Exactly solvable Ising-Heisenberg chain with triangular *XXZ*-Heisenberg plaquettes

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A mixed Ising-Heisenberg spin system consisting of triangular *XXZ*-Heisenberg spin clusters assembled into a chain by alternating with Ising spins interacting to all three spins in the triangle is considered. The exact solution of the model is given in terms of the generalized decoration-iteration map and within the transfer-matrix technique. Exact expressions for thermodynamic functions are derived. Ground-state phase diagrams and thermodynamic and magnetic properties of the system are examined.

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I. INTRODUCTION

Frustrated spin systems have been in the focus of intensive investigations during the last decades.[1] Belonging to a separate class of magnetic systems, they possess a number of fascinating features. Geometrically frustrated magnets are of special interest due to their unusual magnetic and thermodynamic properties. In this class of magnets the lattice topology precludes the spins from simultaneously minimizing all spin–spin-exchange interactions. The simplest example of frustrated spin cluster is given by the triangular arrangement of three spins with antiferromagnetic interaction between each pair.

Numerous variants of lattice spin systems containing triangular plaquettes are, on one hand, widespread structures of magnetic materials and provide, on the other hand, a theoretical prototype models for investigating the geometrically frustrated systems and their unusual features. Among the important classes of geometrically frustrated two-dimensional systems, it is worth mentioning the triangular antiferromagnets[2] and antiferromagnets on kagome lattice.[3] There are few one-dimensional lattices with triangular frustrated units which are famous for their exactly known dimerized ground states: the Majumdar-Ghosh model which is the special case of spin-1/2 chain with competing nearest-neighbor (NN) and next-nearest-neighbor (NNN) interaction[4] and the so-called sawtooth chain (Δ chain), the system of corner-sharing triangles.[5]

Although the properties of the ground states of the above-mentioned systems have been investigated analytically very well, only numerical calculations still remain reliable to gain an insight into the finite-T thermodynamic properties. On the other hand, there is a large class of exactly solvable one-dimensional "classical" lattice models which allow one to obtain an exact expressions for thermodynamic functions using different techniques.[6] The simplest and at the same time key example is the transfer-matrix solution of the one-dimensional Ising model known since the 1920s. Further developments of the transfer-matrix technique which is very powerful and rather simple for the arbitrary one-dimensional lattice systems with discrete commuting variables turned out to be especially useful in the statistical mechanics of macromolecules.[7] However, in the theory of magnetism and strongly correlated systems one-dimensional systems with classical variables have rather "pedagogical" value than practical one.

Nevertheless, it was established in a series of recent publications that considering the Ising counterparts of some Heisenberg one-dimensional spin systems one can obtain, on one hand, the exact thermodynamic description of the problem and, on the other hand, the system which at least on the qualitative level exhibits the magnetic and thermodynamic behaviors very similar to those of the underlying quantum spin model.[8–13] For instance, the form of the magnetization curve does not acquire crucial changes when one replaces some or even all Heisenberg interactions in the chain with Ising ones. So, if the initial quantum spin chain exhibits a magnetization plateau at a certain value of the magnetization, this feature will hold for the corresponding Ising or Ising-Heisenberg chain, whereas quantitative characteristics of the plateau (terminal points, width, etc.) can be different. This feature was reported in Ref. 8 for the spin-1/2 chain with bond-alternating ferromagnetic-ferromagnetic-antiferromagnetic (F-F-AF) interaction, the model of $3CuCl_2 \cdot 2dx$ (dx=1,4-dioxane) compound. In the quantum model describing the magnetic structure of $3CuCl_2 \cdot 2dx$, considered numerically in Ref. 15, the appearance of magnetization plateau at 1/3 of the saturation magnetization value was established. It is worthy to note that experiments have shown no plateau in $3CuCl_2 \cdot 2dx$ which is caused by the insufficient small ratio of the antiferromagnetic and ferromagnetic coupling constants. The corresponding regime of magnetic behavior for F-F-AF Ising chain was also established in Ref. 8. This was the example of the intermediate magnetization plateaus in one-dimensional spin system which in recent decades received considerable attention both in theoretical and experimental aspects.[1,16] Hereafter, the Ising counterpart of this model was solved exactly in thermodynamic context in Ref. 8 demonstrating the same magnetization plateau at $m=1/3$. Almost the same program but with different techniques was performed in Ref. 9 for another bond-alternating chain, the spin-1/2 F-F-AF-AF chain, which is regarded as the model of magnetic structure of $Cu(3\text{-}Clpy)_2(N_3)_2$, where 3-Clpy indicates 3-chloropyridine. The authors considered a simplified Ising-Heisenberg variant of the F-F-AF-AF chain within the method of exact mapping transformation (decoration-iteration transformation).[17] Comparing their results with the experimental and numerical data, they found not only qualitative but also quantitative agreement as well. It is also worthy to mention the works on exact solutions of mixed spin (1/2,1,3/2) and spin 1/2, the so-called diamond chains with the decoration-iteration transformation technique,[10] which revealed series of magnetization plateaus in magnetization process of the system. Also, the magnetization plateaus in one-dimensional spin-1, spin-3/2, and spin-2 Ising chains with single-ion anisotropy have been investigated in Ref. 11 showing good agreement with experimental data obtained for spin-1 Ni compounds. Magnetization plateaus in the Ising limit of the multiple-spin-exchange model on the four-spin cyclic interaction have been considered in Ref. 12.

All these results, unexpected at the first glance, offer the challenge to develop a formalism which, on one hand, leads to the exact analytical treatment for thermodynamic functions of the one-dimensional spin systems and, on the other hand, could be relevant in describing and understanding experimental data for real materials. As mentioned above, the idea is very simple, just replace some (or even all) Heisenberg-type quantum interaction with the Ising ones. Of course, there are many very important features of quantum exchange interaction which are crucial in understanding many phenomena in magnetic systems and which cannot be neglected. But the results of Refs. 8–12 indicate the existence of at least a few quantum spin chains (actually the chains with alternating ferromagnetic and antiferromagnetic couplings), the thermodynamic properties of which do not undergo sizable changes under the replacement of some interaction with more simple Ising ones, allowing an exact solution. In addition to that the spin systems considered here may serve as more or less realistic model for the arrays of single-molecule magnets (SMMs) (Ref. 18) with intermolecular couplings engineered by the methods of the so-called supramolecular chemistry.[19] SMMs recently receive much attention as they are very convenient objects for studying the phenomena which are critical at the nanoscale such as quantum tunneling of magnetization, decoherence, and Berry phases. One of the well-studied specific examples of SMMs, the equilateral spin triangle Cu_3 (Ref. 20) assembled to the one-dimensional arrays with very weak intermolecular coupling, could be the system which approximately can be described by the model considered here.

In this paper we consider a further development of the methods applied in Refs. 8–13 for the chain with frustrated triangular quantum *XXZ*-Heisenberg plaquettes. This chain was introduced in Ref. 14 where the ground-state properties and some numerical results for purely Heisenberg case were obtained. Within the transfer-matrix technique we obtain exact thermodynamic solution of the chain consisting of such spin triangles alternating with the single Ising spins which are coupled by the interaction of Ising type with all six spins of the sites of two neighbor triangular plaquettes. The paper is organized as follows. In Sec. II we formulate the model and present its solution by the decoration-iteration transformation technique. In Sec. III the transfer-matrix solution of the system is given. In Sec. IV, using the transfer-matrix formalism, the exact thermodynamics of the system is discussed. In particular the $T=0$ phase diagram and plots of magnetization vs external magnetic field, specific heat, and magnetic susceptibility are presented. The Appendix contains several technical points of the calculations.

