu_2Mo_3O_{12}$ it is $J_2/J_1 \sim -0.37$.[20,21]

The Hamiltonian of the F-AF model is

$$H = -\sum_{n=1}^{N} (\mathbf{S}_n \cdot \mathbf{S}_{n+1} - s^2) + J\sum_{n=1}^{N} (\mathbf{S}_n \cdot \mathbf{S}_{n+2} - s^2), \qquad (1)$$

where we put $J_1=-1$ and $J_2=J$, s is a spin value, and periodic boundary conditions are imposed. The constant shifts in Eq. (1) secure the energy of the ferromagnetic state to be zero.

Unfortunately, this model is not solved exactly. As was noted above, the ground state of the model (1) is ferromagnetic at $0 < J < 1/4$ and it becomes a singlet incommensurate state for $J > 1/4$. Though the transition point between these phases is $J=1/4$ for any s,[18] the spectra of the model with $s=1/2$ and $s \geqslant 1$ in this point are different. For $s=1/2$, the singlet ground-state wave function in the transition point is known exactly.[19,22] It is degenerate with the ferromagnetic state for any even N. For $s \geqslant 1$, the singlet ground-state wave function is unknown. Finite-size calculations shows that at $J=1/4$, the singlet state lies slightly higher than the ferromagnetic level and the energies of the singlet and the ferromagnetic states are equal in the limit $N \to \infty$ only.

In the vicinity of the transition point at $0 < \gamma \ll 1$ ($\gamma = J - 1/4$), the singlet ground-state energy E_0 behaves as $E_0 \sim \gamma^{\beta}$, where β is a critical exponent. The classical approximation gives $\beta=2$. The spin-wave theory as well as some other approximations[5,10] do not change this critical exponent. Unfortunately, the exact diagonalization of finite chains shows a complicated irregular size dependence of the ground-state energy, which makes the numerical estimation of the critical exponent β impossible. In the paper,[23] we conjectured that for $s=1/2$, strong quantum fluctuation changes the critical exponent and $\beta=5/3$.

We note that the model (1) with $s \geqslant 1$ has not been studied before and the critical exponent for these cases is unknown. In this paper, we confirm our conjecture for $s=1/2$ using scaling estimates of the perturbation theory (PT) in small parameter γ. We show also that $\beta=2$ for $s \geqslant 1$, though the corresponding factor at γ^2 is different from the classical value and it depends on s.

One of the most important and open questions in the zigzag model (1) is the possibility of the spontaneous dimerization of the system in the singlet phase accompanied by a gap in the spectrum. This problem has been mostly studied in the limit of two weakly coupled AF $s=1/2$ chains ($J \gg 1$). The one-loop renormalization-group analysis indicates[24,25] that the gap is open. However, the existence of the gap has not been verified numerically.[25] On the basis of a field theory consideration, it has been proposed[26] that a finite gap exists, but it is so tiny that it cannot be observed numerically. On the opposite side of the singlet phase, $J \to 1/4$, there are no reliable results about the dimerization and the gap. Strong nonmonotonic finite-size effects do not allow us to study the dimerization numerically.

In order to study the problem of the spontaneous dimerization in the singlet phase of the model (1) close to the transition point $J=1/4$, we consider a generalization of the model (1) by adding to the Hamiltonian H the perturbation in the form of a dimerization term. Unfortunately, the used special version of the PT did not give us a rigorous answer about the spontaneous dimerization in the model (1). However, it allowed us to estimate the critical exponent of the dimer order in case if the spontaneous dimerization in the model (1) exists. Besides, it allowed us to obtain the critical exponents of the ground-state energy and the dimer order for the dimerized version of the model (1).

The paper is organized as follows. In Sec. II, we present the scaling estimate of the critical exponent β using the PT in γ for the Hamiltonian (1) starting from the singlet ground state at $J_c=1/4$. In Sec. III, we analyze the PT for the Hamiltonian, which is transformed to new local axes forming a spiral structure. We establish the scaling behavior associated with γ and with the pitch angle of the spiral. It is shown that the critical exponents for the ground-state energy are different for the spins $s=1/2$ and $s \geqslant 1$. In Sec. IV, we study the problem of the spontaneous dimerization in the model (1). In Sec. V, we summarize our results.

II. SCALING ESTIMATE OF THE CRITICAL EXPONENT NEAR THE TRANSITION POINT $J=1/4$

We are interested in the behavior of the model (1) in the vicinity of the transition point $J_c=1/4$. For this aim, it is natural to develop the perturbation theory

$$H = H_0 + V_\gamma,$$

$$H_0 = -\sum (\mathbf{S}_n \cdot \mathbf{S}_{n+1} - s^2) + \frac{1}{4}\sum (\mathbf{S}_n \cdot \mathbf{S}_{n+2} - s^2),$$

$$V_\gamma = \gamma \sum (\mathbf{S}_n \cdot \mathbf{S}_{n+2} - s^2) \qquad (2)$$

with a small parameter $\gamma = J - 1/4 \ll 1 (\gamma > 0)$.

At $\gamma > 0$, the ground state of the Hamiltonian H is a singlet. Since the perturbation V_γ conserves the total spin S^2, the PT to the lowest singlet state $|\Psi_0\rangle$ of the Hamiltonian H_0 involves only singlet excited states. The low-lying singlet excitations at the transition point have very small energies as shown in Figs. 1 and 2, where we present finite-size calculations of the energy gap between the two lowest singlets. These calculations show that the low-lying singlet excitations have different powers in N for the cases $s=1/2$ and $s \geqslant 1$. As will be shown below, this fact leads to different critical exponents for spin systems with $s=1/2$ and $s \geqslant 1$.

