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Energy levels and their degeneracies for two-ring Ising chains of spins-$\frac{1}{2}$ with NN and NNN couplings: spin frustration of ferromagnetic and antiferromagnetic orders

H. Fakhri[a], **S. B. Seyedein Ardebili**[b]

Department of Theoretical Physics and Astrophysics, Faculty of Physics, University of Tabriz, P. O. Box 51666-16471, Tabriz, Iran

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Abstract In an Ising linear chain of spins-$\frac{1}{2}$ with the periodic conditions in NN and NNN interactions as a two-ring structure of two different coupling constants, all or half spins contribute to the NNN couplings, depending on whether the total number of spins is odd or even. In this article, we formulate precise predictions on the values, degeneracy factors, and the number of allowed energy levels for the two-ring Ising chains with any arbitrary number of spins in two different forms for odd and even number of spins. We confirm the validity of our formulations firstly by comparing them with the data obtained from the manual search for small finite-size two-ring Ising chains. Secondly, the validity of the formulations is verified by comparing the obtained partition functions by energy levels with the other forms obtained from the change of variable method. We study analytically the ground levels and show that they exhibit the maximal spin frustration when the ferromagnetic and antiferromagnetic orders are demanded via the NN and NNN coupling constants, respectively. Finally, we show that the low-temperature behavior of the entropy and specific heat capacity per spin in the maximally frustrated regime matches with the analytical results.

1 Introduction

In statistical mechanics, a key step to calculate the thermodynamics properties of a system in thermal equilibrium is evaluating the partition function, which is a sum of Boltzmann factors over energy levels of the model by including the degeneracy of each energy level. Every allowed energy level of a classical Ising chain specifies one or more microstates by one or more spin configurations. Studies on the values, degeneracy factors, and the number of allowed energy levels for Ising chains are of great importance; therefore, it has been considered by several authors. In quantum statistical mechanics, this can be a much more difficult issue to address, especially when Ising, Heisenberg and Heisenberg-Ising models in different dimensions and lattices are considered. For this, many authors have to investigate the

[a] e-mail: hfakhri@tabrizu.ac.ir (corresponding author)

[b] e-mail: b.seyedein@tabrizu.ac.ir

ground state energy of statistical systems in detail and discuss thermodynamics properties at low temperatures. This is justified because the dominant contribution to the partition function arises from the ground state, as the system is not gapless. For example, in Ref. [1], upper and lower bounds have been considered for the ground-state energy of the rectangular one-, two-, and three-dimensional lattices of the Heisenberg-Ising type with anisotropic couplings between nearest neighbors (NNs). The authors have also shown that the ground-state energy per NN pair is not decreased by increasing the dimension of the lattice. In Ref. [2], spin configurations have been considered for the ground state of an Ising model on a flat triangular lattice with the competing interactions between spins at the nearest and next-nearest neighbors (NNNs) as well as a coupling between three spins at the vertices of a NN triangle, and an external magnetic field. In Ref. [3], analytical expressions for the eigenvalues and eigenstates of the Ising Hamiltonians in one-, two- and three-dimensional lattices of arbitrary size have been derived in the absence of an external magnetic field using unitary transformations and combinatorics. The authors have used transfer matrix properties of which the models can include a magnetic field along the z-axis and generalize to a higher number of spin components on each site. The accurate determination of the energy levels and their degeneracy factors in the Ising chains with arbitrary sizes may be very complex, even from the viewpoint of classical statistical mechanics. However, so many attempts have been made to study the spectra of Ising chains, especially on the ground energies. For example, in Ref. [4], the author has studied the degeneracy of the ground state for an open finite one-dimensional chain of Ising spins-$\frac{1}{2}$ with the ferromagnetic and antiferromagnetic competing interactions for nearest neighbors and kth neighbors, respectively. He has shown that when the magnitude of the ratio of the first coupling constant to the second one is k, the ground state is highly degenerate with the residual entropy per spin. The existence of the ferromagnetic and antiferromagnetic competing interactions in a chain causes all interactions not to be satisfied simultaneously [5–7]. In this case, there is no way to simultaneously satisfy all interactions and, consequently, the total energy of the chain cannot be minimized by minimizing all the spin–spin interactions simultaneously. In other words, the ground-state becomes highly degenerate, and some spins behave as free spins. Such a model is generally known in the literature as a frustrated model, and the present paper aims to investigate spin frustration by analyzing energy levels for a two-ring Ising chain with the NN and NNN coupling constants. Some other relevant studies of both classical and quantum-mechanical viewpoints can be mentioned through Refs. [8–16].

