Frustration and ordering in Ising chain in an external magnetic field with third-neighbor interactions

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In this paper, the frustration properties of the Ising model on a one-dimensional monoatomic equidistant lattice in an external magnetic field are investigated, taking into account the exchange interactions of atomic spins at the sites of the first, second, and third neighbors. Exact analytical expressions for the thermodynamic functions of the system are obtained by the Kramers–Wannier transfer-matrix method. A magnetic phase diagram of the ground state of such a spin system is constructed and studied thoroughly. The points and lines of frustrations of the system depending on the values and signs of exchange interactions and on an external magnetic field are found. The criteria for the occurrence of magnetic frustrations in the presence of competition between the energies of exchange interactions and an external magnetic field are formulated. The peculiar features are investigated and the values of entropy and magnetization of the ground state of this model are obtained in the frustration regime and beyond it. Various types of behavior of entropy, magnetization, and magnetic susceptibility depending on the model parameters are revealed.

I. INTRODUCTION

At the present time, spin systems with magnetic frustrations are being studied extremely intensively both theoretically and experimentally [1][5].

The study of frustrated systems makes it possible to understand the mechanisms of particular magnetic states, such as a spin liquid, spin ice, and also explain the existence of various incommensurate, helicoidal, chiral, and other exotic structures (see, for example, Refs. [7–13]).

Magnetic structures with frustrations have been studied since the second half of the last century, but the phenomenon of magnetic frustrations was discovered in the mid-seventies of the twentieth century in magnets exhibiting unusual properties, which was explained by a strong degeneration of the ground state of the system and the impossibility of magnetic ordering even at zero temperature. Such magnets by Gerard Toulouse in 1977 were called frustrated [14][15].

A crucial point in the study of frustrated systems is the search for theoretical solutions that allow us to understand the nature of the occurrence of frustrations in magnetic systems, as well as to adequately interpret experimental data on magnetic materials containing information about new phenomena and their unusual properties.

The Ising model is one of the basic models of the theory of magnetism, for which there is a well-known set of solutions [16][13] that allow one to describe some spin systems (see, for example, Refs. [19][20]).

In the present paper, we study the frustrating properties of an one-dimensional Ising model on a monoatomic equidistant lattice in an external magnetic field, taking into account the exchange interactions of atomic spins at the sites of the first, second, and third neighbors. Such a model makes it possible to obtain an exact solution in the thermodynamic limit, which allows to qualitatively consider the desired characteristics, including explaining the properties of magnets caused by frustrations that are not available for description in the framework of a perturbation theory [21].

Our study of the frustration properties of the model is associated with the investigation of the full magnetic phase diagram of the ground state, as well as the behavior of the zero-temperature entropy and magnetization of the system.

Note that this paper is a continuation of the study of the one-dimensional Ising model, taking into account the exchange interactions of atomic spins at the sites of the first, second, and third neighbors without taking into account an external magnetic field, the paper to be referred to as [22].

II. THERMODYNAMIC FUNCTIONS OF THE ISING CHAIN

We will consider the one-dimensional classical Ising model in an external magnetic field, taking into account the exchange interactions between atomic spins at the sites of the first (nearest), second (next-nearest), and third neighbors, which is given by the Hamiltonian of the form

\[ \mathcal{H} = -\sum_{p=1}^{b} \sum_{n=1}^{N-p} J_{p} \sigma_n \sigma_{n+p} - \mu_0 gH \sum_{n=1}^{N} \sigma_n, \] (1)

where \( b \) is the number of exchange interactions of the chain spins in the model (in this case \( b = 3 \)), \( J_1 \) is the parameter of the exchange interaction between the spins at the nearest neighbor sites of the linear lattice, \( J_2 \) is the parameter of the exchange interaction between the spins at the next-nearest neighbor lattice sites, \( J_3 \) is the parameter of the exchange interaction between the spins at the sites of the third neighbors sites of the lattice, \( H \) is the value of an external uniform magnetic field (directed along the \( z \)-axis), \( \mu_0 \) is the Bohr magneton, \( g \) is the Landé \( g \)-factor, the symbol \( \sigma_n \) denotes the \( z \)-projection of the atomic spin operator located at the \( n \)-site and is equal to \( \sigma = \pm 1(\uparrow, \downarrow) \), and \( N \) is the number of sites in the spin chain.

In the Kramers–Wannier transfer matrix method [21][23] used and with the imposition of cyclic Born–von Kármán

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boundary conditions, the partition function is equal to

$$Z = \text{Tr} \, V^N,$$

(2)

where $V$ is a transfer matrix the elements of which are independent of the site index \([21]\) and are specified by the rule

$$V^{\sigma \sigma' \sigma'' \sigma''' \sigma'''} = \langle \sigma \sigma' | e^{K_1 \sigma \sigma' + K_2 \sigma \sigma'' + K_3 \sigma \sigma''' + B_1 \sigma \sigma'''} | \sigma'' \sigma''' \sigma'''' \rangle = e^{K_1 \sigma \sigma' + K_2 \sigma \sigma'' + K_3 \sigma \sigma''' + B_1 \delta_{\sigma' \sigma''} \delta_{\sigma'' \sigma'''}},$$

through dimensionless coefficients

$$K_{1,2,3} = \beta J_{1,2,3}, \quad B = \beta \mu_0 g H, \quad \beta = \frac{1}{k_B T},$$

and $\delta_{\sigma' \sigma''}$ is the Kronecker symbol.

Note that hereinafter such quantities as the Bohr magneton ($\mu_0$), the Landé $g$-factor ($g$), and the Boltzmann constant ($k_B$) will be put equal to unity, and the quantities are $T$, $H$, $J_2$, and $J_3$ will be measured in $|J_1|$ units, as is commonly accepted in the theory of low-dimensional systems.

The dimension of the square transfer matrix of the one-dimensional spin model is determined by the expression

$$d = c^b,$$

where $c$ is the number of states at the site ($c = 2$ in the classical Ising model), and $b$ is the number of exchange interactions of chain spins in the problem ($b = 3$). Therefore, in the considered problem, the dimension of the transfer matrix is equal to

$$d = 2^3.$$

The construction of the transfer matrix was carried out according to the scheme proposed in \([21]\), and described in detail in \([22]\)\([25]\). Hence, we obtain that the transfer matrix has the following form

$$V = \begin{pmatrix}
V_1 V_2 V_3 V_H & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}.$$

(3)

$$V_1 = e^{K_1}, \quad V_2 = e^{K_2}, \quad V_3 = e^{K_3}, \quad V_H = e^B.$$

The characteristic equation of this matrix is defined as

$$\lambda^8 + a_7 \lambda^7 + a_6 \lambda^6 + a_5 \lambda^5 + a_4 \lambda^4 + a_3 \lambda^3 + a_2 \lambda^2 + a_1 \lambda + a_0 = 0,$$

(4)

where the coefficients are

$$a_7 = -2 e^{K_1 + K_2 + K_3} \cosh B,$$

$$a_6 = 2 e^{2K_3} \sinh[2(K_1 + K_3)],$$

$$a_5 = 4 e^{-K_1 + K_2 + K_3} \sinh[2(K_2 - K_3)] \cosh B,$$

$$a_4 = -2 \{\cosh(4K_2) + \cosh(2B)\} + 4 e^{2K_3} \cos^2 B,$$

$$a_3 = -8 e^{-K_1 - K_2 + K_3} \sinh[2(K_2 + K_3)] \sinh(2K_3) \cosh B,$$

$$a_2 = -8 e^{-2K_3} \sinh[2(K_1 - K_3)] \sin^2(2K_3),$$

$$a_1 = -16 e^{-K_1 - K_2 + K_3} \sinh^3(2K_3) \cosh B,$$

$$a_0 = 16 \sinh^4(2K_3).$$

In the transfer matrix method in the thermodynamic limit ($N \rightarrow \infty$), the partition function \([2]\) is defined as

$$Z = \lambda_1^N,$$

where $\lambda_1$ is the principal (single largest positive real) eigenvalue of the transfer matrix \([3]\), which is the corresponding solution of the equation \((4)\). Note that for the type of matrices under consideration, such a solution always exists by the Frobenius–Perron theorem \([26]\)\([27]\).