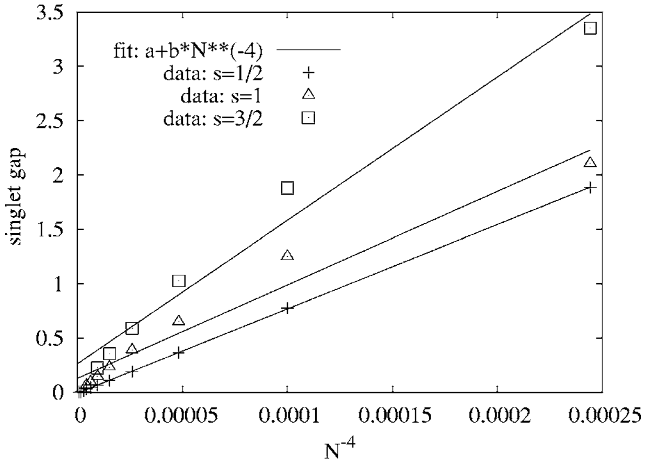

FIG. 1. The gap between two lowest singlet states of the model (1) at the transition point with a different value of spin s vs $1/N^4$. Only the $s=1/2$ curve shows good linear behavior.

The perturbation series for the singlet ground-state energy can be written in the form

$$E_0(\gamma) = \langle \Psi_0 | V_\gamma + V_\gamma \frac{1}{E_0 - H_0} V_\gamma + \cdots | \Psi_0 \rangle. \qquad (3)$$

Suppose that the low-lying excitations acting in the PT behave as

$$E_k - E_0 \sim N^{-\delta}, \qquad (4)$$

where δ is a critical exponents for the excitation spectrum of unperturbed Hamiltonian H_0.

The higher orders of perturbation series contain more dangerous denominators, and, therefore, have higher powers of the infrared divergency. Therefore, we use scaling arguments to estimate the critical exponent for the ground-state energy. Below, we will follow only powers of divergencies and omit all numerical factors.

Suppose that the matrix elements of the perturbation operator V_γ between low-lying states involved in the PT at $N \to \infty$ behave as

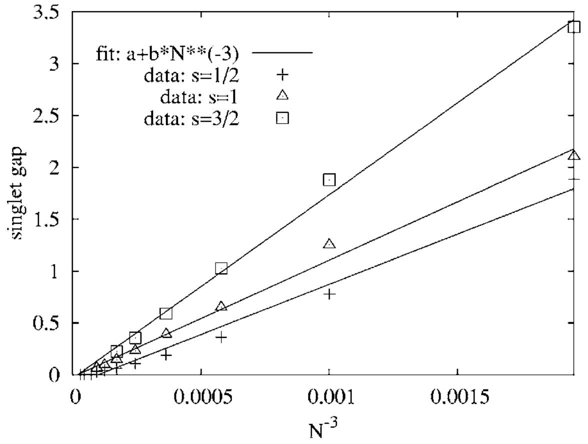

FIG. 2. The gap between two lowest singlet states of the model (1) at the transition point with different value of spin s vs $1/N^3$. $s=1$ and $3/2$ curves have linear dependence.

$$\langle\Psi_i|V_\gamma|\Psi_j\rangle \sim \gamma N^{1-d} \tag{5}$$

with some exponent d.

Looking after powers of infrared divergencies in all orders of the perturbation series, the correction to the ground-state energy takes the form

$$E_0(\gamma) \sim \langle\Psi_0|V_\gamma|\Psi_0\rangle \sum_{m=0}^{\infty} c_m x^m \sim \gamma N^{1-d} f(x), \tag{6}$$

where c_m are unknown constants and

$$x \sim \frac{\langle\Psi_i|V_\gamma|\Psi_k\rangle}{E_k - E_0} \sim \gamma N^{\delta+1-d} \tag{7}$$

is a scaling parameter, which absorbs the infrared divergencies.

The scaling function $f(x)$ at $x \to 0$ is given by the first-order correction. In the thermodynamic limit ($x \to \infty$), the behavior of $f(x)$ is generally unknown, but the natural condition $E_0(\gamma) \sim N$ at $N \to \infty$ requires

$$f(x) \sim x^{d/(\delta+1-d)} \tag{8}$$

and, finally,

$$E_0(\gamma) \sim -N\gamma^{(\delta+1)/(\delta+1-d)} \tag{9}$$

The perturbation series for the lowest excited state $E_1(\gamma)$ has the same form as Eq. (3). But a requirement of a finite mass gap (if any) $m = E_1(\gamma) - E_0(\gamma) \sim O(1)$ leads to another critical exponent

$$m \sim \gamma^{\delta/(\delta+1-d)}. \tag{10}$$

We note that for the models in fixed points with a linear spectrum ($\delta = 1$), a Eqs. (7)–(10) reduce to the well-known formulas[27]

$$x = \gamma N^{2-d},$$

$$E(\gamma) \sim -N\gamma^{2/(2-d)},$$

$$m \sim \gamma^{1/(2-d)}, \tag{11}$$

where the exponent d represents the scaling dimension of the perturbation operator.

However, the transition point $J = 1/4$ is not a fixed point. Finite-size calculations for the gap between lowest singlet states give exponents $\delta = 4$ for the $s = 1/2$ chain and $\delta = 3$ for the $s \geqslant 1$ chain (see Figs. 1 and 2).

