

Exact ground states for a class of one-dimensional frustrated quantum spin models

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We have found the exact ground state for two frustrated quantum spin- $\frac{1}{2}$ models on a linear chain. The first model describes the antiferromagnet-ferromagnet transition point. The singlet state at this point has double-spiral ordering. The second model is equivalent to special case of the spin- $\frac{1}{2}$ ladder. It has a nondegenerate singlet ground state with exponentially decaying spin correlations, and there is an energy gap. The exact ground-state wave function of these models is presented in a special recurrent form, and a recurrence technique for expectation value calculations is developed. [S0163-1829(97)03034-8]

I. INTRODUCTION

Last decade, frustrated Heisenberg models were a subject of intensive studies.¹⁻¹² Of the main interests are ground-state properties with respect to variations of exchange integrals and the character of the phase transitions. In particular, these properties may be important in the theory of high- T_c superconductivity.

There is much interest in quantum spin systems with competing interactions for which an exact ground state can be constructed. An example of such a model has been given by Majumdar and Ghosh.¹³ They have considered an $s = \frac{1}{2}$ chain with antiferromagnetic nearest- and next-nearest-neighbor interactions, and the strength of the second interaction is one-half of the first. The ground state of this model is two-fold degenerate, it consists of dimerized singlets, and there is a gap in the spectrum of excited states.

Another example found by Affleck Kennedy, Lieb, and Tasaki¹⁴ (AKLT) is an $S = 1$ spin chain with special bilinear and biquadratic interactions. This model has a unique valence-bond-solid ground state, and ground-state correlations have an exponential decay. Besides there is the gap between the ground and excited states. Further generalizations of the AKLT model have been studied in a number recent papers.¹⁵

In this paper we present two classes of $s = \frac{1}{2}$ chains for which the exact ground-state wave function has a special recurrent form. These models have competing ferro- and antiferromagnetic interactions, and their ground states can be either ferromagnetic or singlet depending on the relation between the exchange integrals. The first type of exactly solvable models is related to systems at the ferromagnet-antiferromagnet transition point when the ferromagnetic and singlet states are degenerate. The calculation of the spin correlation function in the singlet ground state shows spiral magnetic order at this point.

The model of the second type has the nearest-, next-nearest-, and next-next-nearest-neighbor interactions depending on one parameter. This model has a nondegenerate singlet ground state for cyclic chains and for a certain region of the parameter, and its ground-state properties are similar to that of the AKLT model. In other words, this model has some properties of the "Haldane scenario,"¹⁶ though it is the model with half-integer spin. We note, however, that the

considered model has two sites in a unit cell, and it is equivalent to the special case of a spin ladder. In some limit this model reduces to the effective spin-1 chain for which the ground-state wave function coincides with that for the AKLT model.

This paper is organized as follows. In the Sec. II we will consider a model of the first type and describe the exact singlet ground-state wave function as well as details of the spin correlation function calculations. Section III and the Appendix present the study of a model of the second type. The results of the paper will be summarized in Sec. IV.

II. FRUSTRATED SPIN CHAIN AT ANTIFERROMAGNET-FERROMAGNET TRANSITION POINTS

A. Exact ground-state wave function

Let us consider an $s = \frac{1}{2}$ spin model with nearest- and next-nearest-neighbor interactions given by the Hamiltonian

$$\hat{H} = - \sum_{i=1}^M \left(\mathbf{S}_{2i-1} \cdot \mathbf{S}_{2i} - \frac{1}{4} \right) + J_{23} \sum_{i=1}^M \left(\mathbf{S}_{2i} \cdot \mathbf{S}_{2i+1} - \frac{1}{4} \right) + J_{13} \sum_{i=1}^N \left(\mathbf{S}_i \cdot \mathbf{S}_{i+2} - \frac{1}{4} \right), \quad (1)$$

with periodic boundary conditions and even $N = 2M$.

If $J_{23} < 1$, then the ground state of Eq. (1) is ferromagnetic (singlet) at $\delta < 0$ ($\delta > 0$), where $\delta = J_{13} + J_{23}/2(1 - J_{23})$ (Fig. 1). The equation $\delta = 0$ defines the line of transition points from the ferromagnetic to the singlet state, when energies of these states are zero. The model (1) along this line is given by the Hamiltonian depending on the parameter ν ($\nu > 0$):

$$\hat{H} = - \sum_{i=1}^M \left(\mathbf{S}_{2i-1} \cdot \mathbf{S}_{2i} - \frac{1}{4} \right) - (\nu - 1) \sum_{i=1}^M \left(\mathbf{S}_{2i} \cdot \mathbf{S}_{2i+1} - \frac{1}{4} \right) + \frac{\nu - 1}{2\nu} \sum_{i=1}^N \left(\mathbf{S}_i \cdot \mathbf{S}_{i+2} - \frac{1}{4} \right), \quad (2)$$

with periodic boundary conditions.

We note that Hamiltonian (2) has a symmetry: Its spectrum coincides with the spectrum of $\tilde{H}(\nu)$ obtained by the transformation

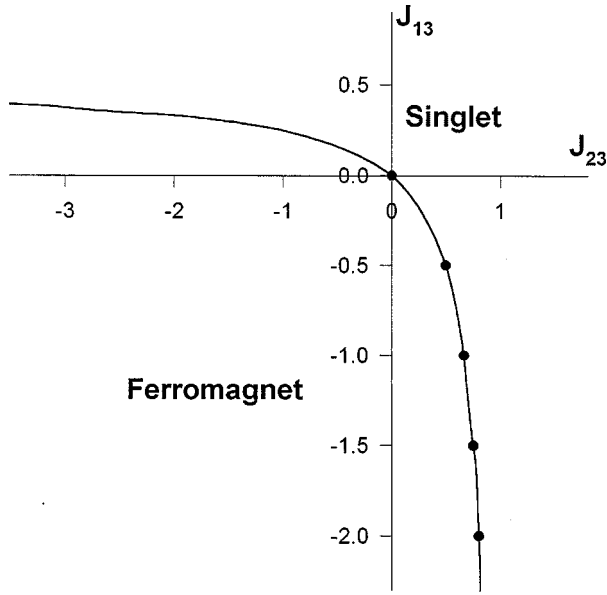


FIG. 1. $T=0$ phase diagram of model (1). The solid line is the boundary between the ferromagnetic and singlet phases. Model (1) along this line is given by Hamiltonian (2). Circles correspond to the special cases of this Hamiltonian.

$$\tilde{H}(\nu) = (\nu - 1)H\left(\frac{\nu}{\nu - 1}\right), \quad \nu > 1.$$

This transformation permutes the factors at the first and second terms in Hamiltonian (2). Thus, due to the symmetry, it is sufficient to consider the range $0 \leq \nu \leq 2$.