As a result, all thermodynamic functions of the system, including the Helmholtz free energy per spin,

$$F = -\frac{T}{N} \ln Z = -T \ln \lambda_1,$$

entropy

$$S = \frac{\partial F}{\partial T} = \ln \lambda_1 + T \frac{\partial \lambda_1}{\lambda_1} \frac{\partial T}{T},$$

(5)

heat capacity

$$C = -T \frac{\partial^2 F}{\partial T^2} = 2 \frac{T}{\lambda_1} \frac{\partial \lambda_1}{\lambda_1} + T^2 \frac{\partial^2 \lambda_1}{\partial T^2} - T^2 \left( \frac{\partial \lambda_1}{\partial T} \right)^2,$$

(6)
magnetization

\[ M = - \frac{\partial F}{\partial H} = \frac{T}{\lambda_1} \frac{\partial \lambda_1}{\partial H}, \tag{7} \]

and magnetic susceptibility

\[ \chi = -\frac{\partial^2 F}{\partial H^2} = \frac{\partial M}{\partial H} = -T \left( \frac{\partial \lambda_1}{\partial H} \right)^2 + T \frac{\partial^2 \lambda_1}{\partial H^2}, \tag{8} \]

are defined only in terms of the principal eigenvalue of the transfer matrix \([21, 28]\).

### III. MAGNETIC PHASE DIAGRAM OF THE GROUND STATE OF THE SYSTEM

The model contains eight variants for the relationship of the parameters of the exchange interactions between the spins at the sites of the first, second, and third neighbors of the chain. These relations are

\( J_1 < 0, J_2 > 0, J_3 < 0, \) \( J_1 > 0, J_2 > 0, J_3 > 0, \) \[ (9) \]

\( J_1 < 0, J_2 > 0, J_3 > 0, \) \( J_1 > 0, J_2 > 0, J_3 < 0, \) \[ (10) \]

\( J_1 < 0, J_2 < 0, J_3 < 0, \) \( J_1 > 0, J_2 < 0, J_3 > 0, \) \[ (11) \]

\( J_1 < 0, J_2 < 0, J_3 > 0, \) \( J_1 > 0, J_2 < 0, J_3 < 0. \) \[ (12) \]

The first two sets \([9]\) correspond to the aggravated antiferromagnetic and ferromagnetic types of the exchange interactions. The last six sets of the parameters \([10, 12]\) define the system with competing exchange interactions between spins.

The presence of an external magnetic field complicates the magnetic phase diagram of the ground state (MPDGS) of the model, which is determined by the behavior of the minimum energy of the spin system configurations at zero temperature, depending on the parameters of the model

\[ E_0 = \min \{ E \}, \]

where the configuration energy itself is the internal energy

\[ U = -T^2 \frac{\partial F}{\partial T} = \frac{T^2 \partial \lambda_1}{\lambda_1 \partial T}, \]

per lattice site at zero temperature,

\[ E = \lim_{T \to 0} U, \]

which is explicitly specified by the total energy operator of the system \([1]\) and is found from the function

\[ E = \frac{1}{m} \sum_{i=1}^{m} e_i, \]

where \( m \) is the number of sites in the configuration, \( b \) is the number of exchange interactions of the chain spins in the problem \((b = 3)\), \( J_p \) is the parameter of the exchange interaction between spins at neighboring sites of the \( p \)-level.

Building complete MPDGS depending on the parameters of the model is an intricate problem and has not been fully carried out. In the papers \([29, 30]\), only some aspects of the change in the MPDGS model in the absence and presence of an external magnetic field were touched upon.

Thus, only seven types of spin configurations with a minimum energy are realized in the ground state of the system, depending on the signs of the parameters of the exchange interactions of the chain spins and the value of an external magnetic field.

The first type of spin configurations is characterized by ferromagnetic ordering, which at \( H = 0 \) corresponds to the set

\[ C_{F2} = \{ \uparrow \uparrow \cdots \}, \tag{13} \]

consisting of two sequences (with spin projections along and against the direction of the \( z \)-axis) with equal energies

\[ E_{F2} = -(J_1 + J_2 + J_3), \tag{14} \]

and when taking into account an external magnetic field \((H > 0)\) directed along the \( z \) spin projection, the set of configurations already consists of one sequence (along the direction of the \( z \)-axis)

\[ C_{F1} = \{ \uparrow \uparrow \cdots \} \tag{15} \]

with energy

\[ E_{F1} = -(J_1 + J_2 + J_3 + H). \tag{16} \]

For such configurations, we introduce index designations F2 and F1, used in \([22, 23]\).

The second type of spin configurations is characterized by antiferromagnetic ordering (configuration designation A2) with the set

\[ C_{A2} = \{ \uparrow \downarrow \cdots \}, \tag{17} \]

consisting of two sequences (with alternating spin projections along and against the direction of the \( z \)-axis) with equal energies

\[ E_{A2} = J_1 - J_2 + J_3. \tag{18} \]

This configuration has the indicated energy both in and without an external magnetic field.

The third type of spin configurations is characterized by magnetic ordering with a tripling of the translation period.
(configuration designation A3), which at \( H = 0 \) has the following set

\[
C_{A3} = \left\{ \begin{array}{c}
\uparrow \uparrow \downarrow \ldots \\
\uparrow \downarrow \uparrow \ldots \\
\downarrow \uparrow \uparrow \ldots \\
\downarrow \downarrow \downarrow \ldots
\end{array} \right\},
\]

consisting of six configurations with equal energies

\[
E_{A3} = \frac{J_1 + J_2 - 3J_3}{3},
\]

and for \( H > 0 \), the set of sequences is halved and consists of

\[
C_{A31} = \left\{ \begin{array}{c}
\uparrow \uparrow \uparrow \ldots \\
\uparrow \uparrow \downarrow \ldots \\
\uparrow \downarrow \uparrow \ldots \\
\downarrow \downarrow \uparrow \ldots
\end{array} \right\},
\]

(configuration designation A31). Such a set consists of three configurations with equal energies

\[
E_{A31} = \frac{J_1 + J_2 - 3J_3 - H}{3}.
\]

The fourth type of configurations is determined by magnetic ordering with a quadrupling of the period of translations (configuration designation A4),

\[
C_{A4} = \left\{ \begin{array}{c}
\uparrow \uparrow \downarrow \downarrow \ldots \\
\uparrow \downarrow \uparrow \downarrow \ldots \\
\downarrow \uparrow \uparrow \downarrow \ldots \\
\downarrow \downarrow \uparrow \uparrow \ldots
\end{array} \right\},
\]

which consists of four configurations with equal energies

\[
E_{A4} = J_2,
\]

regardless of the presence or absence of an external magnetic field.