In order to determine the value of the exponent d, we notice that the singlet ground state of H_0 has a spiral ordering at $N \to \infty$ with a period of the spiral equal to N,

$$\langle\Psi_0|\mathbf{S}_n \cdot \mathbf{S}_{n+l}|\Psi_0\rangle = s^2 \cos\frac{2\pi l}{N}. \tag{12}$$

For the case $s = 1/2$, this expression is an exact one,[19,22] while for $s \geqslant 1$ we have observed the spin spiral structure in exact diagonalization of finite-size systems (the spin correlation function for the spin $s = 1$ chain of size $N = 20$ is shown in Fig. 3). This means that the first-order correction to the ground-state energy in γ is

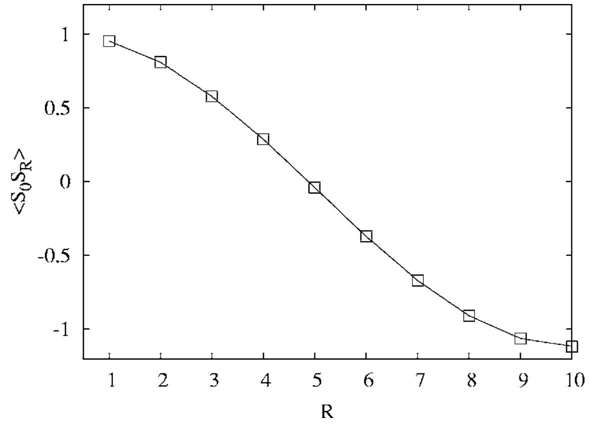

FIG. 3. The spin correlation function $\langle\mathbf{S}_n \cdot \mathbf{S}_{n+l}\rangle$ in the lowest singlet state at the transition point for the spin $s = 1$ chain of size $N = 20$. The spin spiral structure is obvious.

$$\langle\Psi_0|V_\gamma|\Psi_0\rangle = -\gamma\frac{(4\pi s)^2}{N}. \tag{13}$$

We assume that all matrix elements between any low-lying singlet states $|\Psi_i\rangle$ and $|\Psi_j\rangle$ have the same N dependence,

$$\langle\Psi_i|V_\gamma|\Psi_j\rangle \sim \frac{\gamma}{N}, \tag{14}$$

and, therefore, the exponent $d = 2$.

Thus, as follows from Eq. (9), the critical exponents for the ground-state energy are different for $s = 1/2$ and $s \geqslant 1$,

$$E_0(\gamma) \sim -N\gamma^{5/3}, \quad s = 1/2,$$

$$E_0(\gamma) \sim -N\gamma^2, \quad s \geqslant 1. \tag{15}$$

For the case $s \geqslant 1$, the above scaling estimates reproduce the classical value for the critical exponent of the ground-state energy. But in the special case $s = 1/2$, the quantum fluctuations are strong enough to change the critical exponent. In order to understand the nature of the difference between $s = 1/2$ and $s \geqslant 1$ systems and determine factors in Eqs. (15), in the next section we develop a special version of the PT.

III. PERTURBATION THEORY FOR THE TRANSFORMED HAMILTONIAN

Let us start from the classical picture of the ground state of the model (1). In the classical approximation, the spins are vectors that form the spiral structure with a pitch angle φ between neighboring spins. The classical energy per site,

$$E_{\mathrm{cl}}(\varphi) = Ns^2\{1 - \cos\varphi - J[1 - \cos(2\varphi)]\}, \tag{16}$$

is minimized by the angle

$$\varphi_{\mathrm{cl}} = \cos^{-1}\frac{1}{4J}. \tag{17}$$

The classical ground-state energy is

$$E_{\text{cl}}(\varphi_{\text{cl}}) = -N\frac{2s^2}{J}\gamma^2. \tag{18}$$

Following this picture, we transform local axes on the nth site by a rotation about the Y axis by φn. This rotation transforms the original spin wave functions $|\psi_n\rangle$ to a new basis depending on the angle φ,

$$|\psi_{n,\varphi}\rangle = U_\varphi|\psi_n\rangle, \tag{19}$$

where

$$U_\varphi = \exp\left(i\varphi\sum_{n=1}^{N} nS_n^y\right) \tag{20}$$

is the rotation operator and $U_\varphi^\dagger = U_{-\varphi}$. For finite cyclic systems, the pitch angle φ takes quantized values $\varphi_m = \frac{2\pi m}{N}$.

Under the unitary transformation U_φ, the Hamiltonian H takes the form

$$H_\varphi = U_\varphi H U_{-\varphi} = H + V_\varphi,$$

$$\begin{aligned} V_\varphi = {} & (1-\cos\varphi)\sum[S_n^xS_{n+1}^x + S_n^zS_{n+1}^z] \\ & - J(1-\cos 2\varphi)\sum[S_n^xS_{n+2}^x + S_n^zS_{n+2}^z] \\ & - \sum[\sin\varphi(S_n^xS_{n+1}^z - S_n^zS_{n+1}^x) \\ & - J\sin 2\varphi(S_n^xS_{n+2}^z - S_n^zS_{n+2}^x)]. \end{aligned} \tag{21}$$