First, we will show that the ground-state energy of Eq. (2) is zero. Let us represent Hamiltonian (2) as a sum of Hamiltonians H_n of cells containing three sites:

$$\hat{H} = \sum_{i=1}^M (H_{2i-1} + H_{2i}), \quad (3)$$

where

$$\begin{aligned} H_{2i-1} &= -\frac{1}{2} \left(\mathbf{S}_{2i-1} \cdot \mathbf{S}_{2i} - \frac{1}{4} \right) - \frac{\nu-1}{2} \left(\mathbf{S}_{2i} \cdot \mathbf{S}_{2i+1} - \frac{1}{4} \right) \\ &\quad + \frac{\nu-1}{2\nu} \left(\mathbf{S}_{2i-1} \cdot \mathbf{S}_{2i+1} - \frac{1}{4} \right), \\ H_{2i} &= -\frac{1}{2} \left(\mathbf{S}_{2i+1} \cdot \mathbf{S}_{2i+2} - \frac{1}{4} \right) - \frac{\nu-1}{2} \left(\mathbf{S}_{2i} \cdot \mathbf{S}_{2i+1} - \frac{1}{4} \right) \\ &\quad + \frac{\nu-1}{2\nu} \left(\mathbf{S}_{2i} \cdot \mathbf{S}_{2i+2} - \frac{1}{4} \right). \end{aligned}$$

Eigenvalues of each H_n are

$$\lambda_1 = \lambda_2 = 0, \quad \lambda_3 = \frac{\nu^2 - \nu + 1}{2\nu} > 0.$$

We will present a singlet wave function which is the exact one of each H_n with zero energy and, therefore, it is the exact ground-state wave function of Eq. (2). This function has a form

$$\Psi_0(M) = P_0 \Psi_M, \quad (4)$$

where

$$\begin{aligned} \Psi_M &= (s_1^+ + \nu s_2^+ + \nu s_3^+ \cdots + \nu s_N^+) (s_3^+ + \nu s_4^+ \cdots + \nu s_N^+) \cdots \\ &\quad \times (s_{2n-1}^+ + \nu s_{2n}^+ \cdots + \nu s_N^+) \cdots (s_{N-1}^+ + \nu s_N^+) |1, 2, \dots, N\rangle, \end{aligned} \quad (5)$$

where s_i^+ is the $s = \frac{1}{2}$ raising operator.

Equation (5) contains $M = N/2$ operator multipliers, and the vacuum state $|1, 2, \dots, N\rangle$ is the state with all spins pointing down. The function Ψ_M is the eigenfunction of S_z with $S_z = 0$, but it is not the eigenfunction of \mathbf{S}^2 . P_0 is a projector onto the singlet state. This operator is¹⁷

$$P_0 = \frac{1}{8\pi^2} \int_0^{2\pi} d\alpha \int_0^{2\pi} d\beta \int_0^\pi \sin\gamma d\gamma e^{i\alpha \hat{S}_z} e^{i\gamma \hat{S}_x} e^{i\beta \hat{S}_z},$$

where $\hat{S}_{x(z)}$ are components of the total spin operator.

The function Ψ_M contains components with all possible values of spin S ($0 \leq S \leq M$), and in fact a fraction of the singlet is exponentially small at large N . This component is filtered out by the operator P_0 .

It is not difficult to check that

$$H_n \Psi_M = 0 \quad (6)$$

for $n = 1, \dots, (N-2)$, and therefore the ground-state energies for all values of spin S of an open chain described by the Hamiltonian

$$H_{\text{op}} = \sum_{n=1}^{N-2} H_n \quad (7)$$

are zero.

The operators H_{N-1} and H_N do not give zero acting on Ψ_M , but

$$H_{N-1(N)} P_0 \Psi_M = P_0 H_{N-1(N)} \Psi_M = 0. \quad (8)$$

The latter equation can be easily checked using the fact the first set of parentheses in Eq. (5) can be replaced by $(1-\nu)s_1^+$ under the projector P_0 .

Equations (6) and (8) mean that $\Psi_0(M)$ is the exact singlet ground-state wave function of Eq. (2) for any M and that the ground-state energy is zero. We note that the ground-state energy coincides with its exact lower bound because H is the sum of non-negative defined operators [Eq. (3)]. Of course, the trivial ferromagnetic state has zero energy as well.

In the particular case $\nu=2$, when $J_{12}=J_{23}=-1$ and $J_{13}=\frac{1}{4}$, another form of the exact singlet ground-state wave function has been found in Ref. 18. It reads

$$\Psi = \sum [i, j][k, l][m, n] \cdots,$$

where $[i, j]$ denotes the singlet pair and the summation is made for any combination of spin sites under the condition that $i < j, k < l, m < n, \dots$. However, it is not clear how this function can be generalized to $\nu \neq 2$.

The following general statements relevant to Hamiltonian (2) can be proved.

(1) The ground states of open chains described by Eq. (7) in the sector with fixed total spin S are nondegenerate and their energies are zero.

(2) For cyclic chains the ground state in the $S=0$ sector is nondegenerate and has momentum π . The ground-state energies for $0 < S < M$ are nonzero.

(3) The singlet ground-state wave functions for open and cyclic chains coincide with each other.

(4) The singlet ground-state wave function $\Psi_0(M)$ is superstable¹⁹ with respect to any cell operator H_n ; i.e., $\Psi_0(M)$ is the ground-state wave function of the Hamiltonian $H + \lambda H_n$ for $-1 < \lambda < \infty$.

B. Norm of the ground-state wave function

Let us return to the problem of the projection of the function Ψ_M . As one can see from Eq. (5), the function Ψ_M satisfies a recurrent equation

$$\Psi_M = [(s_1^+ + \nu s_2^+) + \nu S^+(N-2)] |1,2\rangle \Psi_{M-1}, \quad (9)$$

where Ψ_{M-1} is the function (5) for the system of $(N-2)$ spins on sites $3, 4, \dots, N$ and $S^+(N-1) = \sum_{i=l+1}^N S_i^+$.

In principle, it is possible to generate $\Psi_0(M)$ starting from $M=1$ and using Eqs. (4) and (9). However, it is more convenient to obtain the recurrent formulae for expectation values (norm and correlators) with respect to the function $\Psi_0(M)$ directly.

First, we consider a norm of $\Psi_0(M)$, which has a form

$$\begin{aligned} G_M &= \langle \Psi_0(M) \Psi_0(M) \rangle = \langle \Psi_M P_0 \Psi_M \rangle \\ &= \frac{1}{2} \int_0^\pi \Phi_M(\gamma) \sin \gamma \, d\gamma, \end{aligned} \quad (10)$$

where

$$\Phi_M(\gamma) = \Phi_M(\gamma_1, \gamma_2) |_{\gamma_1 = \gamma_2 = \gamma}$$

and

$$\Phi_M(\gamma_1, \gamma_2) = \left\langle \Psi_M \exp \left(i \frac{\gamma_1}{2} S^+(N) + i \frac{\gamma_2}{2} S^-(N) \right) \Psi_M \right\rangle. \quad (11)$$

Commuting operators in Eq. (11) and using the fact that $S_z \Psi_M = 0$, we rewrite Eq. (11) in the form

$$\Phi_M(\gamma_1, \gamma_2) = \langle \Psi_M \exp[iz S^-(N)] \exp[iz' S^+(N)] \Psi_M \rangle, \quad (12)$$

where

$$z = \sqrt{\frac{\gamma_2}{\gamma_1}} \tan \frac{\sqrt{\gamma_1 \gamma_2}}{2}, \quad z' = \sqrt{\frac{\gamma_1 \sin \sqrt{\gamma_1 \gamma_2}}{\gamma_2}}.$$

It follows from Eqs. (9) and (12) that the function $\Phi_M(\gamma_1, \gamma_2)$ satisfies the equation

$$\begin{aligned} \Phi_M(\gamma_1, \gamma_2) &= \left[1 + \nu^2 - (1 + \nu)^2 z z' + \nu(\nu + 1)(1 - z z') \right] \\ &\quad \times \left(z \frac{\partial}{\partial z} + z' \frac{\partial}{\partial z'} \right) \end{aligned}$$

$$- \nu^2 (1 - z z')^2 \frac{\partial^2}{\partial z \partial z'} \Big] \Phi_{M-1}(\gamma_1, \gamma_2).$$

Using this equation, we obtain, for $\Phi_M(\gamma)$,

$$\begin{aligned} \Phi_M(\gamma) &= \left[1 + \nu^2 - (1 + \nu)^2 \sin^2 \frac{\gamma}{2} + \nu(\nu + 1) \sin \gamma \frac{d}{d\gamma} \right. \\ &\quad \left. - \nu^2 \cos^2 \frac{\gamma}{2} \left(\frac{d^2}{d\gamma^2} + \frac{1}{\sin \gamma} \frac{d}{d\gamma} \right) \right] \Phi_{M-1}(\gamma). \end{aligned} \quad (13)$$

The solution of Eq. (13) is

$$\Phi_M(y) = L^M(y) \Phi_0(y), \quad (14)$$

where

$$\begin{aligned} L(y) &= \frac{(1 - \nu)^2}{2} + \frac{(1 + \nu)^2}{2} y - \nu(\nu + 1)(1 - y^2) \\ &\quad \times \frac{d}{dy} - \frac{\nu^2}{2} (1 + y)^2 \frac{d}{dy} (1 - y) \frac{d}{dy}, \end{aligned} \quad (15)$$

$y = \cos \gamma$, and $\Phi_0(y) = 1$.