The authors believe that many issues of analysis and optimization of complex systems in the various fields such as biology, wireless communication, artificial intelligence can be modeled with binary variables and mapped on the basic state of the Ising model. In these papers, different Ising machines have been designated for finding the exact solutions to a variety of hard instances Ising problems. In this regard, a physical system called the coherent Ising machine was designed to calculate the ground states of the Ising-like networks [17–21]. This machine is based on a network of optical oscillators proposed for the Ising problem with specific values of coupling. It calculates the basic states of similar Ising networks and provides relatively accurate or approximate solutions with high accuracy to various Ising problems with more than 100 spins with 10,000 spin-spin connections [22]. For example, in paper [23], the authors simulated a 16-bit coherent Ising machine based on semi-classical models. The 2000-bit system has also been studied in Ref [24]. The significance of this model also has been mentioned in its applications for describing different 1D and quasi-1D systems of various materials, such as a ferroelectric system composed of Ca_3CoMnO_6-type chains [25]. In the paper, the magneto-electric coupling of a material using the transfer matrix method was investigated, and the consistency of the results with experience was confirmed. The work was done in the absence of a magnetic field, and the interactions of NN and NNN were considered. The ferroelectric properties of $Ca_3Co_{2-x}Mn_xO_6$, as an Ising chain magnet, have been studied theoretically and experimentally in the works such as [24,26]. Ising chain also has been found some applications in genetics [23]. In this work, a linear 1D Ising model was studied, and the NN interactions were simulated. The results were comparable to complex genetic algorithms. Ref. [27] is one of the papers in which the conformity of theory with experience was well demonstrated, and the authors have proposed a theoretical approach to obtain magnetic properties and simulate magnetic fields in single-ring magnetic compounds based on spin-Ising rings with a limited number.

Analytical methods have been very useful in evaluating the statistical properties of classical Ising chains incisively. It must be emphasized that the two-ring Ising chains are very well-known in the literature under different names, e.g., ANNNI chain, two-leg ladder, zigzag ladder, sawtooth chain, delta chain, decorated chain, and so on. Without the knowledge of energy levels and their degeneracy factors, they have been comprehensively studied from different perspectives—exact solutions through the change of variable method and transfer-matrix approach, decoration-iteration transformation, disorder solution, ground-state analysis, frustration, etc. (see, for example, Refs. [28–36]). In a recent work [37], by using the Hubbard–Stratonovich transformation without analyzing the energy levels and their degeneracy factors, the author has obtained an exact solution for the partition function of the Ising model with an arbitrary number of spin-$\frac{1}{2}$ sites and with a nonsingular coupling coefficients matrix, whether there is a nonzero external field or not. This partition function is transformed to Kramers–Wannier and Onsager solutions when the Ising model is considered as the z-components of spins localized at the 1- and 2-dimensional lattice sites, respectively. We have analyzed exactly all energy levels and the degeneracy factors for the two Ising models that are the special cases of [37] and then obtained their partition functions, which are in agreement with the above-mentioned reference. The cyclic chains of even- and odd-site spins-$\frac{1}{2}$ with the NN and NNN interactions have necessarily three- and two-ring structures, respectively. It is expected that their behaviors will not be different from each other in the thermodynamic limit. In Ref. [38], the contributions of all spin-$\frac{1}{2}$ sites in the NN and NNN interactions have been studied in the thermodynamic limit when the total number of spins is even. The authors of the latter mentioned reference have used the partition function and analyzed the specific heat capacity per spin in the thermodynamic limit to explain the close competition between ferromagnetic NN and antiferromagnetic NNN interactions for when the value of spin frustration parameter is $\frac{1}{2}$. This is in agreement with our analytical findings for the ground energy levels in this work, the finite-size Ising chains of odd-site spins-$\frac{1}{2}$ with the NN and NNN interactions demonstrate the maximal frustration not only for the value $\frac{1}{2}$ but also for the value 1 of spin frustration parameter, which covers automatically the thermodynamic limit mentioned in the above.

In Refs. [39,40] we have utilized the change of variable method to obtain the exact expressions for the partition functions of the two- and three-ring Ising chains formed by the NN and NNN coupling constants with an arbitrary number of spins-$\frac{1}{2}$ in the absence of an external magnetic field. In Ref. [40], we have formulated the allowed energy levels and their degeneracy factors by aggregating data for small sizes of three-ring Ising chains. Then, the standard energy-based method has been used to calculate the partition function of a three-ring Ising chain with an arbitrary even number of spins-$\frac{1}{2}$, in addition to the method mentioned above. Finally, the validity of our formulation has been justified by comparing partition functions obtained from both methods. Now, the present article, in Sect. 2, formulates the values, degeneracy factors, and the number of the allowed energy levels for the two-ring Ising chains introduced in Ref. [39]. Our analytical considerations in Sect. 3 confirm that the ground levels demonstrate the maximal spin frustration via a competition between ferromagnetic NN and antiferromagnetic NNN couplings in both two-ring Ising chains with any arbitrary (odd and even) number of spins-$\frac{1}{2}$. We show that the ground levels of the two-ring chains with the odd and even number of spins-$\frac{1}{2}$ display the maximal frustration for both values $\frac{1}{2}$ and 1, and only value 1 of the spin frustration parameter, respectively. Section 4 is devoted to considering the low-temperature behavior of entropy and specific heat capacity per spin in the maximally frustrated regime. Finally, Sect. 5 is devoted to summarizing the results of this article.

2 The values, degeneracy factors and number of allowed energy levels for the two-ring Ising chains

For a two-ring Ising spin-$\frac{1}{2}$ chain with NN and NNN interactions, all and half spins contribute to the second ones depending on whether the number of spins is odd or even, respectively. Therefore, we will deal with two different types of formulation for the Hamiltonian and consequently two distinct formulations for the energy spectrum with the odd and even number of spins in the chain. Firstly, we are going to consider our ansatz on the formulation of the energy spectrum for a two-ring Ising spin-$\frac{1}{2}$ chain with the odd number of sites.