Now let us choose some eigenstate $|\psi_n\rangle$ of the Hamiltonian H,

$$H|\psi_n\rangle = E_n|\psi_n\rangle. \tag{22}$$

The state $|\psi_n\rangle$ is the eigenstate of the Hamiltonian H, but not of H_φ. Therefore, if we develop and exactly calculate the perturbation theory in V_φ to this state, we arrive at some eigenstate $|\psi_{m,\varphi}\rangle$ of the Hamiltonian H_φ,

$$H_\varphi|\psi_{m,\varphi}\rangle = E_m(\varphi)|\psi_{m,\varphi}\rangle, \tag{23}$$

corresponding to, generally speaking, another energy level $E_m(\varphi) \neq E_n$. Obviously, the unitary transformation U_φ does not change the spectrum. Therefore, the found energy level $E_m(\varphi)$ is also one of the eigenvalues of the original Hamiltonian H. Thus, taking different values of the pitch angle $\varphi_m = \frac{2\pi m}{N}$ $(m=1,\ldots,N)$ and applying the PT in V_φ to some definite eigenstate $|\psi_n\rangle$ of the Hamiltonian H, we obtain a set of N, generally different, levels $E_m(\varphi)$ of H. So, we do not need to fix the value of φ to its classical value in contrast to the spin-wave approximation. Instead, we are free to pick out the minimal energy from the set of the found N levels $E_m(\varphi)$. In the thermodynamic limit, when φ becomes continuous variable, this procedure means the minimization of the found energy $E(\varphi)$ over φ.

As a "source" function $|\psi_n\rangle$ of H, it is natural to choose the ferromagnetic state with all spins pointing up,

$$|F\rangle = |\uparrow\uparrow\cdots\uparrow\rangle. \tag{24}$$

This choice is equivalent to taking the function $|F_\varphi\rangle = U_\varphi|F\rangle$ as a probe ground state for the model (1). The function $|F_\varphi\rangle$ has a spiral structure arising in the classical approximation. The expectation value of the total S^2 in this state is[10]

$$\langle F_\varphi|S^2|F_\varphi\rangle = \frac{N}{2}. \tag{25}$$

This means that $|F_\varphi\rangle$ is not a pure singlet state, but contains an admixture of states with $S\neq 0$. However, it is clear that the weights of states with $S\neq 0$ are negligible at $N\to\infty$ and we can treat the state $|F_\varphi\rangle$ as a singlet one.

Since we are interested in the behavior of the model near the transition point $J=1/4$, it is convenient to represent the Hamiltonian H_φ in the form

$$H_\varphi = H_0 + V_\gamma + V_\varphi \tag{26}$$

with H_0 and V_γ defined above in Eq. (2) and to develop the perturbation theory to the ferromagnetic state in $V = V_\varphi + V_\gamma$. So, there are two channels V_φ and V_γ in the perturbation theory characterized by two small parameters φ and γ. The ferromagnetic state $|F\rangle$ is the eigenstate of the Hamiltonian H_0 with the energy $E_0=0$ and also of the perturbation V_γ, but not of V_φ. The obvious relation $V_\gamma|F\rangle=0$ means that the perturbation series for the energy contains terms $\sim\varphi^m\gamma^n$, but does not contain terms $\sim\gamma^n$ without φ.

At first glance, it seems that as a result of the rotation Eq. (20), we obtain a more complex Hamiltonian H_φ and a more complicated perturbation theory with two channels. But the advantage of this method is to construct the perturbation theory in $V=V_\varphi+V_\gamma$ to the simple ferromagnetic state instead of the perturbation theory in V_γ to a very complicated (and even unknown for $s\geqslant 1$) lowest singlet state of H_0, which was analyzed using scaling arguments and numerical calculations in the previous section. The fact that we separate the term V_γ from H and treat it as the perturbation does not change our arguments about minimization of the found expression for energy $E(\varphi,\gamma)$ over φ.

The ground state of the Hamiltonian H_0 is manifold degenerate: all the ferromagnetic states $|F_{S_z}\rangle$ with different total $S_z = \Sigma S_n^z$ have zero energy. Therefore, at first we have to split this degeneration of the ground state with use of secular equation. It turns out that diagonal elements are proportional to $\langle F_{S_z}|V|F_{S_z}\rangle \sim N$, while nondiagonal matrix elements are $\langle F_{S_z}|V|F_{S_z'}\rangle \sim O(1)$. Therefore, in the thermodynamic limit we can neglect nondiagonal matrix elements and develop regular perturbation theory directly to the ferromagnetic state $|F\rangle$ with all spins pointing up.

The first-order correction to the energy reproduces the leading terms of the classical result (18),

$$E^{(1)} = \langle F|V_\varphi|F\rangle = -2Ns^2\gamma\varphi^2 + Ns^2\frac{\varphi^4}{8}. \tag{27}$$

The second-order correction to the energy,

$$E^{(2)} = \sum_k{}' \frac{\langle\Psi_k|V|F\rangle^2}{E_0 - E_k}, \tag{28}$$

relates to a two-magnon states, because operator V (actually V_φ) has nonzero matrix elements in Eq. (28) only with the states $|\Psi_k\rangle$ containing two magnons with total quasimomentum $Q=0$ and relative quasimomentum k. Exact calculation of the two-magnon problem gives for the sum the following result:

$$E^{(2)} = -N\frac{3s^2\varphi^4}{16(s+1)}. \tag{29}$$

This sum converges, because a dangerous denominator

$$\varepsilon_2(k) = E_k - E_0 = \frac{s}{2}k^4 \tag{30}$$

for small k is compensated by the matrix elements in a numerator,

$$\langle\Psi_k|V_\varphi|F\rangle = \frac{3s^2\varphi^2}{4(s+1)}k^2. \tag{31}$$

As one can see, the two-magnon spectrum of H_0 at $Q=0$ and $k \ll 1$ is simply twice an energy of one magnon $\varepsilon_2(k)=2\varepsilon_1(k)$, where the one-magnon spectrum of H_0 is

$$\varepsilon_1(k) = 2s(1-\cos k) - \frac{s}{2}[1-\cos(2k)] \tag{32}$$

and $\varepsilon_1(k)=sk^4/4$ at small k. So, the low-lying states of H_0 with a small number of magnons have energies $\varepsilon_m = m\varepsilon_1(k) \sim sN^{-4}$, which leads to infrared divergencies in the next-order corrections to the energy. Similar to Eq. (3), we sum them up using the scaling arguments.