The fifth type of configurations is determined by magnetic ordering with a quintupling of the period of translations (configuration designation A41),

\[
C_{A41} = \left\{ \begin{array}{c}
\uparrow \uparrow \uparrow \downarrow \downarrow \ldots \\
\uparrow \uparrow \downarrow \uparrow \downarrow \ldots \\
\uparrow \downarrow \uparrow \uparrow \downarrow \ldots \\
\downarrow \downarrow \uparrow \downarrow \uparrow \ldots
\end{array} \right\},
\]

which consists of four configurations with equal energies

\[
E_{A41} = \frac{-H}{2}.
\]

The sixth type of configurations is characterized by magnetic ordering with sextupling of the period of translations (configuration designation A6),

\[
C_{A6} = \left\{ \begin{array}{c}
\uparrow \uparrow \uparrow \uparrow \downarrow \downarrow \ldots \\
\uparrow \uparrow \uparrow \downarrow \uparrow \downarrow \ldots \\
\uparrow \downarrow \uparrow \uparrow \uparrow \downarrow \ldots \\
\downarrow \downarrow \uparrow \uparrow \uparrow \uparrow \ldots
\end{array} \right\},
\]

which consists of five configurations with equal energies

\[
E_{A6} = \frac{-J_1 - 3(J_2 + J_3) + H}{5}.
\]

The seventh type is characterized by magnetic ordering with a sextuple period of translations (configuration designation A6),

\[
C_{A6} = \left\{ \begin{array}{c}
\uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \downarrow \ldots \\
\uparrow \uparrow \uparrow \uparrow \downarrow \uparrow \downarrow \ldots \\
\uparrow \downarrow \uparrow \uparrow \uparrow \downarrow \uparrow \ldots \\
\downarrow \downarrow \uparrow \uparrow \uparrow \uparrow \uparrow \ldots
\end{array} \right\},
\]

which consists of six configurations with equal energies

\[
E_{A6} = \frac{-J_1 - J_2 - 3J_3}{3}.
\]

From this we obtain that in the absence of an external magnetic field, spin configurations that survive in the ground state correspond to the following designations $C_i$, and $F_j$ (configuration designation A6), introduced in the papers [31, 32] and widely used in the ANNNI model [33–35].

Other types of magnetic ordering, that is, spin configurations with septupling or higher increase in the translation period, do not have a minimum ground state energy at any ratios of the exchange parameters of the system.

Thus, the considered spin configurations have the corresponding minimum energies in the ground state (at $T = 0$) in the following ranges of the model parameters

\[
\begin{align*}
P_{F1} &= \{ H \geq -2(J_1 + J_2) \land H \geq -2(J_1 + J_3) \land H \geq -2(J_1 + 2J_2 + J_3) \} \\
P_{A2} &= \{ J_1 - J_2 \leq 0 \land J_1 - 2J_2 + J_3 \leq 0 \land H \leq -2(J_1 - J_2 + J_3) \land H \leq -2(J_1 - 2J_2 + 3J_3) \land H \leq -2(3J_1 - 4J_2 + J_3) \}.
\end{align*}
\]
From the expression for the minimum energy of the ground state \( \mathcal{E}_G \), it is easy to obtain all ratios of the parameters of the considered model, under which the structure of the magnetic ordering of the spin configurations of the ground state is rearranged with the formation of the structure of the boundaries of the regions of these configurations on the MPDGS of the spin system, shown in Figs. 1, 10.

As noted earlier, all model parameters are measured in units of \( |J| \), therefore, for the convenience of constructing phase diagrams, the quantity \( |J| \) was chosen to be equal to unity. Of course, another choice of the value of the exchange interaction of the nearest neighbors \( |J| \) will not fundamentally change of the MPDGS.

The expressions for the minimum energy of spin configurations \( \mathcal{E}_G \) depend on four model parameters \( J_1, J_2, J_3, H \), so the complete MPDGS is cumbersome.

Note that the presence of competing exchange interactions of spins at the sites of the first, second, and third neighbors affects the complexity of the MPDGS itself.

The MPDGS can be plotted as a dependence of the values of the exchange interactions \( J_3 \) and \( J_2 \) on various values of an external magnetic field \( H \) (Figs. 1 and 2), or as a dependence of the values of \( H \) and \( J_2 \) on various values of the exchange interaction \( J_3 \) (Figs. 3, 4, 5 and 6), and also as a dependence of the values of \( H \) and \( J_3 \) on different values of the exchange interaction \( J_2 \) (Figs. 7, 8, 9 and 10).

Thus, the lines on the MPDGS demonstrate the boundaries of the regions of spin configurations, at which a qualitative change in the structure of the magnetic ordering of the ground state of the spin system occurs.

This magnetic phase diagram is complex; it demonstrates not only the existence of boundaries between two regions of spin configurations, but also the existence of the intersections of such lines (points) that delimit three or more regions of spin configurations. (Note that this situation was considered in detail in [22, 25, 30].)

The dashed lines on the MPDGS indicate the boundaries at which the ground state ordering is rearranged, and the number of configurations of the system with the minimum energy is equal to the sum of the configurations of the regions adjacent to the boundary.

The solid lines on the MPDGS indicate the boundaries at which the number of configurations of the system with the minimum energy is greater than the sum of the configurations of the regions of the phase diagram adjacent to it.

The existence of such set of spin configurations of the system at zero temperature at the boundaries and at points of the phase space is associated with the rearrangement of the magnetic structure and the appearance at a given phase point (in the thermodynamic limit) of an infinite number of spin configurations, including those without any translational invariance.

Crossing the boundaries of spin configurations on the MPDGS with the formation of triple, quadruple or with higher multiplicity points are marked on the plots by round dots.

It should be noted that (in the terminology of the papers [32, 33, 35, 37, 39]) on the MPDGS, the solid lines described above are called multiphase lines, and triple, quadruple and points with higher multiplicity are called multiphase points.

IV. THERMODYNAMICS OF THE SYSTEM AT ZERO TEMPERATURE WITHOUT AN EXTERNAL MAGNETIC FIELD

Taking into account the exchange interactions between atomic spin at the sites of the first, second, and third neighbors, and in the absence of an external magnetic field \( (H = 0) \), the characteristic equation (4) is defined as

\[
\lambda^4 + b_3 \lambda^3 + b_2 \lambda^2 + b_1 \lambda + b_0 = 0,
\]

where the coefficients are

\[
b_3 = -2e^{K_2} \cosh(K_1 + K_3), \quad b_2 = -2e^{K_2} \sinh(K_1 + K_3),
\]

\[
b_1 = 4e^{K_2} \sinh(2K_3) \sinh(K_1 - K_3),
\]

\[
c_1 = -4e^{-K_2} \sinh(2K_3) \cosh(K_1 - K_3),
\]

\[
b_0 = c_0 = 4 \sinh^2(2K_3).
\]

The principal eigenvalue of the transfer matrix determined from the equation (32), is expressed in radicals and has the following form

\[
\lambda_1 = \frac{b_3}{4} - \frac{1}{2} \sqrt{-4\Psi^2 - 2p + \frac{q}{\bar{S}}},
\]
FIG. 1. MPDGS of the Ising chain in an external magnetic field, taking into account the exchange interaction of spins at the sites of the first, second, and third neighbors with antiferromagnetic ($J_1 = -1$) exchange interaction of the nearest neighbors, at the values of an external magnetic field $H = 0$ (a), $H = 4/5$ (b), $H = 4/3$ (c), $H = 9/5$ (d), $H = 2$ (e), and $H = 5/2$ (f).