Remark 1 Let p be an integer number greater than or equal to 2. As illustrated in Fig. 1, consider $2p+1$ Ising spins $S_1, S_2, \cdots, S_{2p+1}$ ($\equiv \pm 1$) on a one-dimensional two-ring chain in which all spins contribute to the interaction with their NNs and NNNs via different coupling constants J and K, respectively. Hamiltonian for the chain in Fig. 1 is

$$H_{J,K}^{2p+1} = -J \sum_{i=1}^{2p+1} S_i S_{i+1} - K \left(\sum_{i=0}^{p} S_{2i+1} S_{2i+3} + \sum_{i=1}^{p} S_{2i} S_{2i+2} \right), \tag{1}$$

with the periodic boundary conditions $S_{2p+2} \equiv S_1$ and $S_{2p+3} \equiv S_2$. Let (m, n) be an ordered pair of nonnegative integer numbers defined by $n = 0$ for $m = 0$ as well as $n = \left[\frac{m+1}{2}\right], \left[\frac{m+1}{2}\right]+1, \left[\frac{m+1}{2}\right]+2, \cdots, p - \left[\frac{m}{2}\right]$ for $m = 1, 2, 3, \cdots, p$, where the symbol [.] denotes the integer part. Then, the allowed energy levels of the Hamiltonian (1) are

$$E_{m,n}^{2p+1}(J, K) = (4n - 2p - 1)\, J + (4m - 2p - 1)\, K. \tag{2}$$

Fig. 1 Plot of the two-ring Ising chain with the NN and NNN coupling constants J and K for the spins $S_1, S_2, \cdots, S_{2p+1}$

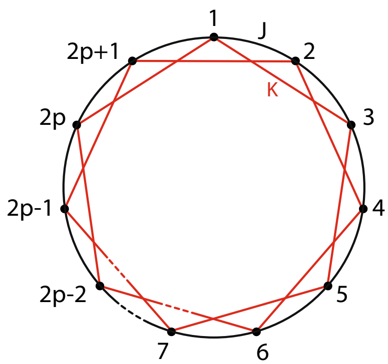


Table 1 The values, degeneracy factors and number of allowed energy levels for the two-ring Ising chains $p = 2, 3, 4, 5$ of Remark 1

$p = 2$, $N^5 = 4$

m	n	$E^5_{m,n}$	$g^5_{m,n}$
0	0	$-5J-5K$	2
1	1	$-J-K$	10
	2	$3J-K$	10
2	1	$-J+3K$	10

$p = 3$, $N^7 = 7$

m	n	$E^7_{m,n}$	$g^7_{m,n}$
0	0	$-7J-7K$	2
1	1	$-3J-3K$	14
	2	$J-3K$	14
	3	$5J-3K$	14
2	1	$-3J+K$	28
	2	$J+K$	42
3	2	$J+5K$	14

$p = 4$, $N^9 = 11$

m	n	$E^9_{m,n}$	$g^9_{m,n}$
0	0	$-9J-9K$	2
1	1	$-5J-5K$	18
	2	$-J-5K$	18
	3	$-3J-5K$	18
	4	$-7J-5K$	18
2	1	$-5J-K$	54
	2	$-J-K$	108
	3	$3J-K$	90
3	2	$-J+3K$	108
	3	$3J+3K$	60
4	2	$-J+7K$	18

$p = 5$, $N^{11} = 16$

m	n	$E^{11}_{m,n}$	$g^{11}_{m,n}$
0	0	$-11J-11K$	2
1	1	$-7J-7K$	22
	2	$-3J-7K$	22
	3	$J-7K$	22
	4	$5J-7K$	22
	5	$9J-7K$	22
2	1	$7J-3K$	88
	2	$-3J-3K$	198
	3	$J-3K$	220
	4	$5J-3K$	154
3	2	$-3J+K$	330
	3	$J+K$	440
	4	$5J+K$	154
4	2	$-3J+5K$	110
	3	$J+5K$	220
5	3	$J+9K$	22

If we denote the degeneracy factor of the energy $E^{2p+1}_{m,n}$ as $g^{2p+1}_{m,n}$, then we have

$$g^{2p+1}_{0,0} = 2, \; g^{2p+1}_{m,n} = \frac{2(2p+1)}{m} C^{2n-1}_{m-1} C^{2p-2n}_{m-1}. \tag{3}$$

The symbol C: stands for the binomial coefficient. The total number of microstates accessible to the two-ring chain in Fig. 1 is estimated by summation of all possible degeneracy configurations:

$$\begin{aligned} 2^{2p+1} &= g^{2p+1}_{0,0} + \sum_{m=1}^{p} \sum_{n=\left[\frac{m+1}{2}\right]}^{p-\left[\frac{m}{2}\right]} g^{2p+1}_{m,n} \\ &= 2 + 2\sum_{m=1}^{p} \sum_{n=\left[\frac{m+1}{2}\right]}^{p-\left[\frac{m}{2}\right]} \frac{2p+1}{m} C^{2n-1}_{m-1} C^{2p-2n}_{m-1}. \end{aligned} \tag{4}$$