According to Eq. (15), $\Phi_M(y)$ is a polynomial in y of order M . It turns out that further calculations will be simplified if $\Phi_M(y)$ is expanded over Legendre polynomials $P_n(y)$:

$$\Phi_M(y) = \sum_{n=0}^M c_n(M) P_n(y). \quad (16)$$

The coefficients $c_n(l)$ are defined by the recurrent equation

$$\begin{aligned} c_n(l+1) &= \frac{n}{2n-1} \frac{(\nu n + 1)^2}{2} c_{n-1}(l) \\ &\quad + \frac{\nu^2(n^2 + n) + (\nu - 1)^2}{2} c_n(l) \\ &\quad + \frac{n+1}{2n+3} \frac{(\nu n + \nu - 1)^2}{2} c_{n+1}(l), \end{aligned} \quad (17)$$

with initial condition $c_0(0) = 1$. Besides, $c_n(l) = 0$ at $n > l$. The norm G_M is given by

$$G_M = \frac{1}{2} \int_{-1}^1 \Phi_M(y) dy = c_0(M). \quad (18)$$

C. Spin correlations

The spin correlation functions can be found in the same way as G_M . It is convenient to express the scalar product $\mathbf{S}_i \cdot \mathbf{S}_j$ by the permutation operator $p_{ij} = 2\mathbf{S}_i \cdot \mathbf{S}_j + \frac{1}{2}$. Then non-normalized expectation value $Q(i, j) = \langle \Psi_0(M) (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4}) \Psi_0(M) \rangle$ is

$$\begin{aligned} Q(i, j) &= -\frac{1}{4} \langle \Psi_0(M) (p_{i,j} - 1)^2 \Psi_0(M) \rangle \\ &= -\frac{1}{4} \langle \Psi_M (p_{i,j} - 1) P_0 (p_{i,j} - 1) \Psi_M \rangle. \end{aligned} \quad (19)$$

The equations for $Q(i, j)$ can be obtained as in the derivation of Eqs. (14) and (15). They are somewhat different for even and odd i . For example, the equations for $Q(1, n)$ have the forms

$$Q(1, 2l) = -\frac{(\nu-1)^2}{4} \int_{-1}^1 \frac{1+y}{2} (L^{l-2} L_1 L^{M-1}) dy, \tag{20}$$

$$Q(1, 2l-1) = -\frac{\nu^2(\nu-1)^2}{4} \int_{-1}^1 \frac{1+y}{2} (L^{l-2} L_2 L^{M-1}) dy, \tag{21}$$

where

$$L_1 = 1 - 2\nu(1-y) \frac{d}{dy} - \nu^2(1+y) \frac{d}{dy} (1-y) \frac{d}{dy},$$

$$L_2 = 1 - 2(1-y) \frac{d}{dy} - (1+y) \frac{d}{dy} (1-y) \frac{d}{dy}.$$

It is clear, that

$$Q(2, n+2) = Q(1, N-n+1).$$

Making use consequent integration of Eqs. (20) and (21), we obtain

$$\begin{aligned} & \int_{-1}^1 \frac{1+y}{2} (L^{l-2} L_{1(2)} L^{M-1}) dy \\ &= \int_{-1}^1 \frac{1+y}{2} (\tilde{L}^{l-2} 1) (L_{1(2)} L^{M-1}) dy \\ &= \int_{-1}^1 (\tilde{L}_{1(2)} \tilde{L}^{l-2} 1) (L^{M-1}) dy, \end{aligned}$$

where

$$\begin{aligned} \tilde{L} &= \tilde{L}_1 = \frac{1}{2} + \frac{(2\nu-1)^2}{2} y - \nu(2\nu-1)(1-y^2) \frac{d}{dy} \\ &\quad - \frac{\nu^2}{2} (1+y)^2 \frac{d}{dy} (1-y) \frac{d}{dy}, \\ \tilde{L}_2 &= \frac{1+y}{2} - (1-y^2) \frac{d}{dy} - \frac{(1+y)^2}{2} \frac{d}{dy} (1-y) \frac{d}{dy}. \end{aligned}$$

So Eqs. (20) and (21) can be rewritten as

$$Q(1, 2l) = -\frac{(\nu-1)^2}{4} \int_{-1}^1 \tilde{\Phi}_{l-1}(y) \Phi_{M-l}(y) dy, \tag{22}$$

$$Q(1, 2l-1) = -\frac{\nu^2(\nu-1)^2}{4} \int_{-1}^1 (\tilde{L}_2 \tilde{\Phi}_{l-2}(y)) \Phi_{M-l}(y) dy, \tag{23}$$

where

$$\tilde{\Phi}_l(y) = \tilde{L}^l(y) 1. \tag{24}$$

The function $\tilde{\Phi}_l(y)$ can be expanded over Legendre polynomials similarly to $\Phi_l(y)$,

$$\tilde{\Phi}_l(y) = \sum_{n=0}^l a_n(l) P_n(y), \tag{25}$$

and the coefficients $a_n(l)$ satisfy the equations

$$\begin{aligned} a_n(l+1) &= \frac{n}{2n-1} \frac{(\nu n + \nu - 1)^2}{2} a_{n-1}(l) \\ &\quad + \frac{\nu^2(n^2+n)+1}{2} a_n(l) \\ &\quad + \frac{n+1}{2n+3} \frac{(\nu n + 1)^2}{2} a_{n+1}(l). \end{aligned} \tag{26}$$

with initial conditions $a_0(0) = 1$ and $a_n(l) = 0$ at $n > l$.

Using Eqs. (18), (22), and (23), we can express the correlation function $K(1, n) = \langle \mathbf{S}_1 \cdot \mathbf{S}_n \rangle / G_M$ in the forms

$$K(1, 2l) = \frac{1}{4} - \frac{(\nu-1)^2}{2c_0(M)} \sum_{n=0}^{l-1} \frac{a_n(l-1) c_n(M-l)}{2n+1}, \tag{27}$$

$$K(1, 2l-1) = \frac{1}{4} - \frac{\nu^2(\nu-1)^2}{2c_0(M)} \sum_{n=0}^{l-1} \frac{b_n(l-1) c_n(M-l)}{2n+1}, \tag{28}$$

where coefficients $b_n(l-1)$ are defined by $a_n(l-2)$ as follows:

$$\begin{aligned} b_n(l-1) &= \frac{1}{2} \frac{n^3}{2n-1} a_{n-1}(l-2) + \frac{n^2+n+1}{2} a_n(l-2) \\ &\quad + \frac{1}{2} \frac{(n+1)^3}{2n+3} a_{n+1}(l-2). \end{aligned} \tag{29}$$

Therefore, the calculation of the spin correlation function reduces to the solution of the recurrent equations (17) and (26), which were used for numerical calculations of the spin correlation function for finite systems.