FIG. 2. MPDGS of the Ising chain in an external magnetic field, taking into account the exchange interaction of spins at the sites of the first, second, and third neighbors with ferromagnetic ($J_1 = +1$) exchange interaction of the nearest neighbors, at the values of an external magnetic field $H = 0$ (a), $H = 1$ (b), and $H = 2$ (c).
FIG. 3. MPDGS of the Ising chain in an external magnetic field, taking into account the exchange interaction of spins at the sites of the first, second and third neighbors with antiferromagnetic ($J_1 = -1$) exchange interaction of nearest neighbors, where $J_3 = 0$ (a), $J_3 = -1/5$ (b), $J_3 = -1/3$ (c), $J_3 = -4/5$ (d), $J_3 = -1$ (e), and $J_3 = -8/5$ (f).

FIG. 4. MPDGS of the Ising chain in an external magnetic field, taking into account the exchange interaction of spins at the sites of the first, second and third neighbors with antiferromagnetic ($J_1 = -1$) exchange interaction of the nearest neighbors, where $J_3 = +1/2$ (a), $J_3 = +1$ (b), and $J_3 = +2$ (c).
FIG. 5. MPDGS of the Ising chain in an external magnetic field, taking into account the exchange interaction of spins at the sites of the first, second and third neighbors with ferromagnetic \((J_1 = +1)\) exchange interaction of the nearest neighbors, where \(J_1 = 0\) (a), \(J_1 = -1/2\) (b), \(J_1 = -1\) (c), \(J_1 = -5/4\) (d), \(J_1 = -2\) (e), and \(J_1 = -3\) (f).

FIG. 6. MPDGS of the Ising chain in an external magnetic field, taking into account the exchange interaction of spins at the sites of the first, second and third neighbors with ferromagnetic \((J_1 = +1)\) exchange interaction of the nearest neighbors, where \(J_1 = +1\) (a), \(J_1 = +3/2\) (b), and \(J_1 = +3\) (c).
FIG. 7. MPDGS of the Ising chain in an external magnetic field, taking into account the exchange interaction of spins at the sites of the first, second and third neighbors with antiferromagnetic \((J_1 = -1)\) exchange interaction of nearest neighbors, where \(J_2 = 0\) (a), \(J_2 = -3/5\) (b), \(J_2 = -2/3\) (c), \(J_2 = -4/5\) (d), \(J_2 = -1\) (e), and \(J_2 = -3/2\) (f).

FIG. 8. MPDGS of the Ising chain in an external magnetic field, taking into account the exchange interaction of spins at the sites of the first, second and third neighbors with antiferromagnetic \((J_1 = -1)\) exchange interaction of the nearest neighbors, where \(J_2 = +1/2\) (a), \(J_2 = +1\) (b), and \(J_2 = +2\) (c).
FIG. 9. MPDGS of the Ising chain in an external magnetic field, taking into account the exchange interaction of spins at the sites of the first, second and third neighbors with ferromagnetic ($J_1 = +1$) exchange interaction of the nearest neighbors, where $J_2 = 0$ (a), $J_2 = -1/2$ (b), $J_2 = -1$ (c), $J_2 = -3/2$ (d), $J_2 = -2$ (e), and $J_2 = -3$ (f).

FIG. 10. MPDGS of the Ising chain in an external magnetic field, taking into account the exchange interaction of spins at the sites of the first, second and third neighbors with ferromagnetic ($J_1 = +1$) exchange interaction of the nearest neighbors, where $J_2 = +1/2$ (a), $J_2 = +1$ (b), and $J_2 = +3/2$ (c).
\[ p = b_2 - \frac{3}{8} b_3, \quad q = b_1 - b_2 b_3 + \frac{b_3^3}{8}, \]
\[ \Psi = \frac{1}{2} \sqrt{\frac{2}{3} p + \frac{1}{3} (\Theta + \Delta_0)}. \]
\[ \Theta = \sqrt{\Delta_1 + \sqrt{\Delta_1^2 - 4\Delta_0^3}}. \]
\[ \Delta_0 = 12b_0 - 3b_1 b_3 + b_2^2, \]
\[ \Delta_1 = -72b_0 b_2 + 27b_2 b_3^2 + 27b_1^2 - 9b_1 b_2 b_3 + 2b_3^3. \]

Using the expression (33), it is possible to calculate all necessary thermodynamic functions of the system.

We also note that the expression for the minimum energy of spin configurations (31) makes it possible to obtain the MPDGS of the system, which is shown in Figs. 1a and 2a.

In the regions beyond the boundaries of spin configurations \( C_{F2}, C_{A2}, C_{A3}, C_{A4}, C_{A6} \) on the MPDGS, the zero-temperature (residual) entropy of the system is always equal to zero,
\[ \lim_{T \to 0} S = S^\circ = 0, \quad (34) \]
and what the system demonstrates in these regions is the equilibrium state of the system.

At the boundaries of the regions of spin configurations \( C_{F2}-C_{A2}, C_{F2}-C_{A3}, C_{A2}-C_{A6}, C_{A2}-C_{A4} (J_1 < 0), \) \( C_{F2}-C_{A4} (J_1 > 0) \), the residual entropy is also equal to zero
\[ S^\circ = 0. \quad (35) \]
As noted earlier, this is due to the fact that at these boundaries such a number of configurations of the system with a minimum energy are formed that is equal to the sum of the configurations of the regions adjacent to this boundary. Therefore, the residual entropy of the equilibrium system (according to the Nernst–Planck theorem) is equal to zero (40, 41).

Such boundaries with zero residual entropy on the MPDGS are marked with dashed lines.

Next, we list the cases when the residual entropy is greater than zero
\[ S^\circ > 0 \]
at the junctions of the regions of the spin configurations of the system on the MPDGS.

Note that this situation is possible and this result does not contradict the third law of thermodynamics (40, 41), and such states of the system in which the entropy of the ground state is greater than zero are frustrated (see the discussion in 22, 25).

Such boundaries with nonzero residual entropy are marked with solid lines on the MPDGS, and triple and with higher multiplicity points are marked with a solid circle. It should also be said that such positions of the frustration of the system on the MPDGS correspond to multiphase lines and multiphase points in the terminology of 33, 38.

Thus, at the boundaries of the regions of spin configurations \( C_{A3}-C_{A4} \) and \( C_{A4}-C_{A6} \) (Figs. 1a and 2a), and at the points \( C_{A2}-C_{A3} (- C_{A5})-C_{A6} (J_1 < 0, \) Fig. 1a), \( C_{F2}-C_{A3}-C_{A4} (- C_{A5}) \) \( (J_1 > 0, \) Fig. 2a), \( C_{F2}-C_{A4}-C_{A5} (- C_{A6}) \) \( (J_1 < 0, H = 0, \) Fig. 3e), \( C_{A1}+C_{A5}-C_{A6} (H = 0, \) Fig. 5c), \( C_{F2}(-C_{A3})-C_{A4} (J_1 > 0, \) Fig. 9c) the residual entropy is
\[ S^\circ = \ln \left[ \frac{1}{3} \left( \vartheta_1 + \frac{3}{\vartheta_2} \right) \right] = 0.2811996, \quad (36) \]
where
\[ \vartheta_1 = \sqrt{\frac{3+3\sqrt{-3D_1}}{2}}, \quad (37) \]
Note that the sublogarithmic expression in Eq. (36) is the single positive largest real (principal) solution of the equation
\[ x^3 - x - 1 = 0, \quad (38) \]
its discriminant is
\[ D_1 = 2^2 - 3^3 = -23. \]