Moreover, the number of allowed distinct values for energy is given by

$$N^{2p+1} = 1 + \frac{1}{2} p(p+1). \tag{5}$$

We introduce two different pieces of evidence in order to confirm the correctness of Remark 1. Firstly, its accuracy can be verified numerically as below. We can directly obtain the values, degeneracy factors and number of allowed energy levels for $p = 2, 3, 4, 5$ as shown in Table 1 by setting spin variables $S_1, S_2, \cdots, S_{2p+1}$ to the values $+1$ and -1 in all different possible ways. For example, the given information in the first column (from the left side) of Table 1 follows from all possible configurations, *up* and *down*, for spins S_1, S_2, S_3, S_4 and S_5 as shown in Table 2. The interaction energies given in this table are obtained by

Table 2 All possible configurations (*up* and *down*) for a two-ring Ising chain of spins S_1, S_2, S_3, S_4 and S_5 with the different exchange coupling constants J and K of NN and NNN interactions, respectively

$E^5_{0,0}=-5J-5K$					$E^5_{1,1}=-J-K$					$E^5_{2,1}=-J+3K$					$E^5_{1,2}=3J-K$				
S_1	S_2	S_3	S_4	S_5	S_1	S_2	S_3	S_4	S_5	S_1	S_2	S_3	S_4	S_5	S_1	S_2	S_3	S_4	S_5
↑	↑	↑	↑	↑	↑	↑	↑	↑	↓	↑	↑	↑	↓	↓	↑	↑	↓	↑	↓
↓	↓	↓	↓	↓	↑	↑	↑	↓	↑	↑	↑	↓	↓	↑	↑	↓	↑	↑	↓
					↑	↑	↓	↑	↑	↑	↓	↓	↑	↑	↑	↓	↑	↓	↑
					↑	↓	↑	↑	↑	↓	↓	↑	↑	↑	↓	↑	↑	↓	↑
					↓	↑	↑	↑	↑	↓	↑	↑	↑	↓	↓	↑	↓	↑	↑
					↑	↓	↓	↓	↓	↑	↑	↓	↓	↓	↑	↓	↑	↓	↓
					↓	↑	↓	↓	↓	↓	↑	↑	↓	↓	↑	↓	↓	↑	↓
					↓	↓	↑	↓	↓	↓	↓	↑	↑	↓	↓	↑	↓	↑	↓
					↓	↓	↓	↑	↓	↓	↓	↓	↑	↑	↓	↑	↓	↓	↑
					↓	↓	↓	↓	↑	↑	↓	↓	↓	↑	↓	↓	↑	↓	↑

setting the spin variables S_1, S_2, S_3, S_4 and S_5 of the Hamiltonian $H^5_{J,K}$ to the values $+1$ and -1 in all different possible ways. One can easily verify that the values, degeneracy factors and the number of allowed energy levels listed in Table 1 are in full compatibility with those found in Remark 1. Secondly, one can obtain the partition function $Z^{2p+1}_{J,K}$ exactly by using $E^{2p+1}_{m,n}$ and $g^{2p+1}_{m,n}$ of Remark 1 as follows

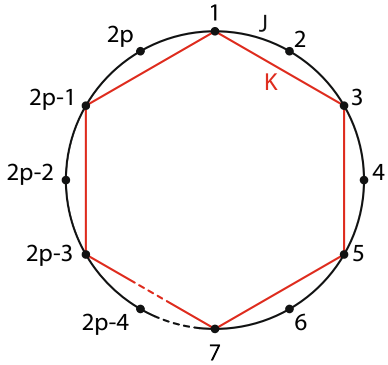
$$
\begin{aligned}
Z^{2p+1}_{J,K} &= g^{2p+1}_{0,0}\, e^{-\beta E^{2p+1}_{0,0}(J,K)} + \sum_{m=1}^{p} \sum_{n=\left[\frac{m+1}{2}\right]}^{p-\left[\frac{m}{2}\right]} g^{2p+1}_{m,n}\, e^{-\beta E^{2p+1}_{m,n}(J,K)} \\
&= 2e^{\beta(2p+1)(J+K)} \left(1 + \sum_{m=1}^{p} \sum_{n=\left[\frac{m+1}{2}\right]}^{p-\left[\frac{m}{2}\right]} \frac{2p+1}{m} C^{2n-1}_{m-1} C^{2p-2n}_{m-1} e^{-4\beta(nJ+mK)} \right),
\end{aligned}
\tag{6}
$$

in which $\beta = 1/k_B T$ and k_B denotes the Boltzmann's constant. This formula is confirmed when it is compared with the relation (1) of Ref. [39] for different values of p. This, in turn, certifies the validity of our formulation in Remark 1 for the spectrum of two-ring Ising chain drawn in Fig. 1.

Remark 2 (Decorated chain) Let p be an integer number greater than or equal to 3. Consider $2p$ Ising spins $S_1, S_2, \cdots, S_{2p}$ ($\equiv \pm 1$) on a one-dimensional chain in which NN spins are coupled to each other by the constant J. Furthermore, we suppose that NNN spins $S_1, S_3, \cdots, S_{2p-1}$ are coupled to each other by the exchange coupling constant K. It is also assumed that the Ising chain is cyclic in both NN and NNN interactions via the boundary condition $S_{2p+1} \equiv S_1$ as shown in Fig. 2. Hamiltonian for two-ring Ising chain described by Fig. 2 is

$$
H^{2p}_{J,K} = -J \sum_{i=1}^{2p} S_i S_{i+1} - K \sum_{i=1}^{p} S_{2i-1} S_{2i+1}. \tag{7}
$$