The PT for Eq. (26) contains two channels V_γ and V_φ, which are described by two independent scaling parameters. In order to determine these scaling parameters, one should estimate large-N behavior of the matrix elements of the operators V_γ and V_φ between low-lying states $|\Psi_i\rangle$ and $|\Psi_j\rangle$, acting in the PT. Since the operators V_γ and V_φ create (annihilate) not more than two magnons, we look after only low-lying states with a small number of magnons and energies,

$$\varepsilon_m \sim sN^{-4}. \tag{33}$$

We note that these states are very different from the singlet states (with $N/2$ magnons) presented in Eq. (3), and this fact is crucial.

The diagonal matrix elements for one-magnon states with small quasimomentum k behave as

$$\langle k|V_\gamma|k\rangle = -4s\gamma k^2,$$

$$\langle k|V_\varphi|k\rangle = \frac{3}{4}s\varphi^2k^2 - s\frac{\varphi^4}{4} + 4s\gamma\varphi^2 \tag{34}$$

(nondiagonal elements in the one-magnon sector are zero).

For a small number of magnons $m \ll N$, we can treat them as almost independent, because the interactions between magnons give only corrections of the order of magnon density $\rho = m/N$ to the excitation energies and to the matrix elements. Therefore, the large-N behavior of the matrix elements ($k \sim 1/N$) is

$$\langle\Psi_i|V_\gamma|\Psi_j\rangle \sim \gamma sN^{-2},$$

$$\langle\Psi_i|V_\varphi|\Psi_j\rangle \sim \varphi^2 sN^{-2}. \tag{35}$$

These formulas are validated by the exact solution of the two-magnon problem.

Now we are ready to identify the scaling parameters of the perturbations V_γ and V_φ. Similar to Eq. (7), they are

$$\frac{\langle\Psi_i|V_\gamma|\Psi_j\rangle}{\varepsilon_m} \sim \gamma N^2,$$

$$\frac{\langle\Psi_i|V_\varphi|\Psi_i\rangle}{\varepsilon_m} \sim \varphi^2 N^2. \tag{36}$$

The scaling parameter φN looks natural, because for the finite cyclic system the pitch angle φ is quantized as $\varphi_m = \frac{2\pi m}{N}$.

The infrared divergencies are absorbed by these scaling parameters so that the divergent part of the perturbation series in both channels has the form

$$E^{(\mathrm{div})} = \langle\Psi_i|V_\varphi|\Psi_j\rangle \sum_{m,n=0}^{\infty} c_{mn}(\varphi N)^{2m}(\gamma N^2)^n \tag{37}$$

with unknown constants c_{mn}.

In order to satisfy the thermodynamic relation $E^{(\mathrm{div})} \sim N$, we rewrite Eq. (37) as

$$E^{(\mathrm{div})} = Ns\varphi^5 \sum_{n=0}^{\infty} g_n(\varphi N)\left(\frac{\gamma}{\varphi^2}\right)^n, \tag{38}$$

where,

$$g_n(\varphi N) = \sum_{m=0}^{\infty} c_{mn}(\varphi N)^{2n+2m-3} \tag{39}$$

are a set of (generally unknown) scaling functions. They should converge in the thermodynamic limit $N \to \infty$ to some constants

$$a_n = \lim_{N\to\infty} g_n(\varphi N), \tag{40}$$

which are Taylor coefficients of an unknown scaling function $f(\frac{\gamma}{\varphi^2})$,

$$E^{(\mathrm{div})} = Ns\varphi^5 \sum_{n=0}^{\infty} a_n\left(\frac{\gamma}{\varphi^2}\right)^n = Ns\varphi^5 f\left(\frac{\gamma}{\varphi^2}\right). \tag{41}$$

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Thus, collecting the converged first-order $E^{(1)}$ and second-order $E^{(2)}$ corrections with the divergent part $E^{(\mathrm{div})}$, the energy takes the form

$$E = -2Ns^2\gamma\varphi^2 + Ns^2\frac{\varphi^4}{8}\frac{s-1/2}{s+1} + Ns\varphi^5 f\left(\frac{\gamma}{\varphi^2}\right). \tag{42}$$

At $\gamma=0$, the estimate of the energy relates to the spectrum of the Hamiltonian H_0. One can see that the energy for $s \geq 1$ is $E \sim N\varphi^4$, which for small $\varphi \sim \frac{1}{N}$ agrees with the numerical estimate $E \sim N^{-3}$ (see Fig. 2). However, in the special case $s=1/2$, the second term in Eq. (42) vanishes and the energy becomes $E \sim N\varphi^5 f(0)$, which for $\varphi \sim \frac{1}{N}$ agrees again with the numerical estimate $E \sim N^{-4}$ (see Fig. 1). From the positivity of the spectrum of the Hamiltonian H_0, we conclude that $f(0) > 0$.