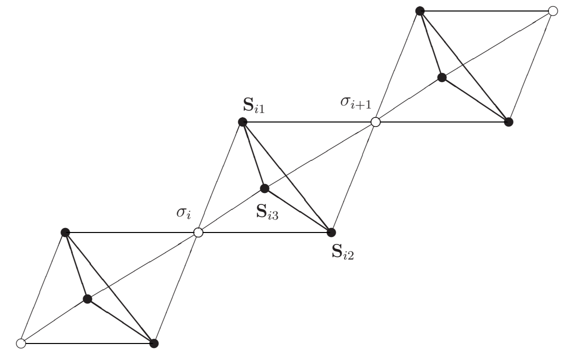

FIG. 1. The schematic picture of the Ising-Heisenberg chain with triangular plaquettes alternating with single sites. The filled (empty) circles indicate Heisenberg (Ising) spins.

II. MODEL AND ITS SOLUTION WITH THE AID OF THE GENERALIZED DECORATION-ITERATION TRANSFORMATION

We begin with the hybrid Ising-Heisenberg spin system consisting of the triangular clusters of Heisenberg $S=1/2$ spins interacting to each other with coupling constant J and axial anisotropy Δ. These triangles are assembled into a chain by alternating with single sites. Each spin at the single site is coupled to all six spins situated at the corners of its two adjacent triangles (see Fig. 1). The interactions of spins at single sites and spins belonging to triangles are all supposed to be of Ising type (the interaction includes only z components of the spins). The corresponding Hamiltonian is suitable to be presented as a sum over the plaquette Hamiltonians each one containing one triangle and its two surrounding single sites,

$$\mathcal{H}=\sum_{i=1}^{N}\mathcal{H}_i,$$

$$\mathcal{H}_i=J\left[\frac{\Delta}{2}(S_{i1}^{+}S_{i2}^{-}+S_{i1}^{-}S_{i2}^{+})+S_{i1}^{z}S_{i2}^{z}+\frac{\Delta}{2}(S_{i1}^{+}S_{i3}^{-}+S_{i1}^{-}S_{i3}^{+})+S_{i1}^{z}S_{i3}^{z}+\frac{\Delta}{2}(S_{i2}^{+}S_{i3}^{-}+S_{i2}^{-}S_{i3}^{+})+S_{i2}^{z}S_{i3}^{z}\right]+K(S_{i1}^{z}+S_{i2}^{z}+S_{i3}^{z})(\sigma_i+\sigma_{i+1})-H_2(S_{i1}^{z}+S_{i2}^{z}+S_{i3}^{z})-\frac{H_1}{2}(\sigma_i+\sigma_{i+1}). \quad (1)$$

Here by σ we denote the z components of the spins at the single sites which, thus, can be identified with the Ising variables taking ± 1 values. K is the Ising coupling between triangle spins and single-site spins and H_1 and H_2 stand for the couplings of Ising and Heisenberg spins to the external magnetic field pointing in the z direction. For convenience we normalize the Heisenberg spin operators in such a way which provides the eigenvalues of S^z to take ± 1 values, which means that our S^α are just the Pauli matrices without spin magnitude multiplier. (In order to recover conventional Heisenberg Hamiltonian parameters one should replace in all our formulas J with $J/4$ and H with $H/2$.) Thus, they obey the commutation relations

$$[S^+_{ia},S^-_{jb}] = \delta_{ij}\delta_{ab}4S^z_{ia},$$
$$[S^z_{ia},S^\pm_{jb}] = \pm 2\delta_{ij}\delta_{ab}S^\pm_{ia} \quad (2)$$

and act on the basic states in the following way:

$$S^z|\uparrow\rangle = |\uparrow\rangle, \quad S^z|\downarrow\rangle = -|\downarrow\rangle,$$
$$S^+|\uparrow\rangle = 0, \quad S^+|\downarrow\rangle = 2|\uparrow\rangle,$$
$$S^-|\uparrow\rangle = 2|\downarrow\rangle, \quad S^-|\downarrow\rangle = 0. \quad (3)$$

In order to describe thermodynamics of the system one need to calculate the partition function

$$\mathcal{Z} = \sum_{(\sigma)} \mathrm{Tr}_{(S)} \exp\left(-\beta\sum_{i=1}^{N}\mathcal{H}_i\right), \quad (4)$$

where the sum is going over all possible configurations of the Ising spins and $\mathrm{Tr}_{(S)}$ denotes the trace over all Heisenberg operators S and β as usual is the inverse temperature. One can easily see that the Hamiltonians corresponding to different plaquettes do commute which allows one to expand the exponent in the partition function obtaining partial factorization of the partition function

$$\mathcal{Z} = \sum_{(\sigma)} \prod_{i=1}^{N} \mathrm{Tr}_i\, e^{-\beta\mathcal{H}_i}. \quad (5)$$

Here Tr_i stands for the trace over the state of ith triangle. Now we can utilize the so-called decoration-iteration transformation[10] which allows us to represent the trace over all states of single triangle interacting with two Ising spin as the elements of the transfer matrix for ordinary one-dimensional Ising model with a certain renormalization of its parameters,

$$\mathrm{Tr}_i\, e^{-\beta\mathcal{H}_i} = \sum_{n=1}^{8} e^{-\beta\lambda_n(\sigma_i,\sigma_{i+1})} = Ae^{\beta R\sigma_i\sigma_{i+1}+\beta(H/2)(\sigma_i+\sigma_{i+1})}. \quad (6)$$

Here $\lambda_n(\sigma_i,\sigma_{i+1})$ are eight eigenvalues of $\mathcal{H}_i$ which depend of the values of its neighbor Ising spins. The parameters of emergent "one-dimensional Ising" model are expressed by the parameters of the initial model in the following way:

$$A = (Z_+Z_-Z_0^2)^{1/4}, \quad \beta R = \frac{1}{4}\log\left(\frac{Z_+Z_-}{Z_0^2}\right),$$
$$\beta H = \beta H_1 + \frac{1}{2}\log\left(\frac{Z_+}{Z_-}\right), \quad (7)$$

where

$$Z_+ = \sum_{n=1}^{8} e^{-\beta\lambda_n(+,+)}, \quad Z_- = \sum_{n=1}^{8} e^{-\beta\lambda_n(-,-)},$$
$$Z_0 = \sum_{n=1}^{8} e^{-\beta\lambda_n(+,-)} = \sum_{n=1}^{8} e^{-\beta\lambda_n(-,+)} \quad (8)$$

are the partition functions for single triangle calculated for certain values of its neighbor Ising spins. The explicit form of these functions can be found in the Appendix. Thus, according to Eqs. (4)–(8) one can obtain an exact solution for the system under consideration in the form corresponding to the well-known solution of one-dimensional Ising model as follows:

$$\mathcal{Z}(\beta;J,K,\Delta,H_1,H_2) = \sum_{(\sigma)}\prod_{i=1}^{N} Ae^{\beta R\sigma_i\sigma_{i+1}+\beta(H/2)(\sigma_i+\sigma_{i+1})}$$
$$= A^N\mathcal{Z}_0(\beta;R,H). \quad (9)$$

