# Antiferromagnet-ferromagnet transition in the one-dimensional frustrated spin model

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The one-dimensional $s=\frac{1}{2}$ quantum spin model with nearest-neighbor ferromagnetic and next-nearest-neighbor antiferromagnetic interactions is considered. The behavior of the system in the vicinity of the transition point from the antiferromagnetic ground state to the ferromagnetic one is studied. The consideration is based on the classical approximation and the regular procedure is proposed to find the corrections to the classical energy. The dependence of the energy on spin $S$ is calculated. We obtain evidence of a phase separation for the state with intermediate $S$.

## I. INTRODUCTION

The quantum spin models with isotropic nearest- and next-nearest-neighbor interactions have been the subject of numerous studies.[1–12] If exchange integrals in these models can be either positive or negative then the ground state can be ferromagnetic or antiferromagnetic depending on a relation between integrals. The study of the character of the transition between these states due to the variation of the exchange integrals has a special interest. In particular, it is not clear whether the transition from the antiferromagnetic state ($S=0$) to the ferromagnetic one ($S=S_{\max}$) comes to pass through states with intermediate values of $S$ or only the two limiting states are possible as the ground states. A similar problem arises in electronic systems with extremely strong interaction, for example, in the Hubbard model with $u=\infty$.[13–15]

The simplest model of such a kind is the one-dimensional (1D) $s=\frac{1}{2}$ quantum spin system given by the Hamiltonian

$$H=-\sum_n \left(\mathbf{S}_n\mathbf{S}_{n+1}-\frac{1}{4}\right)+J\sum_n \left(\mathbf{S}_n\mathbf{S}_{n+2}-\frac{1}{4}\right), \tag{1}$$

with nearest ferromagnetic and next-nearest-neighbor antiferromagnetic ($J>0$) interactions.

Unfortunately, even this simple model is not solved exactly. It is known that the ferromagnetic state is unstable at $J=\frac{1}{4}$,[5,6] and the ground state is nontrivial at $J>\frac{1}{4}$ and can be realized in a form of different phases.[5]

First of all, we are interested in the behavior of the system when $J$ is close to $\frac{1}{4}$. A spin-correlation function for $\gamma=(J-\frac{1}{4})\ll 1$ falls down very slowly ($\sim r^{-\gamma}$). This allows us to use the classical approximation for the zeroth-order state. As it will be shown below a regular procedure is possible to find corrections to the energy as an expansion in powers of $\gamma$. The first three terms of this expansion have been calculated.

## II. PERTURBATION THEORY AT $\gamma\to 0$

The ground state of the Hamiltonian (1) is ferromagnetic at $J\leq\frac{1}{4}$ and $S=S_{\max}=N/2$. (Strictly speaking, energies of states with different $S$ differ by values of order $1/N$, i.e., are degenerate in the thermodynamic limit.) When $J>\frac{1}{4}$ this state is unstable against a creation of a magnon, energy of which is equal to

$$\epsilon(k)=(1-\cos k)-J(1-\cos 2k), \tag{2}$$

where $k$ is a quasimomentum of the magnon.

It follows from this equation that the maximal energy gain of the magnon creation is

$$-\left(\frac{2}{J}\right)\left(J-\frac{1}{4}\right)^2=-\left(\frac{2}{J}\right)\gamma^2. \tag{3}$$

The lowest two-magnon state is a bound one and the binding energy at $\gamma\to 0$ is

$$\epsilon_b=-72\gamma^3 \tag{4}$$

At first glance, one can expect that the magnons are noninteracting to the accuracy of $\gamma^3$ and the total energy of $M$-magnon state with $S=N/2-M$ is

$$E_M=-8M\gamma^2. \tag{5}$$

In fact, $M$ magnons form a bound complex with the energy[16]

$$E=-8M\gamma^2+\epsilon_b\,\frac{M(M^2-1)}{6}. \tag{6}$$

It follows from (6) that Eq. (5) is not correct for finite magnon concentration ($M/N=$const) even with an accuracy of $\gamma^2$. This is confirmed by an exact calculation [Eq. (49)]. Thus, conclusions based on the two-magnon approximation[5] do not give the correct thermodynamic picture in the transition region.