At the boundaries of the regions of spin configurations \( C_{A2}-C_{A3} (J_1 < 0, \) Fig. 1a) and \( C_{F2}-C_{A6} (J_1 > 0, \) Fig. 2a), and also at the points \( C_{F2}-C_{A2}-C_{A3} (J_1 < 0, \) Fig. 1a) and \( C_{F2}(-C_{A2})-C_{A6} (J_1 > 0, H = 0, \) Fig. 5c), \( C_{F2}(-C_{A2})+C_{A6} (J_1 > 0, H = 0, \) Fig. 10b) the residual entropy is
\[ S^\circ = \ln \left[ \frac{1}{3} \left( 1 + \vartheta_2 + \frac{1}{\vartheta_2} \right) \right] \approx 0.3822451, \quad (39) \]
where the sublogarithmic expression is the principal solution of the equation
\[ x^3 - x^2 - 1 = 0, \quad (41) \]
its discriminant is
\[ D_2 = -(2^2 + 3^3) = -31. \]

At triple points \( C_{A2}-C_{A3}-C_{A4} (J_1 < 0, \) Fig. 1a) and \( C_{F2}-C_{A4}-C_{A6} (J_1 > 0, \) Fig. 2a), and also at the points \( C_{F2}-C_{A4} (-C_{A5})-C_{A6} (J_1 > 0, H = 0, \) Fig. 5c) the residual entropy is equal to the natural logarithm of the golden ratio,
\[ S^\circ = \ln \left( 1 + \frac{\sqrt{5}}{2} \right) = \text{arcsch} 2 \approx 0.4812118, \quad (42) \]
where the sublogarithmic expression in (42) is the principal solution of the equation
\[ x^2 - x - 1 = 0, \quad (43) \]
residual magnetic susceptibility has values in the interval

\[ 0 < \chi^o < \infty \]

(blue dashed lines in Figs. 1a and 2a). In the case of frustrated states, the residual magnetic susceptibility is equal to infinity,

\[ \chi^o = \infty \]

(red solid lines in Figs. 1a and 2a).

Note that a detailed study of the temperature dependences of the thermodynamic functions of this model without taking into account an external magnetic field was done in [22].

At the end of this section, we note that in the absence of exchange between the spins of the chain \( J_i = 0 \), a quintuple point is formed on the MPDGS, in which a paramagnetic state is realized, characterized by the fact that all configurations of the system have the same probability and have the same zero energy. The entropy of such a state of the system is equal to the natural logarithm of two,

\[ S = \ln 2 \approx 0.693 147 2, \quad (44) \]

and it is the same (maximum) at any temperature. From this it is clear that the Ising paramagnet is an absolutely frustrated system (see discussion in [22, 25]).

We also recall that in the expression for the Gibbs entropy, the argument of the natural logarithm is the statistical weight of the system \( W \). In the case of \( W = 2 \), which determines the number of possible configurations of the considered model.

V. THERMODYNAMICS OF THE SYSTEM AT ZERO TEMPERATURE IN AN EXTERNAL MAGNETIC FIELD

The inclusion of an external magnetic field exceedingly complicates the behavior of the system. In addition to entropy and heat capacity, one can find the magnetization and magnetic susceptibility of the spin system.

In all possible regions of spin configurations \( (C_{F1}, C_{A2}, C_{A31}, C_{A4}, C_{A41}, C_{A5}, C_{A6}) \), the residual entropy is always equal to zero, and the zero-temperature (residual) magnetization has, among other things, non-zero values.

The residual magnetization of regions with period doubling (antiferromagnetic ordering), period quadrupling and sextupling is equal to zero

\[ M^o_{A2} = 0, \quad M^o_{A4} = 0, \quad M^o_{A6} = 0, \]

and more complicated configurations with period tripling, quadrupling, and quintupling have the following residual magnetizations

\[ M^o_{A31} = 1/3, \quad M^o_{A41} = 1/2, \quad M^o_{A5} = 1/5, \]

also the region with ferromagnetic ordering is equal to unity,

\[ M^o_{F1} = 1. \]
In the presence of an external magnetic field at the junctions of configurations of the MPDGs, the residual entropy and residual magnetization have a wide variety of values, demonstrating both the absence and the presence of frustrations in the corresponding regions of the phase diagram.

In the ground state, at the boundaries of configurations \(C_{A2} - C_{A4}\) and \(C_{A2} - C_{A6}\), the residual specific entropy and residual magnetization are zero,

\[
S^o_{A2 - A4} = 0, \quad M^o_{A2 - A4} = 0, \quad (45)
\]

\[
S^o_{A2 - A6} = 0, \quad M^o_{A2 - A6} = 0 \quad (46)
\]

(green dashed lines on the MPDGs, Figs. [1]-[10]). Recall that on the MPDGs the lines with zero residual entropy are marked with a dashed line.

At the boundaries \(C_{A2} - C_{A5}, C_{F1} - C_{A2}, C_{F1} - C_{A4}, C_{F1} - C_{A31}\), the residual entropy and residual magnetization are, respectively,

\[
S^o_{A2 - A5} = 0, \quad M^o_{A2 - A5} = 1/10, \quad (47)
\]

\[
S^o_{F1 - A2} = 0, \quad M^o_{F1 - A2} = 1/2, \quad (48)
\]

\[
S^o_{F1 - A4} = 0, \quad M^o_{F1 - A4} = 1/2, \quad (49)
\]

\[
S^o_{F1 - A31} = 0, \quad M^o_{F1 - A31} = 2/3 \quad (50)
\]

(blue dashed lines on the MPDGs, Figs. [1]-[10].

Next, we consider the remaining cases where the residual entropy of the spin system is greater than zero. (Such states on the MPDGs are marked with red solid lines, and phase points are marked with red round dots.)

1) At the boundary of the regions of spin configurations \(C_{A2} - C_{A31}\) and at the triple point \(C_{F1} - C_{A2} - C_{A31}\) (see, for example, Fig. [1]), the residual entropy is

\[
S^o = \ln \left[ \frac{1}{3} \left( \theta_1 + \frac{4}{D_1 \zeta_1} \right) \right] \approx 0.2811996, \quad (51)
\]

where the value of \(\theta_1\) is the same as in the case (37), and the residual magnetization is

\[
M^o = \frac{1}{3} \left( 1 + \frac{4}{D_1 \zeta_1} \right) \approx 0.1770088,
\]

where

\[
\zeta_1 = \sqrt[3]{\frac{D_1 + 3 \sqrt{-3D_1}}{D_1^2}}.
\]

In this case, the expression for the residual magnetization is the principal solution to the equation

\[
- D_1 (y^3 - y^2) + 3^2 y - 1 = 0,
\]

where \(D_1 = -23\) is the discriminant of the equation (38).