The partition function of the one-dimensional Ising model with periodic boundary conditions in thermodynamic limit is[6]

$$\mathcal{Z}_0(\beta;R,H) = e^{\beta NR}[\cosh(\beta H) + \sqrt{\sinh^2(\beta H) + e^{-\beta 4R}}]^N. \quad (10)$$

Relation (9) establishes a connection between thermodynamic quantities of the system under consideration and those of one-dimensional Ising model. So, in the thermodynamic limit for free energy per spin we get

$$f = -T\lim_{N\to\infty}\left(\frac{\log\mathcal{Z}}{4N}\right) = \frac{1}{4}(f_0 - T\log A). \quad (11)$$

(We remind that by N we denote the number of the lattice blocks each one containing five spins, so under the periodic boundary conditions the total number of spins is $4N$.) Here by f_0 we denote the corresponding free energy per spin for ordinary Ising chain. Now we can utilize the common thermodynamic relations to obtain expressions for various thermodynamic quantities we are going to investigate. As usual for specific heat, entropy, total magnetization, and susceptibility per spin one has

$$C_H = -T\left(\frac{\partial^2 f}{\partial T^2}\right)_H, \quad S = -\left(\frac{\partial f}{\partial T}\right)_H,$$
$$M = -\left(\frac{\partial f}{\partial H}\right)_T, \quad \chi = \left(\frac{\partial^2 f}{\partial H^2}\right)_T. \quad (12)$$

The thermal averages of various microscopic variables can also be expressed in term of corresponding quantities for the Ising model. The sublattice magnetization and various nearest-neighbor correlation functions can be expressed by the sublattice magnetization and nearest-neighbor correlation functions of ordinary Ising chain given by

$$M_0 = -\left(\frac{\partial f_0}{\partial H}\right)_T = \frac{\sinh(\beta H)}{\sqrt{\sinh^2(\beta H) + e^{-\beta 4R}}}, \quad (13)$$

$$C_0=\langle\sigma_i\sigma_{i+1}\rangle=-\left(\frac{\partial f_0}{\partial R}\right)_{T,H}=1-\frac{2e^{-\beta 4R}}{[\cosh(\beta H)+\sqrt{\sinh^2(\beta H)+e^{-\beta 4R}}]\sqrt{\sinh^2(\beta H)+e^{-\beta 4R}}}. \tag{14}$$

For sublattice and total magnetizations for the model under consideration one obtains

$$M_1=\frac{\left\langle\sum_{i=1}^{N}\sigma_i\right\rangle}{N}=-4\left(\frac{\partial f}{\partial H_1}\right)_T=-\left(\frac{\partial f_0}{\partial H}\right)_T=M_0,$$

$$M_2=\frac{\left\langle\sum_{i=1}^{N}\sum_{a=1}^{3}S_{ia}^z\right\rangle}{3N}=-\frac{4}{3}\left(\frac{\partial f}{\partial H_2}\right)_T=\frac{1}{3}\left[\frac{T}{A}\left(\frac{\partial A}{\partial H_2}\right)_T-\left(\frac{\partial f_0}{\partial R}\right)_T\left(\frac{\partial R}{\partial H_2}\right)_T-\left(\frac{\partial f_0}{\partial H}\right)_T\left(\frac{\partial H}{\partial H_2}\right)_T\right]=\frac{1}{12}(W_++2W_0M_0+W_-C_0),$$

$$M=\frac{1}{4}M_1+\frac{3}{4}M_2, \tag{15}$$

where the corresponding functions $W_\alpha, \alpha=\pm,0$ can be found in Appendix. In the same manner for nearest-neighbor correlation functions we obtain

$$C_{\sigma\sigma}=\langle\sigma_i\sigma_{i+1}\rangle=C_0,$$

$$C_{S\sigma}=\langle S_{ia}^z\sigma_i\rangle=\frac{\left\langle\sum_{i=1}^{N}(\sigma_i+\sigma_{i+i})(S_{i1}^z+S_{i2}^z+S_{i3}^z)\right\rangle}{6N}=\frac{2}{3}\left(\frac{\partial f}{\partial K}\right)_{T,H}=-\frac{1}{12}(V_++2V_-M_0+V_+C_0),$$

$$C_{SS}^{(x,y)}=\langle S_{ia}^xS_{ib}^x\rangle=\langle S_{ia}^yS_{ib}^y\rangle=\frac{2}{3J}\left(\frac{\partial f}{\partial\Delta}\right)_{T,H}=-\frac{1}{12J}(U_++2U_0M_0+U_-C_0),\quad a\neq b,$$

$$C_{SS}^z=\langle S_{ia}^zS_{ib}^z\rangle=\frac{4}{3}\left(\frac{\partial f}{\partial J}\right)_{T,H}-2\Delta C_{SS}^{(x,y)}=\frac{1}{12}\left[\frac{2\Delta}{J}U_+-F_++2\left(\frac{2\Delta}{J}U_0-F_0\right)M_0+\left(\frac{2\Delta}{J}U_--F_-\right)C_0\right],\quad a\neq b. \tag{16}$$

III. SOLUTION WITHIN THE TRANSFER-MATRIX TECHNIQUE

We will use another technique for describing the thermodynamics of the system under consideration. Namely, having the analytical expression for the single-quantum triangle [see the Appendix and Eq. (A5)], one can represent the partition function of the chain under consideration given by Eq. (5) in the form which mimics the partition function of the classical chain with two state variables at each site (the "Ising chain" with arbitrary Boltzmann weights),

$$\mathcal{Z}=\sum_{\sigma}\prod_{i=1}^{N}e^{(\beta/2)H_1(\sigma_i+\sigma_{i+1})}Z(\sigma_i,\sigma_{i+1})=\mathrm{Tr}\,\mathbf{T}^N, \tag{17}$$

where $Z(\sigma_i,\sigma_{i+1})$ is calculated in the Appendix and $\mathbf{T}$ is the following transfer-matrix:

$$\mathbf{T}=\begin{pmatrix}e^{\beta H_1}Z_+ & Z_0\\ Z_0 & e^{-\beta H_1}Z_-\end{pmatrix}. \tag{18}$$

The eigenvalues of $\mathbf{T}$ are

$$\lambda_\pm=\frac{1}{2}[e^{\beta H_1}Z_++e^{-\beta H_1}Z_-\pm\sqrt{(e^{\beta H_1}Z_+-e^{-\beta H_1}Z_-)^2+4Z_0^2}]. \tag{19}$$

Thus, the free energy per one spin in the thermodynamic limit when only maximal eigenvalue survives is

$$f=-\frac{1}{4\beta}\log\left\{\frac{1}{2}[e^{\beta H_1}Z_++e^{-\beta H_1}Z_-+\sqrt{(e^{\beta H_1}Z_+-e^{-\beta H_1}Z_-)^2+4Z_0^2}]\right\}. \tag{20}$$