In the classical approximation the ferromagnetic state is the ground state at $J<\frac{1}{4}$ and a spiral with real-space periodicity $\sim\gamma^{-1/2}$ is formed at $J>\frac{1}{4}$. When $\gamma\ll 1$ it is natural to use the classical approximation with spin-wave correction. This approach allows us to construct a regular expansion in powers of the small parameter $\gamma$ for the system under consideration.

It is convenient to rotate the coordinate system with origin at center $n$ by an angle $\varphi n$ with respect to axis $y$ (as it will be shown below the value $\varphi$ must be chosen equal to an angle of the twist of the spiral). The corresponding transformation to new spin-$\frac{1}{2}$ operators $\boldsymbol{\xi}_n$ has a form

$$S_n^x=\cos(\varphi n)\xi_n^x-\sin(\varphi n)\xi_n^z, \tag{7}$$

$$S_n^y=\xi_n^y,$$

$$S_n^z=\sin(\varphi n)\xi_n^x+\cos(\varphi n)\xi_n^z.$$

In the well-known spin-wave approximation of Anderson[17] for the antiferromagnetic Heisenberg model the angle $\varphi$ is equal to $\pi$.

As a result, the Hamiltonian (1) becomes

$$H=-\cos\varphi\Sigma(\xi_n^z\xi_{n+1}^z+\xi_n^x\xi_{n+1}^x)-\sin\varphi\Sigma(\xi_n^x\xi_{n+1}^z-\xi_n^z\xi_{n+1}^x)-\Sigma\left(\xi_n^y\xi_{n+1}^y-\frac{1}{4}\right)+J\cos2\varphi\Sigma(\xi_n^z\xi_{n+2}^z+\xi_n^x\xi_{n+2}^x)$$
$$+J\sin2\varphi\Sigma(\xi_n^x\xi_{n+2}^z-\xi_n^z\xi_{n+2}^x)+J\Sigma\left(\xi_n^y\xi_{n+2}^y-\frac{1}{4}\right). \tag{8}$$

Let us represent this Hamiltonian in a form

$$H=H_0+V, \tag{9}$$

where

$$H_0=\frac{N}{4}(1-\cos\varphi)-\frac{NJ}{4}(1-\cos2\varphi)-\cos\varphi\Sigma\left(\xi_n^z\xi_{n+1}^z-\frac{1}{4}\right)+J\cos2\varphi\Sigma\left(\xi_n^z\xi_{n+2}^z-\frac{1}{4}\right)$$
$$-\frac{1}{4}(1+\cos\varphi)\Sigma(\xi_n^+\xi_{n+1}^-+\xi_n^-\xi_{n+1}^+)+\frac{J}{4}(1+\cos2\varphi)\Sigma(\xi_n^+\xi_{n+2}^-+\xi_n^-\xi_{n+2}^+), \tag{10}$$

$$V=\frac{1}{4}(1-\cos\varphi)\Sigma(\xi_n^+\xi_{n+1}^++\xi_n^-\xi_{n+1}^-)-\frac{J}{4}(1-\cos2\varphi)\Sigma(\xi_n^+\xi_{n+2}^++\xi_n^-\xi_{n+2}^-)-\sin\varphi\Sigma(\xi_n^x\xi_{n+1}^z-\xi_n^z\xi_{n+1}^x)$$
$$+J\sin2\varphi\Sigma(\xi_n^x\xi_{n+2}^z-\xi_n^z\xi_{n+2}^x). \tag{11}$$

The operator $V$ is the perturbation at $\varphi\ll1$ and the ground-state wave function $\Psi_0$ of $H_0$ corresponds the configuration having all spins pointing, for example, down. Then, the ground-state energy of $H_0$ is

$$E_0=\frac{N}{4}(1-\cos\varphi)-\frac{NJ}{4}(1-\cos2\varphi). \tag{12}$$

The energy $E_0$ has a minimum at $\varphi=\alpha$, where $\alpha$ is the angle of the rotation in $xz$ plane of the classical spiral configuration, and

$$\cos\alpha=\frac{1}{4J},\quad \alpha=\sqrt{8\gamma},\quad \gamma\to0 \tag{13}$$

and

$$E_0=-\frac{N\gamma^2}{2J}. \tag{14}$$

The energy (14) coincides with the energy of the Hamiltonian (1) in the classical approximation. At $\gamma\to0$ we have

$$E_0=-2N\gamma^2. \tag{15}$$

It is easy to check that the ground state at $\varphi=\alpha$ is stable against the spin flip. The operator $V$, which is proportional to $\alpha^2$, can be considered in a framework of the perturbation theory.