At large M the solutions of the recurrent equations (17) and (26) have scaling forms

$$c_n(M) = 2M(M!)^2 \nu^{2M} s \exp\left(M f_0(s) + \frac{2-\nu}{\nu} \ln M + f_1(s)\right), \tag{30}$$

$$\begin{aligned} a_n(M) &= 2M(M!)^2 \nu^{2M} s \\ &\quad \times \exp\left(M f_0(s) - \frac{2-\nu}{\nu} \ln M + g_1(s)\right), \end{aligned} \tag{31}$$

where the parameter

$$s = \frac{2n+1}{2M}$$

can be considered as a continuous variable.

We note that Eqs. (30) and (31) are not valid for special values of ν , $\nu = 1/(m+1)$ ($m = 0, 1, 2, \dots$). For these ν the last term in Eq. (17) vanishes when $n = m$ and Eq. (17) reduces to $(m+1)$ equations for $c_n(l)$ with $n \leq m$.

The recurrent equations (17) and (26) at $M \gg 1$ and $\nu \neq 1/(m+1)$ reduce to differential ones for $f_0(s)$, $f_1(s)$ and $g_1(s)$. For example, $f_0(s)$ satisfies the equation

$$\exp\left(f_0(s) - s \frac{df_0(s)}{ds}\right) = s^2 \cosh^2\left(\frac{1}{2} \frac{df_0(s)}{ds}\right),$$

with the initial condition $f_0(1) = -\ln 4$.

Its implicit solution is

$$f_0(s) = -2 \ln \xi + 2 \frac{\sin \xi}{\xi} \ln \tan \frac{\xi}{2}, \quad (32)$$

where

$$s = \frac{\sin \xi}{\xi}.$$

As follows from Eq. (32), $a_n(M)$ and $c_n(M)$ as functions of n have a sharp maximum at $n/M = 2/\pi$.

The functions $f_1(s)$ and $g_1(s)$ are given by

$$f_1(s) = -\frac{2+\nu}{\nu} \ln \xi + \frac{4-\nu}{2\nu} \ln \sin \xi - \frac{1}{2} \ln \left(\frac{\sin \xi}{\xi^2} - \frac{\cos \xi}{\xi} \right) + C \frac{\nu-1}{\nu^2}, \quad (33)$$

$$g_1(s) = \frac{2-3\nu}{\nu} \ln \xi + \frac{3\nu-4}{2\nu} \ln \sin \xi - \frac{1}{2} \ln \left(\frac{\sin \xi}{\xi^2} - \frac{\cos \xi}{\xi} \right) + C \frac{\nu-1}{\nu^2}, \quad (34)$$

where the constant $C \approx 0.969$.

To obtain $K(1,2l)$ at $N \rightarrow \infty$ we substitute Eqs. (30)–(34) into Eq. (27) and replace the sum over n by the integral over s . This integral is calculated by the method of steepest descent. The saddle point is $s_0 = (1/\pi) \sin(2\pi/N)$, and the integrand does not depend on parameter ν . The final result for the spin correlation function $K(1,2l)$ at $N \rightarrow \infty$ is also independent of ν :

$$K(1,2l) = \frac{1}{4} \cos \frac{2\pi(2l-1)}{N} + O\left(\frac{1}{N}\right). \quad (35)$$

For the particular case $\nu=2$, Eq. (35) has been obtained earlier in Ref. 18.

The corresponding calculations for $K(1,2l-1)$ to within terms $\sim 1/N$ lead to the same expression (35). But taking into account terms $\sim 1/N$, we find that the difference $K(1,2l-1) - K(1,2l)$ is

$$K(1,2l-1) - K(1,2l) = \frac{\pi}{N} \frac{\nu-1}{\nu} \sin \frac{4\pi l}{N} + O\left(\frac{1}{N^2}\right).$$

The latter equation means that the double-spiral structure exists. The pitch angle of each spiral is $4\pi/N$ and there is a small shift angle $\Delta\varphi = (2\pi/N)(2-\nu)/\nu$ between them:

$$K(1,2l) = \frac{1}{4} \cos \left(\frac{2\pi(2l-1)}{N} - \Delta\varphi \right), \quad (36)$$

$$K(1,2l+1) = \frac{1}{4} \cos \frac{4\pi l}{N}. \quad (37)$$

This shift angle reflects the fact that the unit cell contains two sites unless $\nu=2$. Equations (36) and (37) show that long-range spiral order exists in the singlet ground state of Hamiltonian (2) in the thermodynamic limit and that a double-spiral state is formed.

It is interesting to note that correlators (36) and (37) coincide with those obtained by using the simple ‘‘quasiclassical’’ trial wave function in the form

$$\psi_{cl} = \exp\left(\sum_{n=1}^N \zeta_n s_n^+\right) |1,2,\dots,N\rangle,$$

where

$$\zeta_n = \exp\left(\frac{2\pi n}{N} + \frac{(-1)^n \pi}{N} \frac{\nu-2}{\nu}\right).$$

Thus the quantum ground state of the large- N limit resembles the classical one, though for small-size systems quantum fluctuations are essential.

The formation of spirals having a period which is equal to the system size reflects the tendency to the creation of the incommensurate spiral state at the antiferromagnetic region when $\delta > 0$. The behavior of the system in the vicinity of the transition point has been studied by us⁷ for model (1) with $J_{12} = J_{23} = -1$, $J_{13} = \frac{1}{4} + \delta$. For $\delta \ll 1$ the period of the spiral is finite and is proportional to $\delta^{-1/2}$. The transition from the ferromagnetic to the singlet state is a phase transition of the second order with respect to δ .

D. Special cases of the model

There are the special points $\nu = 1/m$ ($m = 1, 2, \dots$) at which Eqs. (36) and (37) are not valid. At $\nu = \frac{1}{2}$ the function (4) reduces to the product of singlets

$$\Psi_0(M) = [2,3][4,5] \cdots [N,1] \quad (38)$$

and $K(2,3) = K(4,5) = \cdots = K(N,1) = -\frac{3}{4}$. Other spin correlators are zero.

Analysis of Eqs. (17), (26), and (27) shows that the ground-state correlations of model (2) with $\nu = 1/m$ ($m \geq 3$) have antiferromagnetic character with an exponentially decay:

$$K(1,n+1) \sim (-1)^n \exp\left(-\frac{n}{r_c}\right),$$

where the correlation length is

$$r_c = -2 \ln^{-1} \left(1 - \frac{2}{m(m-1)} \right). \quad (39)$$

The crossover between the spiral state at $1/m < \nu < 1/(m-1)$ and the antiferromagnetic state at $\nu = 1/m$ occurs in the exponentially small (at $N \gg 1$) vicinity of these special points.

At $m \gg 1$,

$$r_c = m^2 \quad (40)$$

and the correlation length diverges when ν trends to zero along the special points and there is the Néel ordering in this limit.

At $\nu=1$, when $J_{12}=-1$, $J_{23}=J_{13}=0$, the system is divided into ferromagnetic pairs 1-2, 3-4,

Using second-order perturbation theory with respect to $(\nu-1)$, we reduce model (2) at $\nu \rightarrow 1$ to the effective spin-1 Hamiltonian

$$H_{\text{eff}} = \frac{(\nu-1)^2}{8} \sum_{n=1}^M \left\{ -(\mathbf{L}_n \cdot \mathbf{L}_{n+1} - 1) + \mathbf{L}_n \cdot \mathbf{L}_{n+2} - \frac{1}{2} (\mathbf{L}_n \cdot \mathbf{L}_{n+1}) \cdot (\mathbf{L}_{n+1} \cdot \mathbf{L}_{n+2}) - \frac{1}{2} (\mathbf{L}_{n+1} \cdot \mathbf{L}_{n+2}) \cdot (\mathbf{L}_n \cdot \mathbf{L}_{n+1}) \right\}, \quad (41)$$

with M spins $L=1$.