Also, at the boundary of spin configurations \(C_{F1} - C_{A5}\) (see, for example, Fig. [2]), the residual entropy is (51), and the residual magnetization is

\[
M^o \approx 0.5049257.
\]

At the triple point \(C_{A2} - C_{A41} - C_{A5}\) (see Fig. [1]) the residual entropy is (51), and the residual magnetization is

\[
M^o \approx 0.2809997.
\]

At the intersections of spin configurations at points \(C_{A4} - C_{A5} - C_{A6}\) and \(C_{A4} - C_{A5} - (C_{A2} + C_{A6})\), the residual entropy is defined in (51), and the residual magnetization is zero,

\[
M^o = 0.
\]

2) At the triple point \(C_{F1} - C_{A31} - C_{A41}\) (see Fig. [1]), the residual entropy is

\[
S^o = \ln \left[ \frac{1}{3} \left( 1 + \theta_2 + \frac{1}{\theta_2} \right) \right] \approx 0.3822451, \quad (52)
\]

where \(\theta_2\) is defined in (40), and the residual magnetization is

\[
M^o = \frac{1}{3} \left( 1 + \theta_2 + \frac{4}{D_2 \theta_2} \right) \approx 0.6114920,
\]

where

\[
\zeta_2 = \sqrt[3]{4 - D_2 + 3 \sqrt{-3D_2}}.
\]

In this case, the expression for the residual magnetization is the principal solution to the equation

\[
- D_2 (y^3 - y^2) + 3^2 y - 1 = 0,
\]

where \(D_2 = -31\) is the discriminant of the equation (41).

Also at the triple point \(C_{A2} - C_{A31} - C_{A41}\) (see Fig. [1]) the residual entropy is (52), and the residual magnetization is

\[
M^o \approx 0.2730406.
\]

3) At the intersections of spin configurations at the points of the phase diagram \(C_{F1} - C_{A2} - C_{A31} - C_{A41}\) and \(C_{F1} - C_{A2} - C_{A31} - (C_{A41} - J_3) = 0\) (see Fig. [2]), the residual entropy is equal to the natural logarithm of the golden ratio,

\[
S^o = \ln \frac{1 + \sqrt{5}}{2} \approx 0.4812118,
\]

as in (42). In this case, the residual magnetization is equal to

\[
M^o = \frac{1}{\sqrt{2J_3}} \approx 0.4472136,
\]

where the expression for the residual magnetization is the principal solution of the equation

\[
D_3 y^2 - 1 = 0,
\]
where \( \mathcal{D}_3 = 5 \) is the discriminant of the equation (43).

4) At the boundaries of spin configurations \( C_{A31} - C_{A4} \), and at the triple point \( C_{F1} - C_{A31} - C_{A4} \) (see Figs. 1b or 2b), the residual entropy is

\[
S^o = \ln \left( -\psi_4 + \frac{1}{2} \sqrt{\frac{1}{\psi_4} - 4\psi_4^2} \right) \approx 0.199 460 6, \tag{53}
\]

where

\[
\psi_4 = \frac{1}{2} \sqrt{\frac{\theta_4 - 4}{\theta_4}}, \quad \theta_4 = \sqrt{\frac{31 + 3\sqrt{-3\mathcal{D}_4}}{2}}.
\]

That the sublogarithmic expression is the principal solution of the equation

\[
x^4 - x - 1 = 0,
\]

its discriminant is

\[
\mathcal{D}_4 = -(2^8 + 3^3) = -283.
\]

In this case, the residual magnetization is equal to

\[
M^o = -\xi_4 + \sqrt{\frac{3^2}{\mathcal{D}_4} - \xi_4^2} - \frac{2}{\mathcal{D}_4 \xi_4} \approx 0.159 319 6,
\]

where

\[
\xi_4 = \frac{1}{2} \sqrt{\frac{\xi_4 - 2^{10}}{\mathcal{D}_4} - 3^2}.
\]

\[
\xi_4 = \sqrt{\frac{3^{2} + \sqrt{-3\mathcal{D}_4}}{\mathcal{D}_4^2}}.
\]

Here, the expression for the residual magnetization is the principal solution of the equation

\[
-\mathcal{D}_4 x^4 - 2(3^2 y^2 - 2^2 y) - 1 = 0.
\]

Also, at the boundary of spin configurations \( C_{A31} - C_{A41} \) (see Fig. 1b), the residual entropy is also equal to (53), and the residual magnetization is

\[
M^o \approx 0.420 340 2.
\]

5) At the triple point \( C_{F1} - C_{A2} - C_{A41} \) (see Fig. 1b) the residual entropy is

\[
S^o = \ln \left( \frac{1}{4} - \psi_5 + \frac{1}{2} \sqrt{\frac{11}{4} + \frac{3}{8\psi_5} - 4\psi_5^2} \right) \approx 0.414 012 7, \tag{54}
\]

where

\[
\psi_5 = \frac{1}{2} \sqrt{\frac{11}{12} + \frac{1}{3} \left( \theta_5 - \frac{8}{\theta_5} \right)}.
\]

\[
\theta_5 = \sqrt{-2 - 3^4 + 3\sqrt{-3\mathcal{D}_5}}.
\]

The sublogarithmic expression is the principal solution of the equation

\[
x^4 - x^3 - x^2 + x - 1 = 0,
\]

its discriminant is

\[
\mathcal{D}_5 = -[3(2 + 3)^2 + 2^8] = -331.
\]

In this case, the residual magnetization is equal to

\[
M^o \approx 0.526 524 3.
\]

6) At the boundary of spin configurations \( C_{F1} - C_{A4} \) (\( J_3 = 0 \)) or at the triple point \( C_{F1} - C_{A4} - C_{A5} \) (see Fig. 2b), the residual entropy is

\[
S^o = \ln \left( \frac{1}{4} - \psi_6 + \frac{1}{2} \sqrt{\frac{3}{4} - \frac{1}{8\psi_6} - 4\psi_6^2} \right) \approx 0.322 284 6, \tag{55}
\]

where

\[
\psi_6 = \frac{1}{2} \sqrt{\frac{1}{4} + \frac{\theta_6 - 4}{\theta_6}}, \quad \theta_6 = \sqrt{\frac{3^3 - 3\sqrt{-3\mathcal{D}_6}}{2}}.
\]

The sublogarithmic expression is the principal solution of the equation

\[
x^4 - x^3 - 1 = 0,
\]

its discriminant is equal to

\[
\mathcal{D}_6 = -(2^8 + 3^3) = -283.
\]

In this case, the residual magnetization is equal to

\[
M^o \approx 0.396 650 6,
\]

where

\[
\xi_6 = \frac{1}{2} \sqrt{\frac{\xi_6 - 2^{10}}{\mathcal{D}_6} - 3^2}.
\]

\[
\xi_6 = \sqrt{\frac{2^{11} 3^2 + \sqrt{-3\mathcal{D}_6}}{\mathcal{D}_6^2}}.
\]

\[
\mathcal{D}_4 = -(2^8 + 3^3) = -283.
\]

Moreover, the expression for the residual magnetization is the principal solution of the following equation

\[
-\mathcal{D}_4 x^4 - 2(3^2 y^2 + 2^2 y) - 1 = 0.
\]