The expectation value of $S^2$ in the ground state is

$$\langle\Psi_0|S^2|\Psi_0\rangle=\frac{N}{2}. \tag{16}$$

Equation (16) means that $\Psi_0$ is not a pure singlet state but contains an admixture of states with $S\neq0$. Therefore, strictly speaking, the wave function $\Psi_0$ must be projected onto the state with $S=0$. However, it is clear that the weights of states with $S\neq0$ are negligible at $N\to\infty$ and the projection will not influence the leading ($\sim N$) contribution to the energy.

Let us calculate now the second-order term of the perturbation theory. It is easy to see that the third and the fourth terms in (11) do not give contributions to second order and the energy $E^{(2)}$ is

$$E^{(2)}=\sum_m\frac{|\langle\Psi_0|V|\Psi_m\rangle|^2}{E_0-E_m}, \tag{17}$$

where $\Psi_m$ and $E_m$ are the wave function and the energy of the excited two-magnon states of $H_0$ at $J=\frac{1}{4}$.

In other words, the problem of the calculation of $E^{(2)}$ reduces to the consideration of the Hamiltonian

$$\tilde{H}=\tilde{H}_0+\tilde{V}, \tag{18}$$

where

$$\tilde{H}_0=-\Sigma\left(\xi_n^z\xi_{n+1}^z-\frac{1}{4}\right)+\frac{1}{4}\Sigma\left(\xi_n^z\xi_{n+2}^z-\frac{1}{4}\right)-\frac{1}{2}\Sigma(\xi_n^+\xi_{n+1}^-+\xi_n^-\xi_{n+1}^+)+\frac{1}{8}\Sigma(\xi_n^+\xi_{n+2}^-+\xi_n^-\xi_{n+2}^+), \tag{19}$$

$$\tilde{V}=\frac{\alpha^2}{8}\sum[\xi_n^+(\xi_{n+1}^+-\xi_{n+2}^+)+\xi_n^-(\xi_{n+1}^--\xi_{n+2}^-)], \tag{20}$$

and $E^{(2)}$ is given by

$$E^{(2)}=-\left(\frac{\alpha^2}{8}\right)^2\sum_k\frac{|\varphi_{0,k}(1)-\varphi_{0,k}(2)|^2}{\epsilon(0,k)}. \tag{21}$$

Here $\epsilon(Q,k)$ and $\varphi_{Q,k}(n)$ are the energy and the wave function of the two-magnon states of the Hamiltonian (19) with total quasimomentum $Q$ and the relative quasimomentum $k$.

$\epsilon(Q,k)$ and $\varphi_{Q,k}(n)$ are found by the standard way from the solution of the corresponding two-particle problem. We will not present detailed expressions because they are very cumbersome and thus we give only the final result for the sum (21)

$$\frac{1}{N}\sum_k\frac{|\varphi_{0,k}(1)-\varphi_{0,k}(2)|^2}{\epsilon(0,k)}=2. \tag{22}$$

Thus, the second-order quantum correction $E^{(2)}$ coincides with the classical energy and total energy in this approximation is

$$E=-4N\gamma^2. \tag{23}$$

## III. THE CALCULATION OF THE $\gamma^{5/2}$ TERM

The calculation of the third and higher orders of the perturbation theory in $V$ leads to infrared-divergent integrals and it is necessary to sum them in all orders to obtain the contributions proportional to $\gamma^{5/2}$, $\gamma^3$, etc. Here we will calculate the term proportional to $\gamma^{5/2}$.

The well-known regular way of summation of these divergent diagrams is the construction of a bilinear Bose-Hamiltonian.[18] It is necessary to keep in mind that the bare bosonic interaction has to be replaced by an amplitude of two-magnon scattering with zero relative quasimomentum.