Now we need to minimize the ground-state energy over φ. As follows from Eq. (42), this procedure is different for $s=1/2$ and $s \geqslant 1$. For the case $s=1/2$,

$$E = -N\frac{\gamma\varphi^2}{2} + N\frac{\varphi^5}{2} f\left(\frac{\gamma}{\varphi^2}\right). \tag{43}$$

The comparison of powers in φ and γ of two terms in Eq. (43) shows that the minimum of E is reached at $\varphi_{\min} \sim \gamma^{1/3}$. Therefore, $f\left(\frac{\gamma}{\varphi_{\min}^2}\right) \to f(0)$ at $\gamma \to 0$ and the expression for $\varphi_{\min}$ takes the form

$$\varphi_{\min}(\gamma) = \left(\frac{2\gamma}{5f(0)}\right)^{1/3}. \tag{44}$$

As was shown above, $f(0) > 0$, which justifies Eq. (44). The corresponding minimal energy is

$$E_{\min} = -\frac{6}{5[20f(0)]^{2/3}} N\gamma^{5/3}. \tag{45}$$

For the case $s \geqslant 1$, the minimum is defined by the first two terms in Eq. (42) and

$$\varphi_{\min} = \sqrt{8\frac{s+1}{s-1/2}}\sqrt{\gamma},$$

$$E_{\min} = -8Ns^2\frac{s+1}{s-1/2}\gamma^2. \tag{46}$$

The last term in Eq. (42) gives the correction to the energy proportional to $\sim Ns\gamma^{5/2}$.

Thus, we reproduce the critical exponents obtained in Sec. II. However, this special type of the PT allowed us to determine also the factor at γ^2 for the case $s \geqslant 1$, which at $s \to \infty$ tends to the classical result Eq. (18).

According to Eqs. (44) and (46), the pitch angle $\varphi_{\min}$ has different behavior at $\gamma \to 0$ for $s=1/2$ and $s \geqslant 1$. It does not coincide with its classical value (17) for any s, but it naturally tends to φ_{cl} at $s \to \infty$. The found nonzero pitch angle $\varphi_{\min}$ indicates the helical (spiral) structure of the ground state. Of course, this does not imply the helical long-range order, which is destroyed by strong quantum fluctuations. Instead, this means an incommensurate behavior of the spin correlation function and the pitch angle $\varphi_{\min}$ can be identified with the quasimomentum $q_{\max}$ at which the static structure factor takes its maximal value.

IV. DIMERIZED ZIGZAG MODEL

In order to study the problem of the spontaneous dimerization in the zigzag model (1) close to the transition point $J=1/4$, we add to the Hamiltonian H the dimerization perturbation V_α,

$$H_d = H + V_\alpha,$$

$$V_\alpha = \alpha \sum (-1)^n \mathbf{S}_n \cdot \mathbf{S}_{n+1}. \tag{47}$$

Then, the behavior of the ground-state energy $E_0(\alpha,\gamma)$ of the model (47) gives us the dimerization order parameter,

$$p(\alpha,\gamma) = \frac{1}{N}\left\langle \sum (-1)^n \mathbf{S}_n \cdot \mathbf{S}_{n+1} \right\rangle = -\frac{1}{N}\frac{\partial E_0(\alpha,\gamma)}{\partial \alpha}. \tag{48}$$

If $E_0(\alpha,\gamma) \sim -N\alpha p(0,\gamma)$ at $\alpha \to 0$, then the singlet phase of the model (1) is spontaneously dimerized and $p(0,\gamma)$ is the corresponding order parameter.

The classical approximation for the model (47) shows that the spins form a double-spiral structure defined by two pitch angles φ and θ so that the rotation angle about the Y axis on the nth site is

$$\varphi_n = n\varphi + \frac{(-1)^n}{2}\theta. \tag{49}$$

The expansion of the classical energy at $(\alpha,\gamma,\varphi,\theta) \ll 1$,

$$E_{\text{cl}}(\alpha,\gamma,\varphi,\theta) = Ns^2\left(\frac{\varphi^4}{8} + \frac{\theta^2}{2} - 2\gamma\varphi^2 - \alpha\varphi\theta\right), \tag{50}$$

is minimized by the angles

$$\varphi_{\text{cl}} = \sqrt{8\gamma + 2\alpha^2},$$

$$\theta_{\text{cl}} = \alpha\varphi_{\text{cl}}, \tag{51}$$

which give the ground-state energy at $\alpha, \gamma \ll 1$,

$$E_{\text{cl}}(\alpha,\gamma) = -\frac{1}{2}Ns^2(4\gamma + \alpha^2)^2. \tag{52}$$

As follows from Eq. (52), $E_{\text{cl}}(\alpha,\gamma)$ vanishes on the line

$$4\gamma + \alpha^2 = 0, \tag{53}$$

which determines the transition line between the ferromagnetic and the singlet phases for the model (47).

For the case $s=1/2$, the exact singlet ground state on this line is known.[22,28] It has double-spiral long-range order,

$$\langle \mathbf{S}_i \cdot \mathbf{S}_{i+n} \rangle = \frac{1}{4}\cos\varphi_n,$$

where the angles φ_n are defined by Eq. (49) with pitch angle $\varphi = \frac{2\pi}{N}$ and small shift angle between spirals $\theta = \frac{2\pi}{N}\alpha$. It is interesting that the classical relation $\theta = \alpha\varphi$ [see Eq. (51)] remains for the strong quantum $s=1/2$ case on the transition line. The dimerization parameter on the transition line behaves as

$$p_{\text{tr}} = \frac{\varphi\theta}{4} = \frac{\pi^2}{N^2}\alpha. \tag{54}$$

Though $p_{\text{tr}} \neq 0$, the spontaneous dimerization is absent on the transition line in the thermodynamic limit.