Fig. 2 Plot of the two-ring (decorated) Ising chain with the NN and NNN coupling constants J and K for the spins $S_1, S_2, \cdots, S_{2p}$ and $S_1, S_3, \cdots, S_{2p-1}$, respectively



Consider ordered pairs (m, n) of nonnegative integer numbers defined by $n = m, m+1, m+2, \cdots, p-m$ for $m = 0, 1, 2, \cdots, \left[\frac{p}{2}\right]$. In this way, the allowed energy levels of the Hamiltonian (7) are given by

$$E^{2p}_{m,n}(J, K) = (4n - 2p)\, J + (4m - p)\, K. \tag{8}$$

Then, the degeneracy factor $g^{2p}_{m,n}$ for the energy $E^{2p}_{m,n}$ is given by

$$g^{2p}_{m,n} = 2^{2m+1} C^{p}_{m+n} C^{m+n}_{2m}. \tag{9}$$

The total number of microstates accessible for the two-ring chain given in Fig. 2 is evaluated by summation of all possible degeneracy configurations:

$$\begin{aligned} 2^{2p} &= \sum_{m=0}^{\left[\frac{p}{2}\right]} \sum_{n=m}^{p-m} g^{2p}_{m,n} \\ &= \sum_{m=0}^{\left[\frac{p}{2}\right]} \sum_{n=m}^{p-m} 2^{2m+1} C^{p}_{m+n} C^{m+n}_{2m}. \end{aligned} \tag{10}$$

Also, the number of allowed values of energy for the decorated chain is given by

$$N^{2p} = \left(\left[\frac{p}{2}\right] + 1\right)\left(p - \left[\frac{p}{2}\right] + 1\right). \tag{11}$$

Again, our claims in Remark 2 about the values, degeneracy factors and the number of allowed energy levels for the decorated two-ring Ising chain given in Fig. 2 with the even number $2p$ of spins are verified by a direct calculation. For example, we have included the results in Table 3 for $p = 3, 4, 5, 6$, where one can match data with the formulation of Remark 2. Furthermore, the partition function $Z^{2p}_{J,K}$ corresponding to two-ring Ising chain of Fig. 2 is derived by using the values of $E^{2p}_{m,n}$ and $g^{2p}_{m,n}$ given in Remark 2 as follows

$$\begin{aligned} Z^{2p}_{J,K} &= \sum_{m=0}^{\left[\frac{p}{2}\right]} \sum_{n=m}^{p-m} g^{2p}_{m,n} e^{-\beta E^{2p}_{m,n}(J,K)} \\ &= e^{\beta p(2J+K)} \sum_{m=0}^{\left[\frac{p}{2}\right]} \sum_{n=m}^{p-m} 2^{2m+1} C^{p}_{m+n} C^{m+n}_{2m} e^{-4\beta(nJ+mK)}. \end{aligned} \tag{12}$$

Table 3 The values, degeneracy factors and number of allowed energy levels for the two-ring Ising chains $p = 3, 4, 5, 6$ of Remark 2

$\mathbf{p=3,\ N^6=6}$			
m	**n**	$\mathbf{E^6_{m,n}}$	$\mathbf{g^6_{m,n}}$
0	0	$-6J-3K$	2
	1	$-2J-3K$	6
	2	$2J-3K$	6
	3	$6J-3K$	2
1	1	$-2J+K$	24
	2	$2J+K$	24

$\mathbf{p=4,\ N^8=9}$			
m	**n**	$\mathbf{E^8_{m,n}}$	$\mathbf{g^8_{m,n}}$
0	0	$-8J-4K$	2
	1	$-4J-4K$	8
	2	$-4K$	12
	3	$4J-4K$	8
	4	$8J-4K$	2
1	1	$-4J$	48
	2	0	96
	3	$4J$	48
2	2	$4K$	32

$\mathbf{p=5,\ N^{10}=12}$			
m	**n**	$\mathbf{E^{10}_{m,n}}$	$\mathbf{g^{10}_{m,n}}$
0	0	$-10J-5K$	2
	1	$-6J-5K$	10
	2	$-2J-5K$	20
	3	$2J-5K$	20
	4	$6J-5K$	10
	5	$10J-5K$	2
1	1	$-6J-K$	80
	2	$-2J-K$	240
	3	$2J-K$	240
	4	$6J-K$	80
2	2	$-2J+3K$	160
	3	$2J+3K$	160

$\mathbf{p=6,\ N^{12}=16}$			
m	**n**	$\mathbf{E^{12}_{m,n}}$	$\mathbf{g^{12}_{m,n}}$
0	0	$-12J-6K$	2
	1	$-8J-6K$	12
	2	$-4J-6K$	30
	3	$-6K$	40
	4	$4J-6K$	30
	5	$8J-6K$	12
	6	$12J-6K$	2
1	1	$-8J-2K$	120
	2	$-4J-2K$	480
	3	$-2K$	720
	4	$4J-2K$	480
	5	$8J-2K$	120
2	2	$-4J+2K$	480
	3	$2K$	960
	4	$4J+2K$	480
3	3	$6K$	128

However, we previously obtained another form for the partition function $Z^{2p}_{J,K}$ in the relation (14) of Ref. [39] by the change of variable method. Finally, one can show that the above-mentioned two expressions for the partition function $Z^{2p}_{J,K}$ are equal when p is fixed to $p = 3, 4, 5, 6$, etc., which is another certification of the validity of Remark 2.