Replacing $\xi_n^+$ by the Bose-operator $b_n^+$ and neglecting terms containing four Bose-operators in (8) we arrive at the Bose-Hamiltonian

$$H_B=E_0+\sum_k\lambda_1(k)b_k^+b_k+\sum_k\lambda_2(k)(b_k^+b_{-k}^++b_{-k}b_k), \tag{24}$$

where $E_0$ is given by (15),

$$\lambda_1(k)=\cos\alpha-J\cos2\alpha-\frac{1}{2}(1+\cos\alpha)\cos k+\frac{J}{2}(1+\cos2\alpha)\cos2k,$$

$$\lambda_2(k)=\frac{1}{2}(1-\cos\alpha)\cos k-\frac{J}{2}(1-\cos2\alpha)\cos2k, \tag{25}$$

and $\lambda_1(k)$ and $\lambda_2(k)$ are the bare interactions.

As already mentioned above, these expressions must be modified in two respects. First, we need to expand them up to terms $\sim\alpha^4$, and, second, to replace $\lambda_2(k)$ by the correct scattering amplitude $F(k)$. Then,

$$\lambda_1(k)\to\tilde{\lambda}_1(k)=\frac{\alpha^4}{16}+2\sin^4\left(\frac{k}{2}\right)+\frac{\alpha^2k^2}{8},$$

$$\lambda_2(k)\to\tilde{\lambda}_2(k)=\frac{\alpha^2}{4}\left(F(k)-\frac{\alpha^2}{4}\right). \tag{26}$$

It follows from the consideration of the two-magnon problem that

$$F(k)=\frac{k^2}{2},\quad k\to0.$$

Diagonalizing the Hamiltonian (24), we arrive at

$$H_B=E+\sum_{k>0}\sqrt{\tilde{\lambda}_1^2(k)-\tilde{\lambda}_2^2(k)}(\beta_k^+\beta_k+\beta_{-k}^+\beta_{-k}), \tag{27}$$

where $\beta_k$ are new Bose operators. The ground-state energy $E$ is

$$E=E_0+\sum_{k>0}[\sqrt{\tilde{\lambda}_1^2(k)-\tilde{\lambda}_2^2(k)}-\tilde{\lambda}_1(k)]. \tag{28}$$

The expansion of (28) up to second order of $\gamma$ reproduces (23). The contribution of the term $\sim\gamma^{5/2}$ is given by the integral

$$\frac{N}{2\pi}\int_0^\infty dk\left\{\sqrt{\left(\frac{\alpha^4}{16}+\frac{k^4}{8}+\frac{\alpha^2k^2}{8}\right)^2-\frac{\alpha^4}{16}\left(\frac{k^2}{2}-\frac{\alpha^2}{4}\right)^2}-\left(\frac{\alpha^4}{16}+\frac{k^4}{8}+\frac{\alpha^2k^2}{8}\right)+\frac{\alpha^4}{16}\right\}. \tag{29}$$

The numerical calculation of the integral (29) gives $4.146\gamma^{5/2}$. Thus, the ground-state energy calculated up to terms $\sim\gamma^{5/2}$ is

$$E=-4N\gamma^2+4.146N\gamma^{5/2}. \tag{30}$$

As to the excitation spectrum it has the soundlike behavior and the corresponding sound velocity is