For sublattice and total magnetization one obtains

$$M_1=\frac{e^{\beta H_1}Z_+-e^{-\beta H_1}Z_-}{\sqrt{(e^{\beta H_1}Z_+-e^{-\beta H_1}Z_-)^2+4Z_0^2}},$$

$$M_2=\frac{e^{\beta H_1}X_++e^{-\beta H_1}X_-+\dfrac{Z_+(e^{\beta H_1}X_+-X_-)+Z_-(e^{-\beta H_1}X_--X_+)+4Z_0X_0}{\sqrt{(e^{\beta H_1}Z_+-e^{-\beta H_1}Z_-)^2+4Z_0^2}}}{3[e^{\beta H_1}Z_++e^{-\beta H_1}Z_-+\sqrt{(e^{\beta H_1}Z_+-e^{-\beta H_1}Z_-)^2+4Z_0^2}]},$$

$$M = \frac{\left\langle \sum_{i=1}^{N} \left(\sigma_i + \sum_{a=1}^{3} S_{ia}^z \right) \right\rangle}{4N} = \frac{1}{4}M_1 + \frac{3}{4}M_2, \tag{21}$$

where the functions X_+, X_-, X_0 are defined in the Appendix. If one assume $H_1 = H_2 = H$ which means the equality of the g factors for S and σ spins the expression for the total magnetization per spin takes the following form:

$$M = \frac{e^{\beta H}(Z_+ + X_+) - e^{-\beta H}(Z_- - X_-) + \dfrac{(e^{\beta H}Z_+ - e^{-\beta H}Z_-)[e^{\beta H}(Z_+ + X_+) + e^{-\beta H}(Z_- - X_-)] + 4Z_0X_0}{\sqrt{(e^{\beta H}Z_+ - e^{-\beta H}Z_-)^2 + 4Z_0^2}}}{4[e^{\beta H}Z_+ + e^{-\beta H}Z_- + \sqrt{(e^{\beta H}Z_+ - e^{-\beta H}Z_-)^2 + 4Z_0^2}]}, \tag{22}$$

where $H_2 = H$ should be put in all X_α and Z_α functions.

IV. THERMODYNAMIC AND MAGNETIC PROPERTIES

In this section we examine the thermodynamic and magnetic properties of the model under consideration. Having the exact explicit expressions for the magnetization, specific heat, entropy, and nearest-neighbor correlation functions, one can easily obtain their plot vs temperature or external magnetic field despite of their complicated form. Also, analyzing the low-temperature region one can obtain the ground-state properties and corresponding phase diagrams. In what follows, we restrict ourselves in the case of all antiferromagnetic couplings, $J>0$, $K>0$, and $\Delta>0$.

A. Zero-temperature ground-state phase diagrams

Let us analyze the possible ground state of the system at $T=0$ and for positive values of all model parameters J, K, Δ. According to the possible states of three $s=1/2$ spins one can distinguish the following spin configurations on the chain under consideration. First of all, the ground states in the absence of magnetic field depending on the values of model parameters can be either ferrimagnetic (F) or AF,

$$|F\rangle = \prod_{i=1}^{N} |3/2, 3/2\rangle_i \otimes |\downarrow\rangle_i,$$

$$|\mathrm{AF}\rangle = \prod_{i=1}^{N} |1/2, 1/2\rangle_i \otimes |\downarrow\rangle_i, \tag{23}$$

where $|l, m\rangle_i$ stands for the spin state of triangle at ith plaquette with total spin equal to l and $S^z = m$ and $|\uparrow\rangle, |\downarrow\rangle$ are the standard "up" and "down" states of the Ising spins. Expanding the states of quantum triangles by the single-spin basis one finds

$$|3/2, 3/2\rangle = |\uparrow\uparrow\uparrow\rangle,$$

$$|1/2, 1/2\rangle_{R,L} = \frac{1}{\sqrt{3}}(|\uparrow\uparrow\downarrow\rangle + e^{\pm(2\pi i/3)}|\uparrow\downarrow\uparrow\rangle + e^{\mp(2\pi i/3)}|\downarrow\uparrow\uparrow\rangle), \tag{24}$$

where the choice of the sings of the coefficients in $|1/2, 1/2\rangle$ state is connected with the its chirality. For the interactions considered here these two states are degenerated by energy and there is no need to distinguish them in our consideration, so we will omit R, L indices. Thus, here the manifestation of frustration consists in this degeneracy. Every triangle can spontaneously pass from $|1/2, 1/2\rangle_R$ to $|1/2, 1/2\rangle_L$ and vice versa. Therefore, due to the frustration the system possesses nonzero entropy at $T=0$. It is worth mentioning that considering the Ising limit of the system, $\Delta=0$, one can obtain essential enhancement of frustration at $J=K$. Indeed, if one takes only one plaquette which consists of five Ising spins with nine uniform couplings between them, the ground state will be a disordered one with three spins pointing up and the remaining two pointing down or vise versa. So, the number of possible degenerated configuration for one plaquette and for fixed orientation of the total magnetization will be 10. The energies per one plaquette and magnetizations corresponding to $|F\rangle$ and $|\mathrm{AF}\rangle$ configurations are

$$\varepsilon_F = 3\eta - 2h - 6, \quad M_F = 1/2,$$

$$\varepsilon_{\mathrm{AF}} = -\eta(1+2\Delta) - 2, \quad M_{\mathrm{AF}} = 0, \tag{25}$$

where the following dimensionless parameters are introduced: $\varepsilon = E/NK$, $\eta = J/K$, and $h = H/K$. Thus, the ground state of the system at $T=0$ and $h=0$ is ferrimagnetic when $\eta \le \frac{2}{2+\Delta}$ and antiferromagnetic otherwise. The corresponding

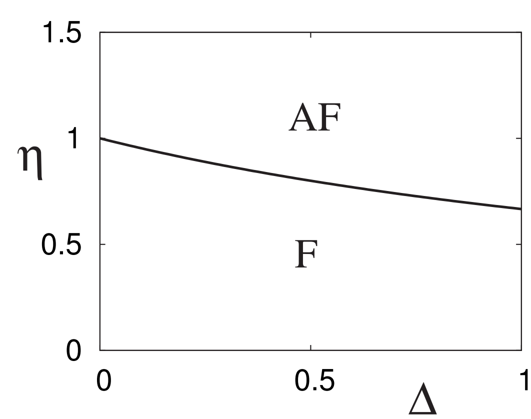

FIG. 2. $T=0$, $H=0$ ground-state phase diagram in the Δ-η plane. The boundary between ferrimagnetic (F) and antiferromagnetic (AF) ground states are given by $\eta = \frac{2}{2+\Delta}$.