The exact singlet ground-state wave function of Hamiltonian (41) can be obtained from the Eqs. (4) and (5). It has the form

$$\Psi_0(M) = P_0 L_1^+ (L_2^+ + L_3^+ + \dots + L_M^+) \dots (L_{M-1}^+ + L_M^+) L_M^+ | -1, \dots, -1 \rangle, \quad (42)$$

where L_i^+ are raising operators of spin 1.

The ground-state correlation function of Eq. (41), $K(1, n+1) = \langle \mathbf{L}_1 \cdot \mathbf{L}_{n+1} \rangle / G_M$, is found from Eqs. (36) and (37). It is

$$K(1, n+1) = \cos \frac{2\pi n}{M}.$$

Finally, we note that it is possible to calculate higher terms of the perturbation theory and to obtain effective spin-1 Hamiltonians which are proportional to the third, fourth, and higher power of the small parameter $(\nu-1)$. All of them have zero ground-state energy as well as Eq. (41).

III. FRUSTRATED SPIN CHAIN

WITH AN ANTIFERROMAGNETIC GROUND STATE

A. Model and its exact ground state

In the preceding section the spin model at the ferromagnet-antiferromagnet transition point has been studied. The exact singlet ground-state wave function at this point is given by Eq. (4). In this section function (4) will be generalized to give the exact ground-state wave function of a special one-dimensional frustrated spin- $\frac{1}{2}$ model. This model has a unique singlet ground state (for the cyclic chain) with an exponential decay of correlations, and there is a gap to the excitations.

Let us consider the wave function which depends on two parameters and has form (4):

$$\Psi_0(M) = P_0 \Psi_M, \quad (43)$$

where

$$\Psi_M = (s_1^+ + \nu_1 s_2^+ + \nu_2 s_3^+ + \dots + \nu_2 s_N^+) (s_3^+ + \nu_1 s_4^+ + \nu_2 s_5^+ + \dots + \nu_2 s_N^+) \dots (s_{N-1}^+ + \nu_1 s_N^+) | 1, 2, \dots, N \rangle. \quad (44)$$

We will construct the Hamiltonian for which $\Psi_0(M)$ is the exact ground-state wave function as the sum of the local four-sites Hamiltonians

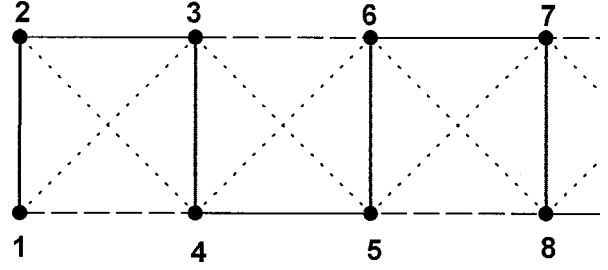


FIG. 2. Spin ladder representation of model (45). Different lines correspond to different exchange interactions.

$$H = H_{1,2,3,4} + H_{3,4,5,6} + \dots + H_{N-3,N-2,N-1,N} + H_{N-1,N,1,2}. \quad (45)$$

The Hamiltonians $H_{i,i+1,i+2,i+3}$ are chosen in the form

$$H_{i,i+1,i+2,i+3} = J_{12} \left[\left(\mathbf{S}_i \cdot \mathbf{S}_{i+1} - \frac{1}{4} \right) + \left(\mathbf{S}_{i+2} \cdot \mathbf{S}_{i+3} - \frac{1}{4} \right) \right] + 2J_{13} \left[\left(\mathbf{S}_i \cdot \mathbf{S}_{i+2} - \frac{1}{4} \right) + \left(\mathbf{S}_{i+1} \cdot \mathbf{S}_{i+3} - \frac{1}{4} \right) \right] + 2J_{23} \left(\mathbf{S}_{i+1} \cdot \mathbf{S}_{i+2} - \frac{1}{4} \right) + 2J_{14} \left(\mathbf{S}_i \cdot \mathbf{S}_{i+3} - \frac{1}{4} \right). \quad (46)$$

Thus, the model has nearest- (J_{12} and J_{23}), next-nearest- (J_{13}), and next-next-nearest- (J_{14}) neighbor interactions. In fact, this model is equivalent to the spin- $\frac{1}{2}$ ladder with different interactions, as is shown in Fig. 2.

We demand that $\Psi_0(M)$ be the eigenfunction of each local Hamiltonian with the eigenvalue $\varepsilon < 0$, i.e.,

$$H_{i,i+1,i+2,i+3} \Psi_0(M) = \varepsilon \Psi_0(M). \quad (47)$$

The exchange integrals J_{ij} and the energy ε are defined by the Schrödinger equation

$$H_{1,2,3,4} \Psi_M = \varepsilon \Psi_M. \quad (48)$$

Let us represent the function Ψ_M in the form

$$\Psi_M = [\hat{q}_1 + \nu_2 \hat{q}_2 S^+(N-4) + \nu_2^2 S^{+2}(N-4)] | 1, 2, 3, 4 \rangle \Psi_{N-2}, \quad (49)$$

where

$$\hat{q}_1 = s_1^+ s_3^+ + \nu_1 (s_1^+ s_4^+ + s_2^+ s_3^+) + \nu_1^2 s_2^+ s_4^+ + \nu_2 (1 + \nu_1) s_3^+ s_4^+, \\ \hat{q}_2 = s_1^+ + \nu_1 s_2^+ + (1 + \nu_2) s_3^+ + (\nu_1 + \nu_2) s_4^+.$$

The equation

$$H_{1,2,3,4} \hat{q}_1 | 1, 2, 3, 4 \rangle = \varepsilon \hat{q}_1 | 1, 2, 3, 4 \rangle \quad (50)$$

reduces to five equations for four exchange integrals and the energy ε . The necessary condition of the existence of a solution with $\varepsilon < 0$ is

$$1 + \nu_1 + \nu_2 = 0. \quad (51)$$

So under this condition there is only one parameter of Hamiltonian (45). It is convenient to take the value $\mu = (2 + \nu_1) / (2\nu_1 + 1)$ as a system parameter. Then, the solu-

tion of Eq. (50) at $\nu_1=(2-\mu)/(2\mu-1)$ and $\nu_2=(\mu+1)/(1-2\mu)$ yields the following expressions for J_{ij} and ε :

$$J_{12}=\frac{(1-2\mu)(2-\mu)}{9}, \quad J_{23}=-\frac{1}{3}\frac{\mu(2-\mu)^2(\mu-1)}{(\mu+1)^2},$$

$$J_{13}=\frac{(2\mu-1)(2-\mu)(\mu-1)^2}{6(\mu+1)^2}, \quad J_{14}=\frac{(2\mu-1)^2(\mu-1)}{3(\mu+1)^2}, \quad (52)$$

$$\varepsilon=-\frac{3\mu(\mu-1)^2}{(\mu+1)^2}.$$

It turns out that the equation

$$H_{1,2,3,4}\hat{q}_2|1,2,3,4\rangle=\varepsilon\hat{q}_2|1,2,3,4\rangle$$

with J_{ij} and ε given by Eq. (52), is satisfied automatically.

As will be proven in the Appendix, the function Ψ_M with $\nu_1=-\nu_2-1$ contains singlet and triplet components only, i.e.,

$$S^{+2}(N)\Psi_M=0. \quad (53)$$

Therefore, the last term in Eq. (49) vanishes and Ψ_M is the eigenfunction of $H_{1,2,3,4}$ with the eigenvalue ε .

Generally, the Hamiltonian $H_{1,2,3,4}$ has following eigenstates: one quintet, three triplets, and two singlets. Two of them (one singlet and one triplet) have energy ε , while other four states have higher energies at $\mu>0$ ($\mu\neq 1$). At $\mu<0$ the ground state of $H_{1,2,3,4}$ is a quintet with zero energy. In the Appendix we will show that the wave function Ψ_M is an eigenfunction with eigenvalue ε of each local Hamiltonian $H_{i,i+1,i+2,i+3}$ excluding that for $i=N-1$. Therefore, the ground-state energy of the open chain at $\mu>0$ is $(N/2-1)\varepsilon$ and it coincides with the exact lower bound of the energy, similarly to the model of Sec. II. However, in the contrast with the latter, the present model is fourfold degenerate for the open chain.