$$v=4\gamma^{3/2}. \tag{31}$$

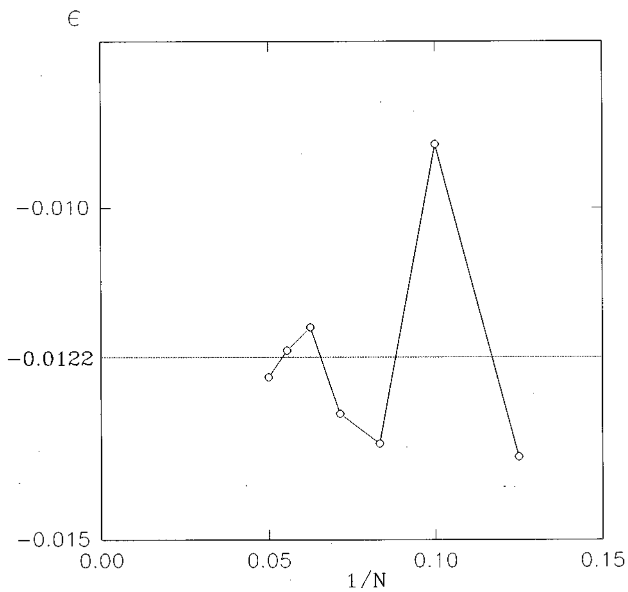


FIG. 1. The ground-state energy per spin $\varepsilon$ of rings with $N=8$–20 for $J=0.3$ ($\gamma=0.5$). The dotted line is the extrapolation to $N\Rightarrow\infty$.

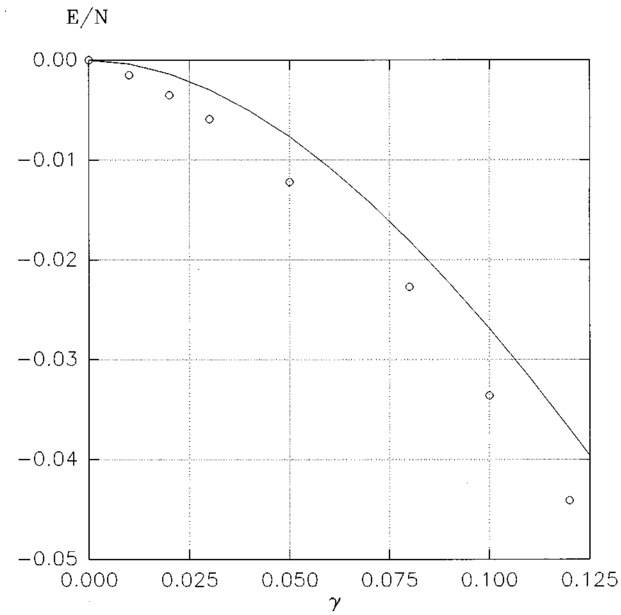


FIG. 2. The ground-state energy given by Eq. (30) (solid line) and the extrapolation of numerical results (circles) as functions of $\gamma$.

## IV. NUMERICAL DIAGONALIZATION OF FINITE RINGS

We have carried out Lanczos calculations on rings with $N=8$–20. These calculations show that the spectrum of the Hamiltonian (1) at $J>\frac{1}{4}$ satisfies the inequality

$$E(S)<E(S+1), \tag{32}$$

where $E(S)$ is the ground-state energy of the Hamiltonian (1) with spin $S$. The inequality (32) coincides with one that takes place in $s=\frac{1}{2}$ Heisenberg antiferromagnet.[19]

At $J<\frac{1}{4}$ and for finite $N$ the state with $S=S_{\max}$ is the ground state. The energies of the singlet and the ferromagnetic states are equal to each other at $J=\frac{1}{4}$. Thus, the transition from the singlet ground state to the ferromagnetic one occurs at $J=\frac{1}{4}$. However, as mentioned above, the energies of states with different $S$ are degenerate at $J\leqslant\frac{1}{4}$ in the thermodynamic limit. Therefore, the energies of states with different $S$ simultaneously go to zero at $\gamma\rightarrow 0$ and $N\rightarrow\infty$ satisfying the inequality (32).

Unfortunately, the problem of an extrapolation of numerical results to $N\rightarrow\infty$ is complicated by the oscillatory dependence of energies on $N$. As an example, the dependence of the ground-state energy ($S=0$) per spin $\epsilon$ on $1/N$ for $J=0.3$ ($\gamma=0.05$) is shown in Fig. 1. Such dependence differs radically from the one for the 1D Heisenberg model with nearest-neighbor antiferromagnetic interactions, where $\epsilon(N)$ is a monotonic function. Apparently, the nonmonotonic behavior of $\epsilon(N)$ in the model under consideration does not depend on the choice of the boundary conditions. We have calculated ground-state energy of open chains and have found that the dependence $\epsilon(N)$ is similar to the one shown in Fig. 1. We note that similar nonmonotonic behavior of $\epsilon(N)$ has been found earlier[4] for the 1D model with nearest-neighbor and next-nearest-neighbor antiferromagnetic interactions in the so-called frustrated regime. Thus, the oscillatory dependence $\epsilon(N)$ is caused by intrinsic properties of frustrated models. In this case it seems natural to choose an average of numerical results of $\epsilon$ for $N=8$–20 as the extrapolation to $N\rightarrow\infty$.