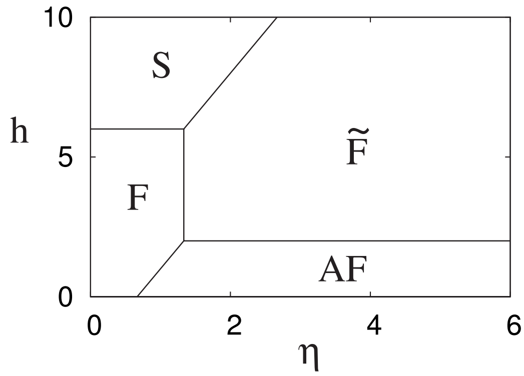

FIG. 3. $T=0$ ground-state phase diagram in the η-h plane for $\Delta=1$. The boundary between F and AF phases is $h=\eta(2+\Delta)-2$; between second ferrimagnetic phase ($\tilde{F}$) and saturate state (S) is $h=\eta(2+\Delta)+2$.

phase diagram is presented in Fig. 2. The appearance of the external magnetic field makes another two ground state possible. Namely, the state with total magnetization $M=1/2$ resulting from AF state by the flip of all Ising spins. This state actually is a ferrimagnetic one differing from F. Another possible state is completely polarized saturated phase,

$$|\tilde{F}\rangle = \prod_{i=1}^{N} |1/2,1/2\rangle_i \otimes |\uparrow\rangle_i,$$

$$|S\rangle = \prod_{i=1}^{N} |3/2,3/2\rangle_i \otimes |\uparrow\rangle_i \tag{26}$$

with

$$\varepsilon_{\tilde{F}} = -\eta(1+2\Delta) - 2h + 2, \quad M_{\tilde{F}} = 1/2,$$

$$\varepsilon_S = 3\eta - 4h + 6, \quad M_S = 1. \tag{27}$$

The corresponding $T=0$ ground-state phase diagram in the (h,η) plane for the case $\Delta=1$ is presented in Fig. 3.

B. Magnetization processes and susceptibility

According to the phase diagram displayed in Fig. 3 one can expect three different kinds of magnetic behavior depending on the relation between parameters η and Δ. The following sequences of transitions occur when the magnitude of external magnetic field is increasing. For the values of η and Δ belonging to the first region given by $\eta \leq \frac{2}{2+\Delta}$, the system undergoes only one transition from $|F\rangle$ to $|S\rangle$ taking place at $h=6$. The next range of parameter values is characterized by $\frac{2}{2+\Delta} < \eta \leq \frac{4}{2+\Delta}$. Here one can occur two consecutive transitions from $|\mathrm{AF}\rangle$ to $|F\rangle$ at $h=\eta(2+\Delta)-2$ and from $|F\rangle$ to $|S\rangle$ at $h=6$. Finally, when η is greater than $\frac{4}{2+\Delta}$ the system undergoes the following transitions: $|\mathrm{AF}\rangle \to |\tilde{F}\rangle$ and $|\tilde{F}\rangle \to |S\rangle$ at $h=2$ and $h=\eta(2+\Delta)+2$, respectively. The corresponding plots of the magnetization processes for finite temperatures are shown in Figs. 4–6. At zero temperature all transitions are obviously jumplike and the corresponding

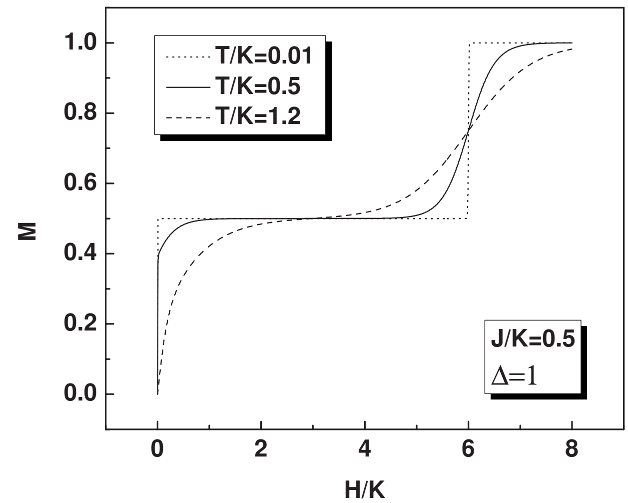

FIG. 4. Total magnetization M as a function of dimensionless external magnetic field h for $\eta=0.5$, $\Delta=1$, and three different dimensionless temperatures $T/K=0.01$, 0.5, and 1.2.

magnetization curves are perfectly steplike. However, at arbitrary finite temperatures all transitions are smeared out within some interval of magnetic field. In Fig. 4 the plots of M vs H/K are presented for $\eta=0.5$ and $\Delta=1$ for several temperatures. One can see the magnetization plateau at $M=1/2$ which corresponds to the zero-temperature stability of $|F\rangle$ state in the interval of h from 0 to 6. The plot for $T/K=0.01$ is very close to this picture, whereas one can see essential shrinkage of the plateau width with increasing temperature. Surely, for large enough temperatures the magnetization curve acquires the form corresponding to the free spins (Langevin curve) with monotonic increase between 0 and 1 values. Generally speaking, at the small values of the ratio η the system under consideration is similar to the mixed antiferromagnetic Ising chain with alternating $s=1/2$ and $s=3/2$ spins, because the strong interaction between the triangle spins makes their behavior very similar to that of one

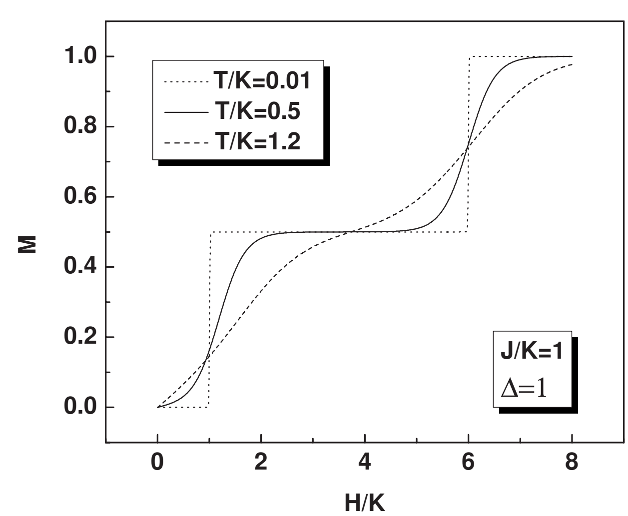

FIG. 5. Total magnetization M as a function of dimensionless external magnetic field h for $\eta=1$, $\Delta=1$, and three different dimensionless temperatures $T/K=0.01$, 0.5, and 1.2.

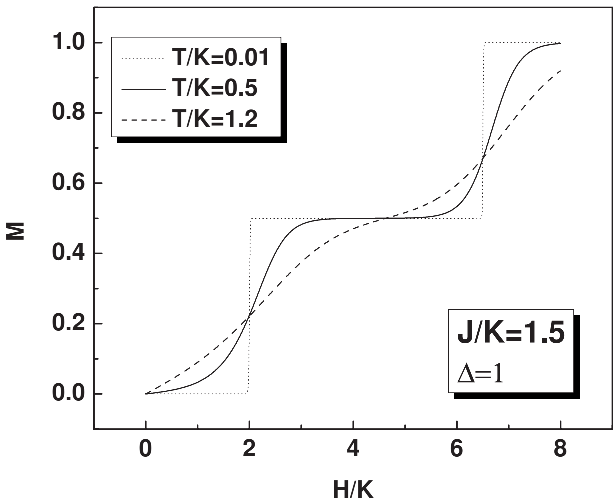

FIG. 6. Total magnetization M as a function of dimensionless external magnetic field h for $\eta=1.5$, $\Delta=1$, and three different dimensionless temperatures $T/K=0.01$, 0.5, and 1.2.