As for the Hamiltonian $H_{N-1,N,1,2}$, the function Ψ_M is not its eigenfunction, but

$$H_{N-1,N,1,2}\Psi_0(M)=\varepsilon\Psi_0(M)$$

(see Appendix) and

$$H\Psi_0(M)=\frac{N}{2}\varepsilon\Psi_0(M).$$

As follows from Eq. (52), the spectrum of $H(\mu)$ coincides with the spectrum of $\tilde{H}(\mu)$ which is connected with $H(\mu)$ by the transformation

$$\tilde{H}(\mu)=\mu^2H\left(\frac{1}{\mu}\right).$$

This transformation permutes the factors at the third and last terms in Eq. (46). Therefore, it is sufficient to consider the Hamiltonian $H(\mu)$ in the region $-1\leq\mu\leq 1$.

The ground state of H is ferromagnetic at $\mu<0$. When $0<\mu<1$ the ground state of the cyclic chain is the nondegenerate singlet. The point $\mu=0$ is the ferromagnet-antiferromagnet transition point. At this point the present

model coincides with model (2) at the special point $\nu=\frac{1}{3}$. As follows from Eq. (52), this transition is the phase transition of first order with respect to μ .

At $\mu=\frac{1}{2}$ the only nonzero exchange integral is J_{23} and the ground state consists of non interacting singlet pairs $2-3, 4-5, \dots, 1-N$. When $\mu\rightarrow 1$ the first term in Eq. (46) dominates and the system is divided into weakly interacting ferromagnetic pairs $1-2, 3-4, \dots$. Using second-order perturbation theory with respect to the small parameter $(\mu-1)$, we reduce the Hamiltonian H [Eq. (45)] to the effective spin-1 model given by

$$H=\frac{(\mu-1)^2}{16}H_{\text{eff}},$$

where

$$H_{\text{eff}}=\sum_{n=1}^M\left\{5\mathbf{L}_n\cdot\mathbf{L}_{n+1}+\mathbf{L}_n\cdot\mathbf{L}_{n+2}+\frac{1}{2}(\mathbf{L}_n\cdot\mathbf{L}_{n+1}-\mathbf{L}_{n+1}\cdot\mathbf{L}_{n+2})^2-6\right\} \quad (54)$$

and \mathbf{L}_n is spin-1 operator.

The ground-state wave function of Eq. (54) can be obtained from Eq. (43) at $\mu=1$. It reads

$$\Psi_0(M)=P_0(\mathbf{L}_1^+-2\mathbf{L}_2^+-\dots-2\mathbf{L}_M^+)(\mathbf{L}_2^+-2\mathbf{L}_3^+-\dots-2\mathbf{L}_M^+)\dots\times(\mathbf{L}_{M-1}^+-2\mathbf{L}_M^+)\mathbf{L}_M^+|-1,-1,\dots,-1\rangle. \quad (55)$$

It is remarkable that the function (55) coincides with the ground-state wave function of the AKLT model. Therefore, the ground-state physics of the model given by Eq. (54) and the AKLT one are the same, though the Hamiltonians of these two models are different.

B. Spin correlations in the ground state

First, we calculate the norm of the ground-state wave function. It is convenient to express the function Ψ_M in terms of the parameter μ and to introduce a new function $\tilde{\Psi}_M$:

$$\Psi_M=(2\mu-1)^{-M}\tilde{\Psi}_M,$$

where

$$\tilde{\Psi}_M=[(2\mu-1)s_1^++(2-\mu)s_2^+-(\mu+1)S^+(N-2)]\times[(2\mu-1)s_3^++(2-\mu)s_4^+-(\mu+1)S^+(N-4)]\dots\times[(2\mu-1)s_{N-1}^++(2-\mu)s_N^+]|1,2,\dots,N\rangle.$$

According to Eq. (18), the norm of $\tilde{\Psi}_0(M)=P_0\tilde{\Psi}_M$ is

$$G_M=\langle\tilde{\Psi}_0(M)\tilde{\Psi}_0(M)\rangle=\frac{1}{2}\int_{-1}^1\Phi_M(y)dy.$$

For the present model the function $\Phi_l(y)$ is defined by the equation

$$\Phi_l(y)=L^l(y)1, \quad (56)$$

where

$$L(y) = \frac{9(1-\mu)^2}{2} + \frac{(1+\mu)^2}{2} \left[y + 2(1-y^2) \frac{d}{dy} - (1+y)^2 \frac{d}{dy} (1-y) \frac{d}{dy} \right].$$

The solution of Eq. (56) is

$$\Phi_l(y) = \frac{\omega_1^l + 3\omega_2^l}{4} + \frac{\omega_1^l - \omega_2^l}{4} y,$$

where

$$\omega_1 = 6(\mu^2 - \mu + 1), \quad \omega_2 = 2(\mu - 2)(2\mu - 1).$$

This form of $\Phi_l(y)$ reflects the fact that the function $\tilde{\Psi}_M$ contains the singlet and triplet components only.

Thus G_M is

$$G_M = \frac{\omega_1^M + 3\omega_2^M}{4}. \quad (57)$$

As $|\omega_2/\omega_1| < 1$, then $G_M = \frac{1}{4}\omega_1^M$ at $M \rightarrow \infty$.

The spin correlation functions can be found in a similar way as in the Sec. II. In analogy with Eqs. (19) and (20), we obtain

$$Q(N-2l-1, N) = -\frac{1}{8} \int_{-1}^1 [L^{M-l-1} \Phi'_{l+1}(y)] dy, \quad (58)$$

where

$$\Phi'_{l+1}(y) = \langle \tilde{\Psi}_{l+1}(p_{N-2l-1, N-1}) P_0(p_{N-2l-1, N-1}) \tilde{\Psi}_{l+1} \rangle.$$

Carrying out the necessary calculations, we find

$$\begin{aligned} \Phi'_{l+1}(y) &= 4(\mu+1)^2(2-\mu)^2\omega_1^{l-1} + \omega_2^{l+1} + (2\mu-1)^2 \\ &\quad \times [(2\mu^2-2\mu+5)\omega_1^{l-1} + (2\mu^2+10\mu-1)\omega_2^{l-1}] \\ &\quad \times (1+y). \end{aligned}$$

Substituting $\Phi'_{l+1}(y)$ into Eq. (58), we obtain, for the spin correlation function $K(1, 2l+2) = K(N-2l-1, N)$,

$$K(1, 2) = \frac{1}{4} \frac{(\mu-1)^2}{2\omega_1} \frac{1+3(\omega_2/\omega_1)^{M-1}}{1+3(\omega_2/\omega_1)^M}, \quad (59)$$

$$\begin{aligned} K(1, 2l+2) &= -\frac{(\mu+1)^2}{27\omega_1\omega_2} \\ &\quad \times \frac{(2\mu-1)^2(\omega_2/\omega_1)^l + (\mu-2)^2(\omega_2/\omega_1)^{M-l}}{1+3(\omega_2/\omega_1)^M}, \end{aligned} \quad (60)$$

where $l = 1, 2, \dots, M-1$.