Also, at the boundary of spin configurations \( C_{F1} - C_{A41} \) (see Fig. 1b), the residual entropy is (55), and the residual magnetization is

\[
M^o \approx 0.698 325 3.
\]
7) At the boundary of spin configurations $C_{A2}–C_{A41}$ (see Figs. 1b, 3c, or 7c), the residual entropy is equal to the natural logarithm of the golden ratio square root,

$$S^\circ = \ln \sqrt{\frac{1 + \sqrt{5}}{2}} \approx 0.2406059,$$

where the sublogarithmic expression is the principal solution of the equation

$$x^4 - x^2 - 1 = 0.$$

And the residual magnetization is equal to

$$M^\circ \approx 0.2763932.$$

8) At the boundary of spin configurations $C_{A41}–C_{A5}$ (see Fig. 1b), the residual entropy is equal to

$$S^\circ = \ln \psi_8 \approx 0.1546968,$$

where the sublogarithmic expression is the principal solution of the equation

$$x^5 - x - 1 = 0.$$

In this case, the residual magnetization is equal to

$$M^\circ \approx 0.3448685.$$

Also at the boundary of spin configurations $C_{A4}–C_{A5}$ and at the triple point $C_{A2}–C_{A4}–C_{A5}$ (see Fig. 1b), the residual entropy is equal to \( \text{(56)} \), and the residual magnetization is

$$M^\circ \approx 0.1034210.$$

9) At the boundary of spin configurations $C_{A31}–C_{A44}–C_{A41}–C_{A5}$, and at the point $C_{A31}–C_{A4}–C_{A41}–C_{A5}$ (see Fig. 1b), the residual entropy is

$$S^\circ = \ln \psi_9 \approx 0.3543820,$$

where the sublogarithmic expression is the principal solution of the equation

$$x^5 - x^2 - 2x - 1 = 0.$$

The residual magnetization is

$$M^\circ \approx 0.2614625.$$

10) At the boundaries of spin configurations $C_{A5}–C_{A6}$ or $C_{A2}–C_{A6}–C_{A5}$, and at the triple point $C_{A2}–C_{A5}–C_{A6}$ (see Figs. 1b or 7b), the residual entropy is

$$S^\circ = \ln \psi_{10} \approx 0.1263896,$$

where the sublogarithmic expression is the principal solution of the equation

$$x^6 - x - 1 = 0,$$

and the residual magnetization is

$$M^\circ \approx 0.0972041.$$

11) At the boundaries of spin configurations $C_{F1}–C_{A6}$ and $C_{F1}–C_{A2}–C_{A6}$, including the triple point $C_{F1}–C_{A2}–C_{A6}$ (see Figs. 2b or 10b), the residual entropy is

$$S^\circ = \ln \psi_{11} \approx 0.2509136,$$

where the sublogarithmic expression is the principal solution of the equation

$$x^6 - x^5 - 1 = 0,$$

and the residual magnetization is

$$M^\circ \approx 0.3688412.$$

12) At the triple point $C_{F1}–C_{A5}–C_{A6}$ (see Fig. 2b), the residual entropy is

$$S^\circ = \ln \psi_{12} \approx 0.3503982,$$

where the sublogarithmic expression is the principal solution of the equation

$$x^6 - x^5 - x - 1 = 0,$$

and the residual magnetization is

$$M^\circ \approx 0.3809168.$$

13) At the triple point $C_{A2}–C_{A31}–C_{A4}$ (see Fig. 1b), the residual entropy is

$$S^\circ = \ln \psi_{13} \approx 0.3373778,$$

where the sublogarithmic expression is the principal solution of the equation

$$x^6 - x^4 - x^3 - x^2 + 1 = 0,$$

and the residual magnetization is

$$M^\circ \approx 0.1544059.$$

14) At the points of the phase diagram $C_{A2}–C_{A31}–C_{A4}–C_{A41}–C_{A5}$ or $C_{A2}–C_{A4}–C_{A41}–(-C_{A31}–C_{A5})$ (see Figs. 1b, 3b, or 7b), the residual entropy is

$$S^\circ = \ln \psi_{14} \approx 0.4469977,$$

where the sublogarithmic expression is the principal solution of the equation

$$x^6 - x^5 - x^3 - x^2 + 1 = 0,$$

and the residual magnetization is

$$M^\circ \approx 0.2389829.$$
FIG. 12. Entropy (a) and magnetization (b) of the ground state of the Ising chain in an external magnetic field, taking into account the interaction of spins at the sites of the first, second, and third neighbors with antiferromagnetic interaction of nearest neighbors \((J_1 = -1)\) and antiferromagnetic interaction of third neighbors \((J_3 = -1/5)\). Red rhombic dots indicate the values of the functions at the boundaries of the spin configurations.

FIG. 13. Magnetization of the ground state of the Ising chain in an external magnetic field, taking into account the exchange interaction of spins at the sites of the first, second, and third neighbors with antiferro-/antiferro-/antiferromagnetic exchange interactions, where \(J_1 = -1, J_3 = -1/5, J_2 = -1\) (red line 1), \(J_2 = -3/5\) (green line 2), and \(J_2 = -1/10\) (blue line 3). Rhombic dots mark frustration magnetization points.

FIG. 14. Entropy (a) and magnetization (b) of the ground state of the Ising chain in an external magnetic field, taking into account the interaction of spins at the sites of the first, second, and third neighbors with antiferromagnetic interaction of nearest neighbors \((J_1 = -1)\) and antiferromagnetic interaction of the second neighbors \((J_2 = -1)\). Red rhombic dots indicate the values of the functions at the boundaries of the spin configurations.

FIG. 15. Magnetization of the ground state of the Ising chain in an external magnetic field, taking into account the exchange interaction of spins at the sites of the first, second, and third neighbors with anti-ferro/anti-ferro/anti-ferromagnetic exchange interactions, where \(J_1 = -1, J_2 = -1, J_3 = -1\) (red line 1), \(J_3 = -3/5\) (green line 2), and \(J_3 = -1/5\) (blue line 3). Rhombic dots mark frustration magnetization points.
As an illustration, consider several examples of the behavior of the residual entropy and residual magnetization in Figs. 12 and 14, which correspond to the phase diagrams shown in Figs. 13 and 15.

In Figs. 13 and 15, the field dependences of residual magnetization are shown for several ratios of the values of exchange interactions presented in Figs. 12 and 14.

In this case, note that in Fig. 15 (line 1) in the case of antiferro-antiferro-antiferromagnetic exchange interaction in the spin chain, a non-trivial behavior of the spin system arises when a non-zero magnetization in the ground state is retained at $H = 0$.

It should be noted that at zero temperature ($T = 0$) in the presence of an external magnetic field ($H > 0$), the other thermodynamic functions of the spin system, such as the residual heat capacity $C^\circ$, for any model parameters, is always equal to zero,

$$C^\circ = 0.$$  

The residual magnetic susceptibility $\chi^\circ$ of the system beyond the boundaries of spin configurations and at the boundaries $C_{A2} = C_{A4}$ and $C_{A2} = C_{A6}$ (marked with green dashed lines on the MPDGS) is zero,

$$\chi^\circ = 0,$$

at the boundaries of spin configurations $C_{A2} = C_{A5}$, $C_{F1} = C_{A2}$, $C_{F1} = C_{A4}$, $C_{F1} = C_{A3}$ (marked with blue dashed lines on the MPDGS) has values in the interval

$$0 < \chi^\circ < \infty,$$

and in the case of frustrated states, the residual magnetic susceptibility is equal to infinity,

$$\chi^\circ = \infty.$$

This situation is of a special interest, which should be considered in the next following paper.

In the end, it should be noted that the Ising paramagnet in the absence of all exchange interactions of spins between neighbors ($J_i = 0$) in an external magnetic field ($H > 0$) in the ground state ($T = 0$) is characterized by only one configuration $C_{F1}$, in which the chain spins are oriented along the direction of an external magnetic field. Therefore, the residual entropy and residual magnetization of the system are respectively equal to

$$S^\circ = 0, \quad M^\circ = 1.$$

There are no relevant frustrated states in the considered range of model parameters.