spin 3/2. So, the region $\eta \leq \frac{2}{2+\Delta}$ can be considered as the spin-3/2–spin-1/2 mixed chain regime. The typical plots for the second range of η are presented in Fig. 5. Here two magnetization jumps corresponding to the transitions $|\text{AF}\rangle \rightarrow |F\rangle$ and $|F\rangle \rightarrow |S\rangle$ occur at $T=0$ in the magnetization curves for the system under consideration for $\eta=1$ and $\Delta=1$. The corresponding plateau at $M=1/2$ as in the previous case appears due to stability of the $|F\rangle$ state between $|\text{AF}\rangle$ and $|S\rangle$. The width of the plateau is $8-\eta(2+\Delta)$. The plots for different finite temperatures from Fig. 5 exhibit the gradual shrinking down of the plateau with the increasing temperature. For the same plateau at $M=1/2$ but with another physical content one can see the magnetization curves for the third region of values of η. In Fig. 6 one can see the plots of M vs H/K for $\eta=1.5$ and $\Delta=1$. All properties mentioned above concerning the temperature effect hold in this case as well. However, the plateau at $M=1/2$ now corresponds to the $|\tilde{F}\rangle$ state of the chain. The two terminal points of the plateau correspond to the zero-temperature transition from $|\text{AF}\rangle$ to $|\tilde{F}\rangle$ and from $|\tilde{F}\rangle$ to $|S\rangle$, respectively. The position of the left end of the plateau ($h=2$) is unaffected by the any changes in interaction parameters provided that the latter stay within $\eta > \frac{4}{2+\Delta}$. (The same phenomenon for the right end of plateau at $h=6$ takes place in the two other regimes of behavior of the system under consideration.) The width of this plateau at $T=0$ is equal to $\eta(2+\Delta)$.

The plots of thermal dependence of magnetic susceptibility times temperature $T\chi$ per one spin are displayed in Figs. 7–9. First of all, zero-field susceptibility diverges at $T=0$ which is a consequence of the fact that $T=0$ is the critical point at which the system possesses an ideal long-range spin order, which is destroyed by any finite temperature. In Fig. 7 the plots of $T\chi$ vs T for the first region parameters are presented for several values of external magnetic field. Here no divergence is observed at $T=0$ because of energy gap opened by magnetic field. A rather sharp peak appears in the curve at extremely weak-field value. This peak corresponds to the thermal instability at the transition from uncorrelated disordered state, which is the ground state at any finite tempera-

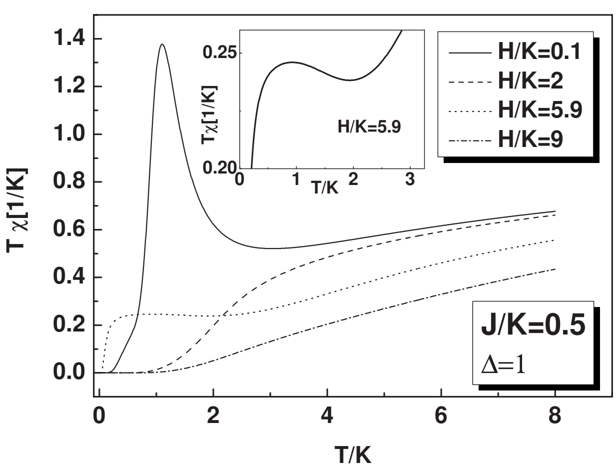

FIG. 7. The temperature dependence of the $T\chi$ product for several values of field strength and $\eta=0.5$, $\Delta=1$. The inset displays the round minimum for $H/K=3$ on an enlarged scale.

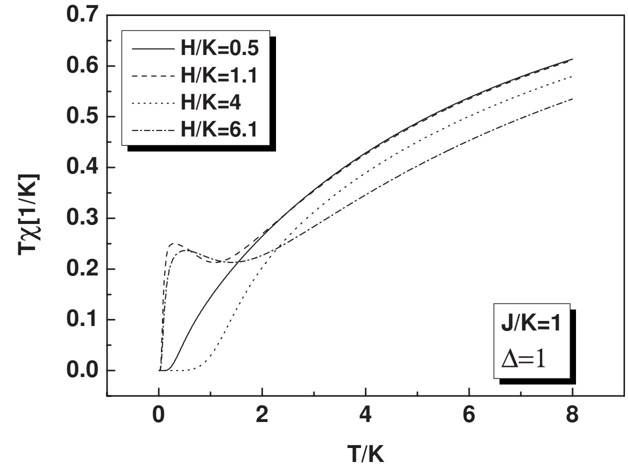

FIG. 8. The temperature dependence of the $T\chi$ product for several values of field strength and $\eta=1$, $\Delta=1$.

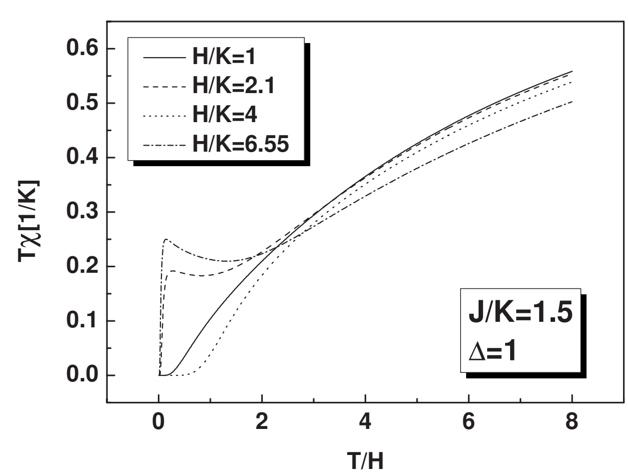

FIG. 9. The temperature dependence of the $T\chi$ product for several values of field strength and $\eta=1.5$, $\Delta=1$.

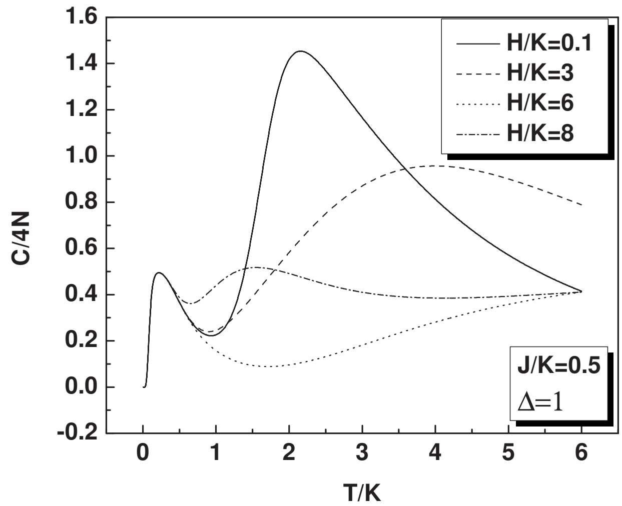

FIG. 10. Specific head per one spin as a function of the dimensionless temperature T/K given in K units for $\eta=0.5$, $\Delta=1$ for various values of h.