Similar calculations for $K(1, 2l+1)$ result in

$$K(1, 2l+1) = \frac{(\mu+1)^2}{6\omega_1} \frac{(\omega_2/\omega_1)^l + (\omega_2/\omega_1)^{M-l}}{1+3(\omega_2/\omega_1)^M}. \quad (61)$$

The correlators $K(2, n)$ have been obtained by using the symmetry of the system (see Fig. 2). For example,

$$K(2, 3) = K(1, N), \quad \text{etc.}$$

In the thermodynamic limit $M \rightarrow \infty$ and $l \ll M$, Eqs. (59)–(61) reduce to

$$K(1, 2) = -\frac{3}{4} \frac{\omega_2}{\omega_1}, \quad (62)$$

$$K(1, 2l+2) = -\frac{(\mu+1)^2(2\mu-1)^2}{27\omega_1\omega_2} \left(\frac{\omega_2}{\omega_1} \right)^l, \quad (63)$$

$$K(1, 2l+1) = \frac{(\mu+1)^2}{6\omega_1} \left(\frac{\omega_2}{\omega_1} \right)^l. \quad (64)$$

The correlators have the exponential decay, and the correlation length r_c is

$$r_c(\mu) = 2 \ln^{-1} \left| \frac{\omega_1(\mu)}{\omega_2(\mu)} \right|. \quad (65)$$

It follows from Eq. (65) that the ground state has ultrashort-range correlations. For example, $r_c(0) = 2 \ln^{-1}(\frac{3}{2})$ [this value coincides with r_c given by Eq. (39) with $m=3$] and $r_c(1) = 2 \ln^{-1} 3$. In the latter case, r_c coincides with correlation length of the AKLT model. At $\mu = \frac{1}{2}$ the only non-zero correlators are $K(2, 3) = K(4, 5) = \dots = K(N, 1) = -\frac{3}{4}$ in accordance with the dimer character of the ground state.

The value $\omega_2(\mu)$ changes the sign at $\mu = \frac{1}{2}$ and as follows from Eqs. (62), (63), and (64), the correlators show an antiferromagnetic structure of the ground state at $0 \leq \mu \leq \frac{1}{2}$, while at $\frac{1}{2} \leq \mu \leq 1$ there are ferromagnetic correlations inside the pairs (1, 2), (3, 4), ... and the antiferromagnetic correlations between the pairs.

C. Energy gap

The Hamiltonian H of the cyclic chain has a singlet-triplet gap Δ for finite N . It is evident that for $\mu = \frac{1}{2}$ the gap exists for $N \rightarrow \infty$ and $\Delta(\frac{1}{2}) = \frac{1}{6}$. The existence of a finite gap at the thermodynamic limit in the range $0 < \mu < 1$ follows from the continuity of the function $\Delta(\mu)$. It is also clear that $\Delta(\mu)$ at $N \rightarrow \infty$ vanishes at the boundary points $\mu = 0$ and $\mu = 1$ when the ground state is degenerate and there are low-lying spin wave excitations.

Unfortunately, the method of the exact calculation of $\Delta(\mu)$ in the thermodynamic limit is unknown. For $\mu \approx \frac{1}{2}$ the gap can be found by using perturbation theory in $(\mu - \frac{1}{2})$. In this case $\Delta(\mu)$ is

$$\Delta(\mu) = \frac{1}{6} + O((\mu - \frac{1}{2})^2), \quad \mu \leq \frac{1}{2}, \quad (66)$$

$$\Delta(\mu) = \frac{1}{6} - \frac{8}{9}(\mu - \frac{1}{2}) + O((\mu - \frac{1}{2})^2), \quad \mu \geq \frac{1}{2}.$$

Equations (66) show that $\Delta(\mu)$ has a cusp at $\mu = \frac{1}{2}$. For the approximate calculation $\Delta(\mu)$, we use the trial function of the triplet state in the form

$$\Psi_t = \sum_{n=1}^N c_n s_n^+ \Psi_0(M), \quad (67)$$

where

$$c_{2l-1} = a e^{ikl}, \quad c_{2l} = b e^{ikl}, \quad k = \frac{4\pi}{N} t, \quad t = 1, \dots, M.$$

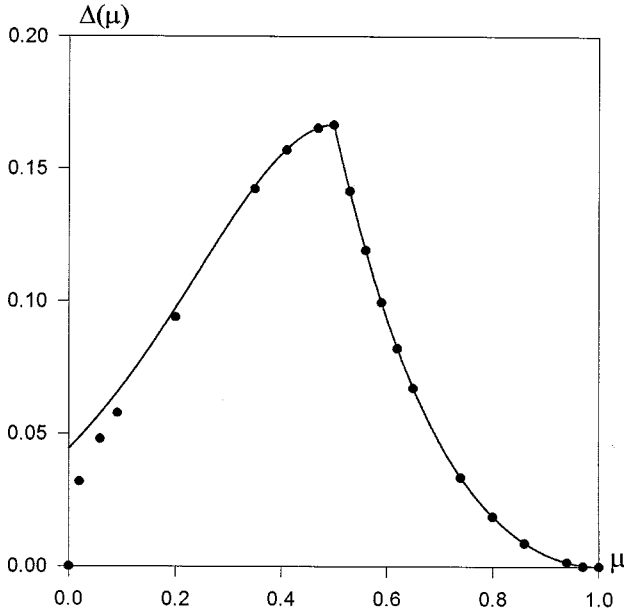


FIG. 3. Singlet-triplet gap of model (45) as a function of the parameter μ . The circles denote the results of the extrapolation of exact finite-chain calculations. The solid line represents the dependence $\Delta(\mu)$ given by Eq. (69).

This trial function gives $\Delta(\mu)$, which is

$$\Delta(\mu) = \frac{2\sum_{n \neq m} c_n^* c_m K(n, m) J_{n, m} - 2\sum_{n \neq m} |c_n|^2 K(n, m) J_{n, m}}{\frac{3}{4}\sum_n |c_n|^2 + \sum_{n \neq m} c_n^* c_m K(n, m)}. \quad (68)$$

Function (68) has minima at $k = 4\pi/N$ and $k = \pi$ for $0 < \mu < \frac{1}{2}$ and $\frac{1}{2} < \mu < 1$, respectively. Then $\Delta(\mu)$ at $N \rightarrow \infty$ is

$$\Delta(\mu) = \frac{8}{243} \frac{(\mu+1)^4 (\mu-1)^2}{\omega_1 (\omega_1 + \omega_2)}, \quad 0 < \mu < \frac{1}{2}, \quad (69)$$

$$\Delta(\mu) = \frac{2}{3} \left(1 + \frac{\omega_2}{\omega_1}\right) (\mu-1)^2, \quad \frac{1}{2} < \mu < 1.$$

The dependence of $\Delta(\mu)$ given by Eqs. (69) is shown in Fig. 3 together with the results of extrapolations of exact finite-chain calculations. Both dependences agree very well for $\mu \geq \frac{1}{2}$. In particular, Eqs. (69) correctly reproduce Eqs. (66) at $\mu \approx \frac{1}{2}$. However, $\Delta(\mu)$ given by Eqs. (69) is not zero at $\mu = 0$, while numerical calculations fit the dependence $\Delta(\mu) \sim \sqrt{\mu}$ at $\mu \rightarrow 0$.

We note that the trial function of the type (67) gives a value 0.7407 for the singlet-triplet gap in the AKLT model. This estimate is close to the value 0.7143 obtained by another approach in Ref. 20.

The above consideration refers to a gap in the cyclic chain. The open chain has a fourfold-degenerate ground state. Finite-chain calculations show that the spin of the lowest excitation is $S=2$. However, there are also two excited singlet and triplet states, the energies of which are close to that of $S=2$. The difference of these three eigenvalues decreases to zero exponentially at $N \rightarrow \infty$. We expect that these states are degenerate in the thermodynamic limit (at $\mu = \frac{1}{2}$ they are degenerate for finite N). The gap in the open chain

equals to the difference between the energies of the degenerate ground state and the lowest excited one. The extrapolation of the results of finite-chain calculations to $N \rightarrow \infty$ gives a finite gap in the open chains at $0 < \mu < 1$. Its value is very close to that for cyclic chains.