For the energies of one- and two-magnon states, which are known exactly at $N\rightarrow\infty$, this procedure gives an accuracy within 5–10 %. The ground-state energy extrapolated in this way is shown in Fig. 2 together with the energy (30). These two dependences are qualitatively similar. Some difference between them is explained, on the one hand, by the approximate extrapolation and, on the other hand, by the neglecting of terms of higher orders in Eq. (30).

## V. THE ENERGIES OF STATES WITH $S\neq 0$

The ground state of the Hamiltonian (8) is a singlet. To consider states with $S\neq 0$ it is necessary to construct the Hamiltonian, the ground state of which has $S\neq 0$. This can be achieved by the additional rotation [along with (7)] of the coordinate system by angle $\theta$ with respect to axis $x$. The spin operator $\boldsymbol{\xi}_n$ are transformed according to the equations

$$\xi_n^x=\eta_n^x,$$

$$\xi_n^y=\cos\theta\,\eta_n^y-\sin\theta\,\eta_n^z,$$

$$\xi_n^z=\sin\theta\,\eta_n^y+\cos\theta\,\eta_n^z. \tag{33}$$

As it will be shown below the angle $\theta$ fixes nonzero spin $S$ of the ground state

$$S=S_{\max}\sin\theta. \tag{34}$$

Under the transformation (33) the original Hamiltonian (1) takes the form

$$H=-\Sigma\left[(\cos\alpha\ \cos^2\theta+\sin^2\theta)\eta_n^z\eta_{n+1}^z+(\cos\alpha\ \sin^2\theta+\cos^2\theta)\eta_n^y\eta_{n+1}^y+\cos\alpha\,\eta_n^x\eta_{n+1}^x-\frac{1}{4}\right]$$
$$+J\Sigma\left[(\cos2\alpha\ \cos^2\theta+\sin^2\theta)\eta_n^z\eta_{n+2}^z+(\cos2\alpha\ \sin^2\theta+\cos^2\theta)\eta_n^y\eta_{n+2}^y+\cos2\alpha\,\eta_n^x\eta_{n+1}^x-\frac{1}{4}\right]$$
$$+\Sigma\left[\frac{\sin2\theta}{2}(1-\cos\alpha)(\eta_n^z\eta_{n+1}^y+\eta_n^y\eta_{n+1}^z)-\frac{J\ \sin2\theta}{2}(1-\cos2\alpha)(\eta_n^z\eta_{n+2}^y+\eta_n^y\eta_{n+1}^z)\right.$$
$$-\sin\alpha\ \cos\theta(\eta_n^x\eta_{n+1}^z-\eta_n^z\eta_{n+1}^x)-\sin\alpha\ \sin\theta(\eta_n^x\eta_{n+1}^y-\eta_n^y\eta_{n+1}^x)+J\ \sin2\alpha\ \cos\theta(\eta_n^x\eta_{n+2}^z-\eta_n^z\eta_{n+2}^x)$$
$$\left.+J\ \sin2\alpha\ \sin\theta(\eta_n^x\eta_{n+2}^y-\eta_n^y\eta_{n+2}^x)\right]. \tag{35}$$

Similarly to the case $S=0$, the perturbation theory up to $\gamma^2$ can be used for the calculation of the ground-state energy of (35). It is not difficult to convince oneself that the third term in (35) does not give the contribution to the second order and (35) reduces to the Hamiltonian