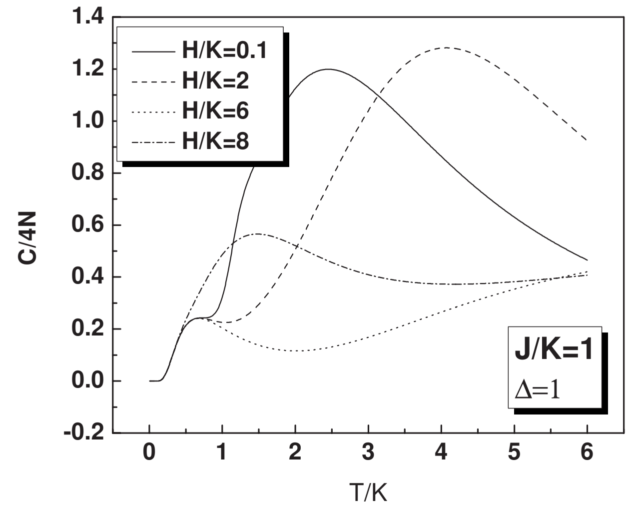

FIG. 11. Specific head per one spin as a function of the dimensionless temperature T/K given in K units for $\eta=1$, $\Delta=1$ for various values of h.

ture and $H=0$, to the ferrimagnetic state $|F\rangle$. At the end of the peak the tiny round minimum is observed. With increasing the field strength the low-temperature peak is smoothed out and the curve becomes monotonically increasing, which is a general feature of antiferromagnetically coupled spin systems. At $H/K=5.9$, i.e., in the vicinity of the transition from $|F\rangle$ to $|S\rangle$, the $T\chi$ vs T curve exhibits a very rapid increase at low temperatures with further narrow plateau formation which is then followed by the slowly and monotonically increasing region. The inset of Fig. 7 shows the small round minimum which accompanies the transition from narrow plateau to increasing monotone behavior of susceptibility. Very similar picture of susceptibility thermal dependence was obtained for the F-F-AF-AF Ising-Heisenberg chain in Ref. 9. In Fig. 8 the plots of $T\chi$ vs T for $\eta=1$, $\Delta=1$ are presented. Here, a little smaller than in the previous case, low-temperature peaks appear at the values of H/K corresponding to the transitions from $|\mathrm{AF}\rangle$ to $|F\rangle$ and from $|F\rangle$ to $|S\rangle$. One can observe a similar picture of the $T\chi$ thermal behavior for the system under consideration when the parameters belong to the third region, $\eta>\frac{4}{2+\Delta}$. The corresponding plots are presented in Fig. 9.

C. Specific heat

As mentioned above, the technique developed in the paper allows one to obtain analytical exact expressions for all thermodynamic functions of the system. Thought, the forms of some of them are extremely cumbersome, one can easily obtain their plots. In Figs. 10–12 the plots of thermal behavior of the specific heat of the system under consideration are presented. Generally, specific heat exhibits two-peak structure, with one sharp low temperature, which is almost unaffected by the value of the magnetic field, and another one with broaden peak, which undergoes considerable changes under increasing magnetic field. Figure 10 demonstrates the corresponding plots for $\eta=0.5$, $\Delta=1$. The second peak is well pronounced here and is strongly field dependent. Thus, one can associate it with Schottky-type anomaly. With the increase in the external magnetic field strength the peak moves to higher-temperature region and, at the same time, drops in magnitude. At the values of field strength close to the transition to saturated state at $T=0$ the second broad peak begins to enhance again for a while; however, with the further increase in the field it gradually gets smoother. In general, one can observe almost the same features in the thermal behavior of the specific heat times temperature per spin for the region $\frac{2}{2+\Delta}\leq\eta<\frac{4}{2+\Delta}$ (Fig. 11). The essential difference with the previous case is complete merging of sharp low-temperature peak and the Schottky-type broad peak at the values of field strength corresponding to the plateau in the magnetization curve at $T=0$. Figure 12 shows typical plots of $T\chi$ vs T for $\eta=1.5$, i.e., for the third region of model parameters, $\eta\geq\frac{4}{2+\Delta}$. Here at low-field strength immediate after the first sharp peak a narrow almost horizontal region of the

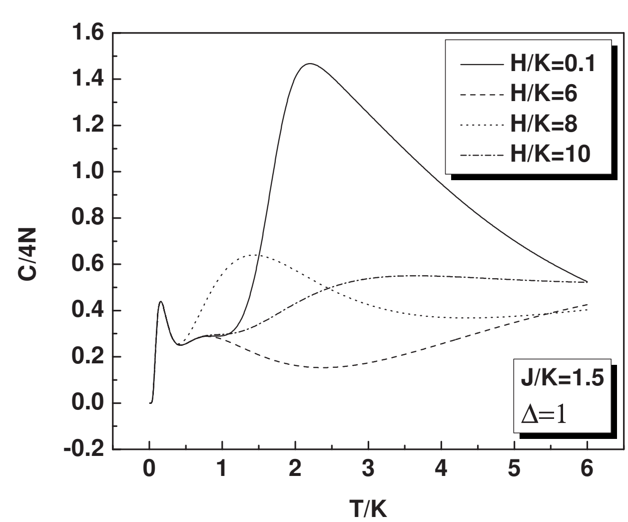

FIG. 12. Specific head per one spin as a function of the dimensionless temperature T/K given in K units for $\eta=1.5$, $\Delta=1$ for various values of h.

curve appears. Increasing the field strength one can observe the enhancement of the slope of the corresponding region accompanying the second broad peak changes described above.

V. CONCLUDING REMARKS

In this paper we considered exactly solvable model of one-dimensional spin system with Heisenberg-*XXZ* triangular spin clusters alternating with single Ising spins. Two different approaches have been discussed: the decoration-iteration transformation[9,10,17] and the transfer-matrix direct formalism. Both approaches lead to the possibility of obtaining exact analytical expressions for the thermodynamic functions of the system. The system considered here, as well as the other systems considered earlier in Refs. 8–12, at first glance is only of academic interest. However, the strict indications of the relevance of the approaches based on the simplification of the spin-exchange interaction scheme in one-dimensional magnetic materials have been given in Refs. 8, 9, and 11. Namely, considering the spin-exchange Hamiltonians for various materials with one-dimensional exchange structure in most cases one can gain insight into description of their properties and understanding of their thermodynamic behavior only within the complicated and laborious numerical calculations demanding some time extremely powerful computing facilities, such as supercomputers. On the other hand, at least for some class of systems, the simplification of the model based on the replacement of all or just some of the exchange Heisenberg interactions with the interactions of Ising type does not affect the prominent properties of their thermodynamics. This fact makes the simplified exactly solvable (in the "thermodynamic" sense) counterpart of the one-dimensional models which describe the magnetism of real materials very promising. Especially this approach can be successful in the series of bond-alternating chain with spatially repeated sequence of ferromagnetic and antiferromagnetic interactions as it has been established for F-F-AF (Ref. 8) and F-F-AF-AF (Ref. 9) chains. Apparently, replacing the ferromagnetic bounds with Ising ones is especially "safe" in that sense because the former ones favor parallel orientation of the spins, which is given by a separable vector of state. Thus, one can lose only a small amount of information of the properties of that bound by regarding it as the Ising one. Antiferromagnetically coupled spins are not so "harmless" because they can be in the superposition and entangled states which cannot be properly translated into the Ising language. Another essential difference between Heisenberg spin chains and their simplifying counterparts is the spin-wave properties. Generally speaking, spin wave cannot propagate through Ising spins, so only localized excitations are relevant in that case. Further applications of the methods discussed in the present paper in other one-dimensional and quasi-one-dimensional Heisenberg models, especially in the models of novel magnetic materials, as well as a comparison of the results with the experimental data, can play a very important role in the understanding of complicated magnetic materials and their thermodynamic properties and can draw the frameworks of applicability of the approach offered in this paper.