As follows from Eq. (48), the classical approximation yields the dimerization order for the model (47),

$$p_{\text{cl}}(\alpha,\gamma) = s^2\varphi_{\text{cl}}\theta_{\text{cl}} = 2s^2\alpha(4\gamma + \alpha^2). \tag{55}$$

Equation (55) shows that the dimerization vanishes on the transition line Eq. (53), which accords with Eq. (54), and it vanishes also at $\alpha=0$, which implies the absence of the spontaneous dimerization for the model (1). Since the classical approximation describes the limit $s\to\infty$, one can expect that at least in the limit $s\to\infty$ the spontaneous dimerization in the model (1) is absent.

Following the classical picture, we transform the local axes on the nth site by a rotation about the Y axis by angle φ_n as written in Eq. (49), but not fixing φ and θ to their classical values. Under this unitary transformation, the Hamiltonian H_d (47) takes the form

$$H_{\varphi,\theta}=H_0+V(\alpha,\gamma,\varphi,\theta), \tag{56}$$

where the perturbation $V(\alpha,\gamma,\varphi,\theta)$ has a very cumbersome form and we do not present it here.

Similar to the analysis done in Sec. III, we develop PT in $V(\alpha,\gamma,\varphi,\theta)$ to the fully polarized state (24). The first order in V exactly reproduces the classical energy (50),

$$E^{(1)}=E_{\mathrm{cl}}(\alpha,\gamma,\varphi,\theta). \tag{57}$$

The second-order correction to the ground-state energy gives

$$E^{(2)}=-Ns^2\left(\frac{3\varphi^4}{16(s+1)}+\frac{(\theta-\alpha\varphi)^2}{2}\right). \tag{58}$$

As one can see, the terms containing the angle θ in the first order $E^{(1)}$ are exactly compensated by the contributions of the second order $E^{(2)}$. This result is rather unexpected. The classical approximation corresponds to the limit $s\to\infty$ and it would seem that the quantum effects will give relative corrections $\sim s^{-1}$ to the energy. However, in this case the quantum corrections have the same order in s as the classical energy.

The next-order corrections contain infrared divergencies and we treat them using the scaling arguments similar to that done in Sec. III. The analysis shows that the most divergent parts of the PT are accumulated in the following scaling parameters:

$$x_\alpha\sim\alpha N,$$

$$x_\varphi\sim\varphi N,$$

$$x_\gamma\sim\gamma N^2. \tag{59}$$

It turns out that the angle θ is not accompanied by the infrared divergencies and, therefore, it does not form a scaling parameter. After the algebraic manipulations with the divergent series of the PT similar to Eqs. (37)–(41), the main contribution of the next-order corrections to the ground-state energy at $N\to\infty$ takes the form

$$E^{(\mathrm{div})}=Ns\varphi^5 f\left(\frac{\gamma}{\varphi^2},\frac{\alpha}{\sqrt{\gamma}}\right), \tag{60}$$

where $f(\frac{\gamma}{\varphi^2},\frac{\alpha}{\sqrt{\gamma}})$ is an unknown scaling function of two scaling variables. The angle θ does not contribute to the most divergent parts of the PT Eq. (60) because it is not accompanied by the infrared divergencies.

Collecting the corrections $E^{(1)}$ and $E^{(2)}$ with the scaling part $E^{(\mathrm{div})}$, we obtain the leading terms for the ground-state energy:

$$E=-\frac{1}{2}Ns^2(4\gamma+\alpha^2)\varphi^2+Ns^2\frac{\varphi^4}{8}\frac{s-1/2}{s+1}+Ns\varphi^5 f_s\left(\frac{\gamma}{\varphi^2},\frac{\alpha}{\sqrt{\gamma}}\right). \tag{61}$$

As follows from Eq. (61), the leading terms do not contain the angle θ. In fact, we have checked that the energy does not contain terms up to $\sim\theta^4$. This result is not surprising. In general, the PT in $V(\alpha,\gamma,\varphi,\theta)$ for the ferromagnetic state results in the energy $E(\alpha,\gamma,\varphi,\theta)$ depending on θ. On the other hand, the spectra of the Hamiltonians H_d (47) and $H_{\varphi,\theta}$ (56) coincide and the eigenvalues $E_n(\alpha,\gamma)$ of both Hamiltonians do not depend on θ and φ. Therefore, for any values of θ and φ, the PT leads to one of the determinate levels $E_n(\alpha,\gamma)$ of the Hamiltonian H. The pitch angle φ is quantized as $\varphi_n=\frac{2\pi n}{N}$ for finite N, and the PT with different φ_n leads to generally different levels $E_n(\alpha,\gamma)$. At the same time, in contrast to the pitch angle φ, the angle θ is a continuous variable even for finite N. Therefore, the continuity condition of the dependence $E(\alpha,\gamma,\varphi,\theta)$ on θ implies that the PT in $V(\alpha,\gamma,\varphi,\theta)$ with any value of θ leads to the same energy level as at $\theta=0$. In other words, the energy obtained in the PT ground state does not depend on θ.

This fact is an argument for the absence of the spontaneous dimerization in the zigzag model (1). Really, the PT with any value of θ arrives at the same state as it does at $\theta=0$. But at $\theta=0$ and $\alpha=0$, the PT in $V(\alpha,\gamma,\varphi,\theta)$ reduces to the PT (21) in V_φ considered in Sec. III. There are no terms in the perturbation V_φ that break translational symmetry and can potentially lead to the dimer order.