3 Spin frustration of ferromagnetic and antiferromagnetic orders

Let us set J and K equal to 1 and $-\alpha$, in both two-ring Ising chains discussed above, and use $\alpha > 0$ as a spin frustration parameter for when the ferromagnetic and antiferromagnetic interactions are carried out via the coupling constants J and K, respectively. This symbolization allows us to consider the spin frustration effect on each of the models, separately, as follows:

(a) *Analysis of spin frustration effect on the two-ring Ising chain of Fig. 1*: We show analytically that the maximal spin frustration in the ground states at the low temperatures occurs when the dimensionless parameter α takes both values $\frac{1}{2}$ and 1. First, we need to get the ground energies, which may sometimes depend on the evenness and oddness of p.

- Our considerations show that the inequality $2n \geq m$ holds by all pairs (m, n) of Remark 1, whether p is even or odd. If we demand that $E^{2p+1}_{0,0}(1, -\alpha)$ with the degeneracy factor 2 be the ground energy, then we obtain the inequality $m\alpha \leq n$ that must be satisfied by all pairs (m, n) belonging to $1 \leq m \leq p$ and $\left[\frac{m+1}{2}\right] \leq n \leq p - \left[\frac{m}{2}\right]$. By comparison with $2n \geq m$, we conclude that, for $\alpha \leq \frac{1}{2}$, the ground energy of the two-ring Ising spins-$\frac{1}{2}$ chain corresponding to Fig. 1 for every $p \geq 2$, whether even or odd, is $E^{2p+1}_{0,0}(1, -\alpha) = (2p + 1)(\alpha - 1)$.

- An immediate consequence of $2n \geq m$ is $(\frac{p}{2} - n)/(p - m) \leq \frac{1}{2}$ which, in turn, results that the ground energy of the two-ring Ising model in Fig. 1 with $p \geq 2$ as an even number is $E^{2p+1}_{p,\frac{p}{2}}(1, -\alpha) = -1 - (2p - 1)\alpha$ for $\alpha \geq \frac{1}{2}$, with the degeneracy factor $2(2p + 1)$.
- From Remark 1, for p as an arbitrary odd number, it becomes clear that $E^{2p+1}_{p-1,\frac{p-1}{2}}(1, -\alpha)$ will be the ground energy, provided that the inequality $\frac{p-1}{2} - n \leq (p - m - 1)\alpha$ is satisfied by α. The satisfaction of this inequality requires that α obeys $\alpha \geq \frac{1}{2}$ and $\alpha \leq 1$ for $0 \leq m \leq p - 3$ and $m = p$, respectively. Moreover, it leads to $\alpha \geq 0$ for $m = p - 2$ while no condition is applied for $m = p - 1$. Therefore, for every odd integer $p \geq 3$, $E^{2p+1}_{p-1,\frac{p-1}{2}}(1, -\alpha) = -3 - (2p - 5)\alpha$ with the degeneracy factor $\frac{1}{3}p(p + 1)(2p + 1)$ is the ground energy of the two-ring Ising chain corresponding to Fig. 1 in the region $\frac{1}{2} \leq \alpha \leq 1$.
- Here, we again assume that p is an odd integer number greater than or equal to 3. If we demand that $E^{2p+1}_{p,\frac{p+1}{2}}(1, -\alpha)$ be the ground energy, we get $\alpha \geq (p + 1)/2p$ and $\frac{p+1}{2} - n \leq (p - m)\alpha$. These inequalities are satisfied by all pairs (m, n) of Remark 1 if inequality $\alpha \geq 1$ is satisfied. Therefore, $E^{2p+1}_{p,\frac{p+1}{2}}(1, -\alpha) = 1 - (2p - 1)\alpha$ is the ground energy for $\alpha \geq 1$ with the degeneracy factor $2(2p + 1)$.

Now, we are in an appropriate position to consider the maximal spin frustration effect for the values $\alpha = \frac{1}{2}$ and $\alpha = 1$:

- **Maximal frustration at $\alpha = \frac{1}{2}$ for even values of p**: For an even $p \geq 2$, the two-ring Ising chain in Fig. 1 takes the energy $-p - \frac{1}{2}$ via two ground levels $E^{2p+1}_{0,0}(1, -\frac{1}{2})$ and $E^{2p+1}_{p,\frac{p}{2}}(1, -\frac{1}{2})$ with the degeneracy factors 2 and $2(2p + 1)$, respectively. The sum of the degeneracy factors at $\alpha = \frac{1}{2}$ is $4(p + 1)$ which is increasing linearly with p and describes itself a type of frustration rate. This, in turn, implies that the chain becomes more frustrated at $\alpha = \frac{1}{2}$ when p is increased.
- **Maximal frustration at $\alpha = \frac{1}{2}$ for odd values of p**: Again, the two ground levels $E^{2p+1}_{0,0}(1, -\frac{1}{2})$ and $E^{2p+1}_{p-1,\frac{p-1}{2}}(1, -\frac{1}{2})$ with the degeneracy factors 2 and $\frac{1}{3}p(p+1)(2p+1)$, respectively, take the same energy, named $-p - \frac{1}{2}$, for an odd $p \geq 3$ in the chain of Fig. 1. Despite the previous case, the sum of the degeneracy factors at $\alpha = \frac{1}{2}$ is a cubic power of p which, in turn, means stronger frustrations for higher values of p.
- **Maximal frustration at $\alpha = 1$ for odd values of p**: For an odd $p \geq 3$, the two-ring Ising chain in Fig. 1 takes the energy $2 - 2p$ via two ground levels $E^{2p+1}_{p-1,\frac{p-1}{2}}(1, -\frac{1}{2})$ and $E^{2p+1}_{p,\frac{p+1}{2}}(1, -\frac{1}{2})$ with the degeneracy factors $\frac{1}{3}p(p + 1)(2p + 1)$ and $2(2p + 1)$, respectively. Therefore, there exists very stronger frustrations due to the fact that the sum of the degeneracy factors not only is a cubic power of p but also is greater than the previous case by $4p$.