$$H(\theta)=H_0(\theta)+V(\theta), \tag{36}$$

where

$$H_0(\theta)=E_0\cos^2\theta-\left(\cos\alpha\ \cos^2\theta+\sin^2\theta\Sigma\left(\eta_n^z\eta_{n+1}^z-\frac{1}{4}\right)+J(\cos2\alpha\ \cos^2\theta)\Sigma\left(\eta_n^z\eta_{n+2}^z-\frac{1}{4}\right)\right.$$
$$-\frac{1}{4}[\cos^2\theta+\cos\alpha(1+\sin^2\theta)]\Sigma(\eta_n^+\eta_{n+1}^-+\eta_n^-\eta_{n+1}^+)$$
$$+\frac{J}{4}[\cos^2\theta+\cos2\alpha(1+\sin^2\theta)]\Sigma(\eta_n^+\eta_{n+2}^-+\eta_n^-\eta_{n+2}^+), \tag{37}$$

$$V=\frac{1}{4}\cos^2\theta(1-\cos\alpha)\Sigma(\eta_n^+\eta_{n+1}^++\eta_n^-\eta_{n+1}^-)-\frac{J}{4}\cos^2\theta(1-\cos2\alpha)\Sigma(\eta_n^+\eta_{n+2}^++\eta_n^-\eta_{n+2}^-), \tag{38}$$

and $E_0$ is given by (15).

The ground state of $H_0(\theta)$ is the state with all spins pointing down, $\xi_n^z=-\frac{1}{2}$. Then, in accordance with (7) and (33) the expectation values of components of total spin in the ground state are

$$\sum_n \langle S_n^z\rangle=\sum_n \langle S_n^x\rangle=0,\quad \sum_n \langle S_n^y\rangle=\frac{N}{2}\sin\theta \tag{39}$$

and the ground-state spin is given by Eq. (34).

The ground-state energy of $H_0(\theta)$ as a function of normalized spin $m=S/S_{\max}$ is

$$E_0(m)=(1-m^2)E_0(0). \tag{40}$$

The energy (40) is the energy of the Hamiltonian (1) with $S\neq0$ in the classical approximation.

The calculation of the quantum correction $E^{(2)}(\theta)$ reduces to the analogous problem for the Hamiltonian (18), and value $\alpha^2$ in (20) is replaced by $\alpha^2(1-m^2)$. According to Eqs. (15) and (21) the ground-state energy of (36) up to order $\gamma^2$ is

$$E(m)=E_0(0)[1-m^2+(1-m^2)^2]. \tag{41}$$

The term $\sim\gamma^{5/2}$ is calculated in the analogy with the case $S=0$ taking into account that $\tilde{\lambda}_1(k)$ and $\tilde{\lambda}_2(k)$ in Eq. (26) depend on $\theta$. At small values of $\alpha$ and $k$

$$\tilde{\lambda}_1(k)=\frac{\alpha^4}{16}\cos^2\theta+\frac{k^4}{8}+\frac{\alpha^2k^2}{8}(1+3\sin^2\theta),$$
$$\tilde{\lambda}_2(k)=\cos^2\theta\left(\frac{\alpha^2}{4}\right)\left(\frac{k^2}{2}-\frac{\alpha^2}{4}\right), \tag{42}$$

and the corresponding contribution to the energy is

$$E^{(3)}(m)=\gamma^{5/2}g(m), \tag{43}$$

where the function $g(m)$ is presented in Fig. 3.

The most interesting peculiarity of the function $E(m)$ can be seen from the first two terms of the expansion $E(m)$ given by Eq. (41). It follows from (41) that $d^2E/dm^2$ becomes zero at $m=1/\sqrt{2}$. This fact signifies the thermodynamic instability of the uniform state against the phase separation. Another manifestation of this instability is a behavior of the function $m(h)$ describing the response of the system to the external magnetic field directed along axis $y$. For example, it turns

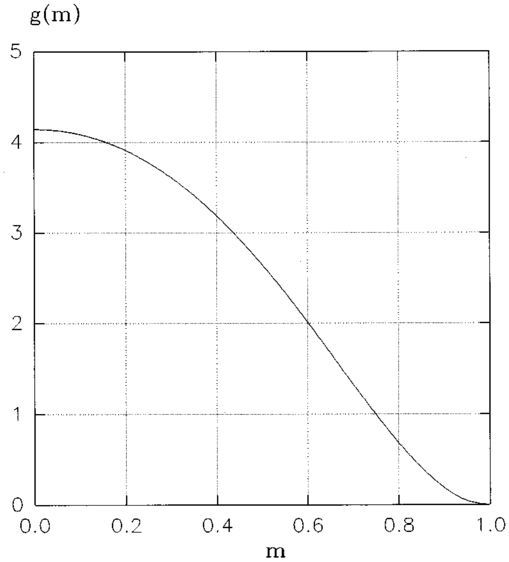


FIG. 3. The dependence of the function $g$ in Eq. (43) on normalized spin.