**VI. CONCLUSIONS**

In this paper, the precise analytical expressions for the entropy, heat capacity, magnetization, and magnetic susceptibility of the one-dimensional Ising model in an external magnetic field, taking into account the exchange interactions of atomic spins at the sites of the first, second, and third neighbors are obtained by the Kramers–Wannier transfer-matrix method. The analysis of the configuration features of the ground state, the description of the boundaries of the transitions of spin configurations and the frustrating properties of the spin system under study are carried out: a complete magnetic phase diagram of the ground state model is constructed.

The criteria are formulated and the relations of the model parameters at which magnetic frustrations occur in the considered one-dimensional spin systems are determined. It was found out that frustrations are caused by competition between the energies of the exchange interactions of spins and an external magnetic field. Thus, it is shown that in the frustration regime, the system undergoes a rearrangement of the structure of the magnetic ordering in the ground state, which begins to include a set of spin configurations comparable to the size of the system, including those without any translational invariance.

The behavior of entropy, magnetization, heat capacity, and magnetic susceptibility in the ground state of the system is analyzed.

A cardinal difference in the behavior of the entropy in the ground state of the magnetic system in the frustration region and beyond it is shown. It is determined that the most important attribute of the existence of magnetic frustrations in the system is the non-zero value of the zero-temperature entropy in this regime, and that this property does not contradict the third law of thermodynamics.

The values of entropy and magnetization for all configurations of the ground state of the spin system depending on the values of the model parameters are calculated. The features of the behavior of the heat capacity and magnetic susceptibility of the system at zero temperature are considered.

The paper also compares the behavior of the entropy, magnetization, and magnetic susceptibility of the system at zero temperature with the magnetic phase diagram of the ground state.

It is found that the entropy, magnetization, and magnetic susceptibility of the ground state exhibit several types of behavior at the boundaries of spin configurations, depending on the presence or absence of frustrations in the spin system.

It is also noted that at a certain ratio of the antiferro-antiferro-antiferromagnetic parameters of the exchange interactions of the model, the spin system can have a non-zero magnetization in the absence of a field and at zero temperature.

As a special example, it is demonstrated that an Ising paramagnetic, which in the absence of an external magnetic field is an absolutely frustrated system, since its entropy is nonzero and does not depend on temperature.

Thus, the proposed analysis scheme allows us to consider a wide range of phenomena in one-dimensional (or quasi-one-dimensional) magnetic systems with frustrations and describe their relationship with the peculiar features of thermodynamic functions. The mathematical apparatus developed in the present paper makes it possible to solve similar problems in more complicated models of statistical physics, in partic-
ular, in multicomponent spin models with discrete symmetry and arbitrary spin value.

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[1] F. A. Kassan-Ogly and B. N. Filippov, Bull. Russ. Acad. Sci. Phys. 74, 1452 (2010).
[2] H. T. Diep, ed., Frustrated spin systems, 3rd ed. (World Scientific, Singapore, 2020).
[3] C. Lacroix, P. Mendels, and F. Mila, eds., Introduction to frustrated magnetism: Materials, experiments, theory (Springer, Berlin, Heidelberg, 2011).
[4] J.-F. Sadoc and R. Moessner, Geometrical frustration (Cambridge University Press, New York, 1999).
[5] Y. B. Kudasov, A. S. Korshunov, V. N. Pavlov, and D. A. Maslov, Phys. Usp. 55, 1169 (2012).
[6] A. N. Vasiliev, O. S. Volkova, E. A. Zvereva, and M. M. Markina, Low dimensional magnetism (Fizmatlit, Moscow, 2018).
[7] M. Voyta, Rep. Prog. Phys. 81, 064501 (2018).
[8] L. Balents, Nature 464, 199 (2010).
[9] C. Balz, B. Lake, J. Reuther, H. Luetkens, R. Schönemann, T. Herrmannsdörfer, Y. Singh, A. T. M. Nazmul Islam, E. M. Wheeler, J. Rodriguez-Rivera, T. Guidi, G. Simeoni, C. Baines, and H. Ryll, Nature Physics 12, 942 (2016).
[10] C. Broholm, R. J. Cava, S. A. Kivelson, D. G. Nocera, M. R. Norman, and T. Senthil, Science 367, eaay0668 (2020).
[11] A. A. Zvyagin, Low Temp. Phys. 39, 901 (2013).
[12] T. Lookman and X. Ren, eds., Frustrated materials and ferroic glasses (Springer, Cham, 2018).
[13] O. A. Starykh, Rep. Prog. Phys. 78, 052502 (2015).
[14] G. Toulouse, Commun. Phys. 2, 115 (1977).
[15] J. Vannimenus and G. Toulouse, J. Phys. C: Solid State Phys. 10, L537 (1977).
[16] E. Ising, Z. Physik 31, 253 (1925).
[17] S. G. Brush, Rev. Mod. Phys. 39, 883 (1967).
[18] M. Niss, Arch. Hist. Exact Sci. 59, 267 (2005).
[19] W. P. Wolf, Braz. J. Phys. 30, 794 (2000).
[20] C. Binek, Ising-type antiferromagnets (Springer, Berlin, Heidelberg, 2003).
[21] R. J. Baxter, Exactly solved models in statistical mechanics (Academic Press, London, 1982).
[22] A. V. Zarubin, F. A. Kassan-Ogly, and A. I. Proshkin, J. Magn. Magn. Mater. 514, 167144 (2020).
[23] H. A. Kramers and G. H. Wannier, Phys. Rev. 60, 252 (1941).
[24] T. Oguchi, J. Phys. Soc. Jpn. 20, 2236 (1965).
[25] A. V. Zarubin, F. A. Kassan-Ogly, A. I. Proshkin, and A. E. Shestakov, J. Exp. Theor. Phys. 128, 778 (2019).
[26] R. A. Horne and C. R. Johnson, Matrix analysis, 2nd ed. (Cambridge University Press, Cambridge, 2013).
[27] C. Domb, Adv. Phys. 9, 149 (1960).
[28] W. Nolting and A. Ramakamth, Quantum theory of magnetism (Springer, Berlin, Heidelberg, 2009).
[29] S. Katsura and A. Narita, Progr. Theor. Phys. 50, 1750 (1973).
[30] Y. Murakoa, M. Kanemaru, and T. Idogaki, J. Magn. Magn. Mater. 177-181, 773 (1998).
[31] M. E. Fisher and W. Selke, Phys. Rev. Lett. 44, 1502 (1980).
[32] M. E. Fisher and W. Selke, Phil. Trans. R. Soc. A 302, 1 (1981).
[33] W. Selke, M. Barreto, and J. Yeomans, J. Phys. C: Solid State Phys. 18, L393 (1985).
[34] W. Selke, Phys. Reports 170, 213 (1988).
[35] J. Yeomans, The theory and application of axial Ising models, in Solid state physics Vol. 41, edited by H. Ehrenreich and D. Turnbull (Academic Press, San Diego, 1988) pp. 151–200.
[36] A. V. Zarubin, F. A. Kassan-Ogly, and A. I. Proshkin, J. Phys.: Conf. Ser. 1389, 012009 (2019).
[37] V. L. Pokrovskii and G. V. Uimin, Sov. Phys. JETP 55, 950 (1982).
[38] M. Barreto and J. Yeomans, Physica A 134, 84 (1985).
[39] J. Yeomans, The application of axial Ising models to the description of modulated order, in Incommensurate crystals, liquid crystals, and quasi-crystals edited by J. F. Scott and N. A. Clark (Plenum Press, New York, 1987).
[40] A. Sommerfeld, Thermodynamics and statistical mechanics (Academic Press, New York, 1956).
[41] W. Nolting, Theoretical physics 8: Statistical physics (Springer, Cham, 2018).