(b) *Analysis of spin frustration effect on the two-ring Ising chain of Fig.* 2: We first obtain the ground-state energies as a function of the frustration parameter α and then show that the maximal frustration occurs when it takes the value 1. Indeed, the classical ground energies of the decorated Ising chain are determined depending upon which of the inequalities $\alpha \leq 1$ or $\alpha \geq 1$ is satisfied by the frustration parameter. Again, for $\alpha \geq 1$, the ground level has two different forms in terms of the parameters p and α, depending on whether p is even or odd.

- An immediate result from Remark 2 is $0 \leq m \leq \left[\frac{p}{2}\right]$ and $m \leq n \leq p - m$. On the other hand, in order to have a minimum value for energy via $E^{2p}_{0,0}(1, -\alpha)$ with the degeneracy factors 2, the inequality $n \geq m\alpha$ must be satisfied by all pairs (m, n) of Remark 2. The last inequality for $n = m = 0$ is fulfilled without imposing any restrictions on α. Otherwise, the condition expression $\alpha \leq \frac{n}{m}$ is evaluated. From this, together with $n \geq m$, we deduce that $\alpha \leq 1$. Therefore, for every $p \geq 2$, whether even or odd, the ground energy of the two-ring Ising spins-$\frac{1}{2}$ chain in Fig. 2 is $E^{2p}_{0,0}(1, -\alpha) = p(\alpha - 2)$ in the case of $\alpha \leq 1$.
- Clearly, if we demand that $E^{2p}_{\frac{p}{2},\frac{p}{2}}(1, -\alpha) = -p\alpha$ with the degeneracy factor 2^{p+1} for a given even number $p \geq 2$ be a ground level, then the inequality $(\frac{p}{2} - m)\alpha \geq \frac{p}{2} - n$ is derived, which, is automatically satisfied by $n = m = \frac{p}{2}$ without any condition on α. This inequality appears in the form of $\alpha \geq \frac{p-2n}{p-2m}$ for the rest of pairs (m, n) of $1 \leq m \leq \left[\frac{p}{2}\right]$ and $m \leq n \leq p - m$, satisfied by $\alpha \geq 1$.
- In the case of odd $p \geq 3$, in computing the lowest level by $E^{2p}_{\frac{p-1}{2},\frac{p-1}{2}}(1, -\alpha) = -2 - (p - 2)\alpha$ with the degeneracy factor $2^p p$, it will be needed to satisfy the inequality $(\frac{p-1}{2} - m)\alpha \geq \frac{p-1}{2} - n$, which is trivially satisfied by $n = m = \frac{p-1}{2}$. While, for the other values of m and n in Remark 2 the inequality $\alpha \geq 1$ must be realized.

Now, we can explain the maximal spin frustration effect at $\alpha = 1$ on the two-ring Ising chain of Fig. 2 in two different forms for the even and odd values of p.

- **Maximal frustration at $\alpha = 1$ for even values of** p: For an even $p \geq 2$, the energy of the two-ring Ising chain in Fig. 2 takes the value $-p$ by ground levels $E^{2p}_{0,0}(1, -1)$ and $E^{2p}_{\frac{p}{2},\frac{p}{2}}(1, -1)$ with the degeneracy factors 2 and 2^{p+1}, respectively. Furthermore, the sum of the degeneracy factors at $\alpha = 1$ is $2(1 + 2^p)$ which is increasing in terms of p.
- **Maximal frustration at $\alpha = 1$ for odd values of** p: Again, the lowest energy $-p$ for an odd $p \geq 3$ in the chain of Fig. 2 is derived by two ground levels $E^{2p}_{0,0}(1, -1)$ and $E^{2p}_{\frac{p-1}{2},\frac{p-1}{2}}(1, -1)$ with the degeneracy factors 2 and $2^p p$, respectively. The sum of the degeneracy factors at $\alpha = 1$ is $2(1 + 2^{p-1} p)$ which, in turn, means a stronger frustration for higher values of p, in comparison with the previous case.

4 The maximally frustrated regime: Low-temperature behavior of entropy and specific heat capacity in the vicinity of the values $\frac{1}{2}$ and 1 of frustration parameter

Now, we investigate the role of the spin frustration parameter α at the low-temperatures on the entropy $S = -\frac{\partial F^N_\alpha}{\partial T}$ and the specific heat capacity $C = \frac{\partial U}{\partial T}$ with $U = -T^2 \frac{\partial}{\partial T} \frac{F^N_\alpha}{T}$ as internal energy that is obtained from the Helmholtz free energy per spin $F^N_\alpha \equiv -\frac{1}{N\beta} \ln Z^N_{1,-\alpha}$. The N refers to the number of spins in the Ising chains of Figs. 1 and 2, namely $2p + 1$ and $2p$, respectively. Therefore, the partition functions obtained in (6) and (12) are used to evaluate the low-temperature behavior of entropy and specific heat capacity in the vicinity of the values $\frac{1}{2}$ and 1 of spin frustration parameter, corresponding to the maximally frustrated regime. From now on, it is assumed that the NN and NNN exchange couplings are given in terms of the unit $k_B \times Kelvin = 1.3807 \times 10^{-23} Joule$, which will be omitted to simplify both text and plots.