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APPENDIX

Here we derive the exact expressions for the functions Z_+, Z_-, Z_0 from Eq. (8). For these purposes one should obtain the eigenvalues of the matrix, corresponding to the Hamiltonian of single triangle. So, we define a partition function for one single triangle

$$\mathcal{Z}_\Delta(\beta;J,\Delta,H) = \mathrm{Tr}\, e^{-\beta\mathcal{H}_\Delta(J,\Delta,H)} = \sum_{n=1}^{8} \langle\psi_n|e^{-\beta\mathcal{H}_\Delta(J,\Delta,H)}|\psi_n\rangle, \tag{A1}$$

where $|\psi_n\rangle$ is an arbitrary orthogonal normalized system of states. Then, one can easily see that the Hamiltonian corresponding to ith plaquette from Eq. (1) has the same form as the Hamiltonian of single isolated triangle if one introduces instead of magnetic field H an "effective field" depending on the values of σ_i and σ_{i+1},

$$\tilde{H} = H_2 - K(\sigma_i + \sigma_{i+1}). \tag{A2}$$

The term corresponding to the interaction of σ_i and σ_{i+1} with magnetic field H_1 adds $-\frac{H_1}{2}(\sigma_i+\sigma_{i+1})$ to each eigenvalue of $\mathcal{H}_\Delta$. It is easy to see that $\mathcal{H}_\Delta$ is diagonal in the symmetry-adapted basis. The higher weight state of which is given by Eq. (25). The rest five states can be easily found by successive actions of the lowering operator $S^-_{\mathrm{tot}}=\frac{1}{2}(S^-_1+S^-_2+S^-_3)$ on $|3/2,3/2\rangle$ and $|1/2,1/2\rangle_{L,R}$ as follows:

$$|3/2,1/2\rangle = \frac{1}{\sqrt{3}}(|\uparrow\uparrow\downarrow\rangle + |\uparrow\downarrow\uparrow\rangle + |\downarrow\uparrow\uparrow\rangle),$$

$$|3/2,-1/2\rangle = \frac{1}{\sqrt{3}}(|\uparrow\downarrow\downarrow\rangle + |\downarrow\uparrow\downarrow\rangle + |\downarrow\downarrow\uparrow\rangle),$$

$$|3/2,-3/2\rangle = |\downarrow\downarrow\downarrow\rangle,$$

$$|1/2,-1/2\rangle_{R,L} = \frac{1}{\sqrt{3}}(|\downarrow\downarrow\uparrow\rangle + e^{\pm(i2\pi/3)}|\uparrow\downarrow\downarrow\rangle + e^{\mp(i2\pi/3)}|\downarrow\uparrow\downarrow\rangle). \tag{A3}$$

Taking into account Eq. (A2) the eight eigenvalues of $\mathcal{H}_i$ are

$$\lambda_{1,2}(\sigma_i,\sigma_{i+1}) = 3(J \pm H) \mp 3K(\sigma_i + \sigma_{i+1}),$$

$$\lambda_{3,4}(\sigma_i,\sigma_{i+1}) = \lambda_{5,6}(\sigma_i,\sigma_{i+1}) = -(1+2\Delta)J \pm H \mp K(\sigma_i + \sigma_{i+1}),$$

$$\lambda_{7,8}(\sigma_i,\sigma_{i+1}) = -(1-4\Delta)J \pm H \mp K(\sigma_i + \sigma_{i+1}). \quad \text{(A4)}$$

Thus, one has

$$Z(\sigma_i,\sigma_{i+1}) = \sum_{i=1}^{8} e^{-\beta\lambda_n(\sigma_i,\sigma_{i+1})} = B_1 \cosh\{\beta[H_2 - K(\sigma_i+\sigma_{i+1})]\} + B_2 \cosh\{\beta 3[H_2 - K(\sigma_i+\sigma_{i+1})]\}, \quad \text{(A5)}$$

where

$$B_1 = 2(e^{\beta(1-4\Delta)J} + 2e^{\beta(1+2\Delta)J}), \quad B_2 = 2e^{-\beta 3J}. \quad \text{(A6)}$$

Now, we can define the functions appearing in Eqs. (15) and (16) as follows:

$$Z_+ = B_1 \cosh[\beta(H_2 - 2K)] + B_2 \cosh[\beta 3(H_2 - 2K)],$$

$$Z_- = B_1 \cosh[\beta(H_2 + 2K)] + B_2 \cosh[\beta 3(H_2 + 2K)],$$

$$Z_0 = B_1 \cosh(\beta H_2) + B_2 \cosh(\beta 3H_2),$$

$$X_\alpha = T\left(\frac{\partial Z_\alpha}{\partial H_2}\right)_T = B_1 \sinh[\beta(H_2 - \alpha 2K)] + 3B_2 \sinh[\beta 3(H_2 - \alpha 2K)], \quad \alpha = \pm, 0,$$

$$Y_\pm = T\left(\frac{\partial Z_\pm}{\partial K}\right)_T = \mp 2\{B_1 \sinh[\beta(H_2 \mp 2K)] + 3B_2 \sinh[\beta 3(H_2 \mp 2K)]\},$$

$$Q_\alpha = T\left(\frac{\partial Z_\alpha}{\partial \Delta}\right)_T = B_3 \cosh[\beta(H_2 - \alpha 2K)], \quad \alpha = \pm, 0,$$

$$P_\alpha = T\left(\frac{\partial Z_\alpha}{\partial J}\right)_T = B_4 \cosh[\beta(H_2 - \alpha 2K)] + B_5 \cosh[\beta 3(H_2 - \alpha 2K)], \quad \alpha = \pm, 0,$$

$$W_\pm = \frac{X_+}{Z_+} + \frac{X_-}{Z_-} \pm 2\frac{X_0}{Z_0}, \quad W_0 = \frac{X_+}{Z_+} - \frac{X_-}{Z_-},$$

$$V_\pm = \frac{Y_+}{Z_+} \pm \frac{Y_-}{Z_-},$$

$$U_\pm = \frac{Q_+}{Z_+} + \frac{Q_-}{Z_-} \pm 2\frac{Q_0}{Z_0}, \quad U_0 = \frac{Q_+}{Z_+} - \frac{Q_-}{Z_-},$$

$$F_\pm = \frac{P_+}{P_+} + \frac{P_-}{Z_-} \pm 2\frac{P_0}{Z_0}, \quad F_0 = \frac{P_+}{Z_+} - \frac{P_-}{Z_-}, \quad \text{(A7)}$$

where

$$B_3 = 16Je^{\beta(1-\Delta)J} \sinh(\beta 3\Delta J)$$

$$B_4 = 2[(1-4\Delta)e^{\beta(1-4\Delta)J} + 2(1+2\Delta)e^{\beta(1+2\Delta)J}],$$

$$B_5 = -6e^{-\beta 3J}. \quad \text{(A8)}$$

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