out that $dm/dh<0$ at $m>1/\sqrt{2}$. In other words, the energy (41) is not minimal at given $S$. This results from the fact that the rotation of the coordinate system is the same for all centers. Another way of fixing $S$ is to introduce the angle $\theta(n)$, depending on $n$. The state with the phase separation is described by the dependence

$$\theta(n)=\theta, \quad 1<n<N_1,$$

$$\theta(n)=\frac{\pi}{2}, \quad N_1<n<N. \tag{44}$$

In this case

$$m=1-c(1-\sin\theta), \quad c=\frac{N_1}{N}. \tag{45}$$

The energy $E(m)$ for this choice of $\theta(n)$ can be found in analogy with the uniform case (neglecting boundary effects) and is given by

$$E(m)=cE_0[(1-x^2)+(1-x^2)^2], \tag{46}$$

where

$$x=1-\frac{1-m}{c}.$$

The minimization of (46) with respect to $c$ gives

$$c=\frac{3(1-m)}{(4-\sqrt{7})}. \tag{47}$$

Thus, at $m<m_0$, where

$$m_0=\frac{\sqrt{7}-1}{3}\simeq 0.5485, \tag{48}$$

Eq. (41) is correct but at $m>m_0$ the energy is

$$E(m)=2.6311E_0\gamma^2(1-m). \tag{49}$$

At $m>m_0$ the system is in the two-phase state, consisting of the ferromagnetic phase of size $N(1-c)$ and the phase with $S=(N/2)m_0$ of size $Nc$. Naturally, Eqs. (47)–(49) can be obtained with the help of the "Maxwell rule."

In connection with Eq. (49) we note the following. As already mentioned above, the binding energy of two-magnon states (4) is proportional to $\gamma^3$ and one can expect that magnons is noninteracting in the accuracy of $\gamma^2$. In this case the energy $E(m)$ would be equal to $2E_0(1-m)$ at $m\to 1$. The difference of this energy from (49) means that this is not the case. Therefore, the interaction of a macroscopic number of magnons is very complicated and leads to the creation of a new phase.

## VI. CONCLUSION

In this work we mainly have been interested in the transition from the antiferromagnetic ground state to the ferromagnetic one. The perturbation theory based on the classical spin configuration has been used and the dependence of the ground-state energy on spin $S$ has been calculated. We have not dwelt on an important question relating to the symmetry and the degeneracy of the ground state. According to the well known Lieb-Shultz-Mattis (LSM) theorem[20,21] the ground state of $s=\frac{1}{2}$ spin chain model with the translationally and rotationally invariant interaction is either degenerate or has gapless excitations. It turns out that in the ground state of the Hamiltonian (27) the nonzero chiral order parameter[5] exists

$$\langle[\mathbf{S}_n\times\mathbf{S}_{n+m}]_y\rangle\sim\sin(m\sqrt{8\gamma}).$$

This expectation value changes the sign under the permutation of spins. This chiral symmetry means that the ground state is twofold degenerate. On the other hand, the spectrum of (27) is gapless. Thus, the ground state of the considered model is degenerate but the spectrum is gapless. This contradicts the LSM theorem. In fact, the expansion of the ground-state energy in small parameter $\gamma$ is asymptotical and, probably, the exponential, with respect to small $\gamma$, terms will restore a rotational symmetry and the ground state will be nondegenerate.

Our main result is that the transition from the state with $S=0$ to the state with $S=S_{\max}$ occurs by passing the states with the intermediate spins. The dependence $E(S)$ in this approximation testifies the instability against the phase separation.

We believe that this approach can be used for the study of a two-dimensional version of the considered model. In addition to that the scenario of the transition from the antiferromagnetic state to the ferromagnetic one is similar to that considered for the 1D model.

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