IV. SUMMARY

We have studied a class of the one-dimensional quantum spin- $\frac{1}{2}$ models with competing interactions. The exact ground-state wave function of these models is found in a special recurrent form. The Hamiltonians of these models are the sums of Hamiltonians that are local and noncommuting with each other. The ground-state wave function of the total Hamiltonian is the ground-state one for each of them. This means that this ground-state wave function is superstable¹⁹ with respect to each local Hamiltonian.

One of the studied models describes the transition point from the ferromagnetic to the spiral state when the energies of these two states are equal to each other. It is interesting to compare the exact quantum singlet state with the classical one. Both states are the states of a helical type (excluding some special cases), and their spin correlation functions are identical in the thermodynamic limit, though quantum effects are essential for finite chains. This fact is rather surprising for the one-dimensional model with spin $\frac{1}{2}$.

Another exactly solvable Hamiltonian has the antiferromagnetic ground state. This state is nondegenerate for closed chains and is fourfold degenerate for open ones. The Hamiltonian depends on the parameter μ , and there are two special values $\mu=0$ and $\mu=1$ where the singlet and ferromagnetic states are degenerate. The value $\mu=0$ is the ferromagnet-antiferromagnet transition point where a phase transition of first order with respect to μ occurs.

The ground state is characterized by the exponential decay of correlators with a very short correlation length, and there is a gap in the excitation spectrum at $0 < \mu < 1$. Thus this model has some properties suggested by Haldane¹⁶ for the one-dimensional Heisenberg antiferromagnet with integer spin. The first model for which these properties have been proved rigorously is the AKLT model. Our model is the one with spin $\frac{1}{2}$. Affleck and Lieb²¹ have shown for translationally invariant and the isotropic Heisenberg Hamiltonians that for a half-integer spin chain either the excitation spectrum is gapless or the ground state is degenerate. The existence of a finite gap in our model does not contradict the Affleck-Lieb theorem because this model is not translationally invariant. It has two sites in the unit cell and is equivalent to the special ladder model. Moreover, in the limit $\mu \rightarrow 1$ its ground-state wave function reduces to that for the AKLT model.

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APPENDIX

We prove that square of the total raising operator annihilates Ψ_M if condition (51) is satisfied. The recurrent equation for $S^{+2}(N)\Psi_M$ is

$$\begin{aligned} S^{+2}(N)\Psi_M &= 2(1 + \nu_1 + \nu_2)s_1^+s_2^+|1,2\rangle S^+(N-2)\Psi_{M-1} \\ &+ [(1 + 2\nu_2)s_1^+ + (\nu_1 + 2\nu_2)s_2^+ \\ &+ \nu_2 S^+(N-2)]|1,2\rangle S^{+2}(N-2)\Psi_{M-1}. \end{aligned} \quad (\text{A1})$$

The first term in Eq. (A1) vanishes under condition (51) and, therefore,

$$\begin{aligned} S^{+2}(N)\Psi_M &= [(1 + 2\nu_2)s_1^+ + (\nu_1 + 2\nu_2)s_2^+ + \nu_2 S^+(N-2)] \\ &\times [(1 + 2\nu_2)s_3^+ + (\nu_1 + 2\nu_2)s_4^+ \\ &+ \nu_2 S^+(N-4)] \cdots (s_{N-1}^+ + s_N^+)^2 \\ &\times [s_{N-1}^+ + \nu_1 s_N^+]|1,2,\dots,N\rangle = 0. \end{aligned}$$

This equation means that the wave function Ψ_M contains singlet and triplet components only.

Now we prove that $\tilde{\Psi}_0(M)$ is the eigenfunction of each local Hamiltonian in Eq. (45). Of course, consequently the same will be true for $\Psi_0(M)$.

The function $\tilde{\Psi}_M$ satisfies the recurrent equation

$$\tilde{\Psi}_M = [\hat{u}_{12}\tilde{\Psi}_{M-1} - (\mu + 1)S^+(N-2)\tilde{\Psi}_{M-1}]|1,2\rangle, \quad (\text{A2})$$

where

$$\hat{u}_{12} = (2\mu - 1)s_1^+ + (2 - \mu)s_2^+.$$

Let us consider functions $\varphi_M^+ = S^+(N)\tilde{\Psi}_M$, $\varphi_M^- = S^-(N)\tilde{\Psi}_M$, and $\chi_M = S^-(N)S^+(N)\tilde{\Psi}_M$. The recurrent equations for these functions are obtained from Eq. (A2) using Eq. (A1). They are

$$\begin{aligned} \varphi_M^+ &= [(\mu + 1)s_1^+s_2^+\tilde{\Psi}_{M-1} + \hat{v}_{12}\varphi_{M-1}^+]|1,2\rangle, \\ \varphi_M^- &= [(\mu + 1)(\tilde{\Psi}_{M-1} - \chi_{M-1}) + \hat{u}_{12}\varphi_{M-1}^-]|1,2\rangle, \quad (\text{A3}) \\ \chi_M &= [(\hat{u}_{12} - \hat{v}_{12})\tilde{\Psi}_{M-1} + \hat{v}_{12}\chi_{M-1} + (\mu + 1) \\ &\times (s_1^+s_2^+\varphi_{M-1}^- - \varphi_{M-1}^+)]|1,2\rangle, \end{aligned}$$

where

$$\hat{v}_{12} = -(2 - \mu)s_1^+ - (2\mu - 1)s_2^+.$$

Equations (A2) and (A3) can be written in a matrix form

$$R(M) = D_{12}R(M-1), \quad (\text{A4})$$

where $R(M)$ and D_{12} are (2×2) matrices:

$$\begin{aligned} R(M) &= \begin{pmatrix} \tilde{\Psi}_M - \chi_M & \varphi_M^+ \\ -\varphi_M^- & \tilde{\Psi}_M \end{pmatrix}, \\ D_{12} &= \begin{pmatrix} \hat{v}_{12} & (\mu + 1)s_1^+s_2^+ \\ -(\mu + 1) & \hat{u}_{12} \end{pmatrix}|1,2\rangle. \end{aligned}$$

Therefore, $R(M)$ is

$$R(M) = D_{12}D_{34} \times \cdots \times D_{N-1,N}. \quad (\text{A5})$$

As $\tilde{\Psi}_M$ contains singlet and triplet components only, the projection of $\tilde{\Psi}_M$ onto the singlet is

$$\tilde{\Psi}_0(M) = P_0\tilde{\Psi}_M = 2\tilde{\Psi}_M - \chi_M. \quad (\text{A6})$$

It follows from Eqs. (A5) and (A6) that

$$\tilde{\Psi}_0(M) = \text{Tr } D_{12}D_{34} \times \cdots \times D_{N-1,N}. \quad (\text{A7})$$

This form of $\tilde{\Psi}_0(M)$ is similar to the matrix product wave function of the AKLT model and its generalizations, which has been found in Ref. 15. Each of four matrix elements of $R(M)$ is the eigenfunction of the local Hamiltonian $H_{i,i+1,i+2,i+3}$ for $i = 1, 3, \dots, N-3$ because of matrix elements of the product $D_{i,i+1}D_{i+1,i+2}$ are the eigenfunctions of this Hamiltonian. Besides, it can be proved¹⁵ that the four matrix elements of $R(M)$ are the only ground states of Eq. (45) and, therefore, the ground state of the open chain is fourfold degenerate.

It is easily to check¹⁵ that the triplet wave functions $R_{12}(M)$ and $R_{21}(M)$ are not eigenfunctions of $H_{N-1,N,1,2}$. On the other hand, using cyclic permutations of matrices under the *trace*, we have

$$H_{N-1,N,1,2}\tilde{\Psi}_0(M) = \varepsilon\tilde{\Psi}_0(M),$$

and, therefore, the ground state of the cyclic chain is the nondegenerate singlet.

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