However, the above arguments do not prove the absence of the spontaneous dimerization in the model (1). The rigorous method is to calculate the dimer order parameter directly from Eq. (48), which we follow below.

The minimization of the ground-state energy over φ is performed in the same manner as was done in Sec. III. For the case $s=1/2$, the second term in Eq. (61) disappears. The comparison of powers in φ of two terms in Eq. (61) shows that the minimum of E is reached at $\varphi_{\min}\sim(4\gamma+\alpha^2)^{1/3}$. Therefore, we substitute $f(\frac{\gamma}{\varphi_{\min}^2},\frac{\alpha}{\sqrt{\gamma}})\to f(0,\frac{\alpha}{\sqrt{\gamma}})$ at $\gamma\to0$ and the expression for $\varphi_{\min}$ becomes

$$\varphi_{\min}(\alpha,\gamma)=(4\gamma+\alpha^2)^{1/3}g(\eta), \tag{62}$$

where $\eta=\frac{\alpha}{\sqrt{\gamma}}$ and $g(\eta)=[10f(0,\eta)]^{-1/3}$.

The corresponding minimal energy is

$$E_{\min}=-\frac{3N}{40}(4\gamma+\alpha^2)^{5/3}g^2(\eta). \tag{63}$$

For the case $s\geqslant1$, the energy minimum is defined by the first two terms in Eq. (61) and

$$\varphi_{\min}=\sqrt{2\frac{s+1}{s-1/2}}\sqrt{4\gamma+\alpha^2},$$

$$E_{\min}=-Ns^2\frac{s+1}{2s-1}(4\gamma+\alpha^2)^2+Ns(4\gamma+\alpha^2)^{5/2}g_s(\eta), \tag{64}$$

where $g_s(\eta)=\left[\frac{2(s+1)}{s-1/2}\right]^{5/2}f_s\left(\frac{\gamma}{\varphi_{\min}^2},\eta\right)$. So, the leading term in the ground- state energy for $s\geqslant 1$ is determined by the regular parts of the PT, while the scaling part [the last term in Eq. (64)] gives only a small correction to the energy.

We see that the difference in the critical exponents for the cases $s=1/2$ and $s\geqslant 1$ remains for the more general dimerized model (56) as well. The pitch angle $\varphi_{\min}$ and the ground-state energy $E_{\min}$ naturally vanish on the transition line Eq. (53) for both cases $s=1/2$ and $s\geqslant 1$.

The dimerization of the model (56) is defined as a derivative of the energy with respect to α (48). As follows from Eqs. (63) and (64), the dimerization at $\gamma=0$ appears with critical exponents

$$p(\alpha,0)\sim\alpha^{7/3},\quad s=1/2,$$

$$p(\alpha,0)\sim\alpha^{3},\quad s\geqslant 1. \tag{65}$$

As for the model (1) ($\alpha=0$), the dimerization depends on the behavior of the scaling functions $f_s(\eta)$ at small η. There are two possible scenarios. First, the expansion of $f_s(\eta)$ at $\eta\to 0$ is $f_s(\eta)=a+b\eta^{\mu}$ with some constants a and b and $\mu>1$, so that $f_s'(0)=0$. In this case, the dimer parameter is zero for the model (1). Second, $f_s(\eta)=a+b\eta$ at $\eta\to 0$ and $f_s'(0)=b$. For this case the translation symmetry of the zigzag model (1) is spontaneously broken and dimer long-range order appears as

$$p(0,\gamma)\sim\gamma^{7/6},\quad s=1/2,$$

$$p(0,\gamma)\sim\gamma^{2},\quad s\geqslant 1. \tag{66}$$

Here the critical exponent for the dimerization (66) for $s\geqslant 1$ comes not from the leading term in Eq. (64), but from the scaling correction (the last term).

Unfortunately, we do not have any information about the behavior of the scaling functions $f_s(\eta)$. Therefore, we can only state that if the zigzag model (1) is in the dimerized singlet phase at $\gamma>0$, then the critical exponents for the dimer LRO are given by Eqs. (66).

V. SUMMARY

We have studied the frustrated Heisenberg chain with the nearest ferromagnetic and the next-nearest-neighbor antiferromagnetic exchange interactions. It was shown that the behavior of the model in the vicinity of the transition point between the ferromagnetic and the singlet phases depends on the value of the spin. For $s=1/2$, the critical exponent characterizing the behavior of the energy is $\beta=5/3$ in contrast to the "classical" exponent $\beta=2$ for $s\geqslant 1$. This difference is a result of different finite-size dependencies of the spectrum at the transition point $\gamma=0$ for the cases $s=1/2$ and $s\geqslant 1$. The pitch angles characterizing the incommensurate behavior of the spin correlation functions are different for $s=1/2$ and $s\geqslant 1$, too. In particular, the pitch angle φ of the spiral is proportional to $\gamma^{1/3}$ for $s=1/2$ and to $\gamma^{1/2}$ for $s\geqslant 1$. This means that the considered model with $s=1/2$ is special and the quantum effects for this value of s are the most strong.

One more intriguing question is related to the existence of the spontaneous dimerization in the singlet phase. In order to study this problem, we added to the Hamiltonian H the dimerization term and treated it as a perturbation. Unfortunately, the used special version of the PT did not give us a rigorous answer about the spontaneous dimerization in the singlet phase. Instead, under assumption of the existence of the spontaneous dimerization, the PT allowed us to estimate the critical exponent of the dimer order parameter. Besides, using the special version of the PT, we obtain the critical exponents of the ground-state energy and the dimer order for the dimerized version of the model (1).

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