In Figs. 3 and 4, we have considered the behavior of the entropy and specific heat capacity per spin as the function of spin frustration parameter $0 < \alpha < 1.5$ at the low-temperatures $T = 0.1K$ and $0.3K$ for the parameters $p = 3, 4, 5, 6, 7, 8$ of size of the two-ring Ising chains in Figs. 1 and 2. Due to the fact that the low-temperatures $T = 0.1K$ and $0.3K$ led to establishing the ground-state energies, the curves indicate the expected behaviors in agreement with our analytical results on the maximally frustrated regime, presented in the previous section. According to Fig. 3a–d for the Ising chains in Fig. 1, the maximum and minimum values for the entropy and specific heat capacity per spin are shown, respectively, in the vicinity of $\alpha = \frac{1}{2}$, whether p is even or odd. Whilst, this happens only for odd values of p in the vicinity of $\alpha = 1$. These are in agreement with the maximal degeneracies $4(p+1)$, $2 + \frac{1}{3}p(p+1)(2p+1)$ and $(2p+1)(2+\frac{1}{3}p(p+1))$ for even p and $\alpha = \frac{1}{2}$, odd p and $\alpha = \frac{1}{2}$, odd p and $\alpha = 1$, respectively. Finally, according to Fig. 4a–d for the Ising chains in Fig. 2, the maximum and minimum values for the entropy and specific heat capacity per spin are exhibited, respectively, in the vicinity of only $\alpha = 1$, for every p, whether even or odd. This assertion is in agreement with the maximal degeneracies $2 + 2^{p+1}$ and $2 + 2^p p$ for even and odd p, respectively, in the vicinity of $\alpha = 1$. We must point out that as it is seen from Fig. 4a–d, there are no extreme values for the entropy and specific heat capacity per spin in the vicinity of $\alpha = \frac{1}{2}$ which, in turn, is in agreement with our analytical results on Remark 2 of the previous section.

5 Concluding remarks

As it has been shown in Fig. 1, a cyclic linear chain of the odd number $2p+1$ of spins-$\frac{1}{2}$ in the NN and NNN interactions with coupling constants J and K, respectively, has to have a two-ring structure so that all spins contribute to the interaction with their NNs and NNNs. Fig. 2 denotes a two-ring (decorated) chain of the even number $2p$ of spins-$\frac{1}{2}$ while all and half spins contribute to the NN and NNN interactions with coupling constants J and K, respectively. Remarks 1 and 2 introduce explicitly the exact forms of the classical energy levels and their corresponding degeneracy factors for these two-ring Ising chains without remarking that the NN and NNN interactions are from which type, ferromagnetic or antiferromagnetic. However, we know that the competing ferromagnetic and antiferromagnetic interactions lead to frustration at the low temperatures, which can be measured in degenerate ground states by the negative ratio of the coupling constants K and J, the so-called frustration parameter α. Maximal frustration occurs when some ground levels for some values of α find the same energy, and consequently, become more degenerated with respect to the other values in their vicinity. In fact, the disorder in the spin orientations induced by competing interactions increases in the ground levels at the last issues. In this work, we have shown that the ground levels of the two-ring Ising spins-$\frac{1}{2}$ chain corresponding to Fig. 1 with p as an even number are $E^{2p+1}_{0,0}(1, -\alpha) = (2p+1)(\alpha - 1)$ and $E^{2p+1}_{p,\frac{p}{2}}(1, -\alpha) = -1 - (2p-1)\alpha$ for $\alpha < \frac{1}{2}$ and $\alpha > \frac{1}{2}$ with the degeneracy factors 2 and $2(2p+1)$, respectively. Furthermore, the ground levels of Fig. 1 with p as an odd number are $E^{2p+1}_{0,0}(1, -\alpha) = (2p+1)(\alpha - 1)$, $E^{2p+1}_{p-1,\frac{p-1}{2}}(1, -\alpha) = -3 - (2p-5)\alpha$ and $E^{2p+1}_{p,\frac{p+1}{2}}(1, -\alpha) = 1 - (2p-1)\alpha$ for $\alpha < \frac{1}{2}$, $\frac{1}{2} < \alpha < 1$ and $\alpha > 1$ with the degeneracy factors 2, $\frac{1}{3}p(p+1)(2p+1)$ and $2(2p+1)$, respectively. These results demonstrate spin frustration effect by the ground levels of Fig. 1 at the low temperatures in the presence of the competing ferromagnetic and antiferromagnetic interactions. Moreover, maximal spin frustration occurs in the ground energy $-p - \frac{1}{2}$ with the degeneracy factors $4(p+1)$ and $2 + \frac{1}{3}p(p+1)(2p+1)$ in the cases p even and odd, respectively, at $\alpha = \frac{1}{2}$, as well as in the ground energy $2 - 2p$ with the degeneracy

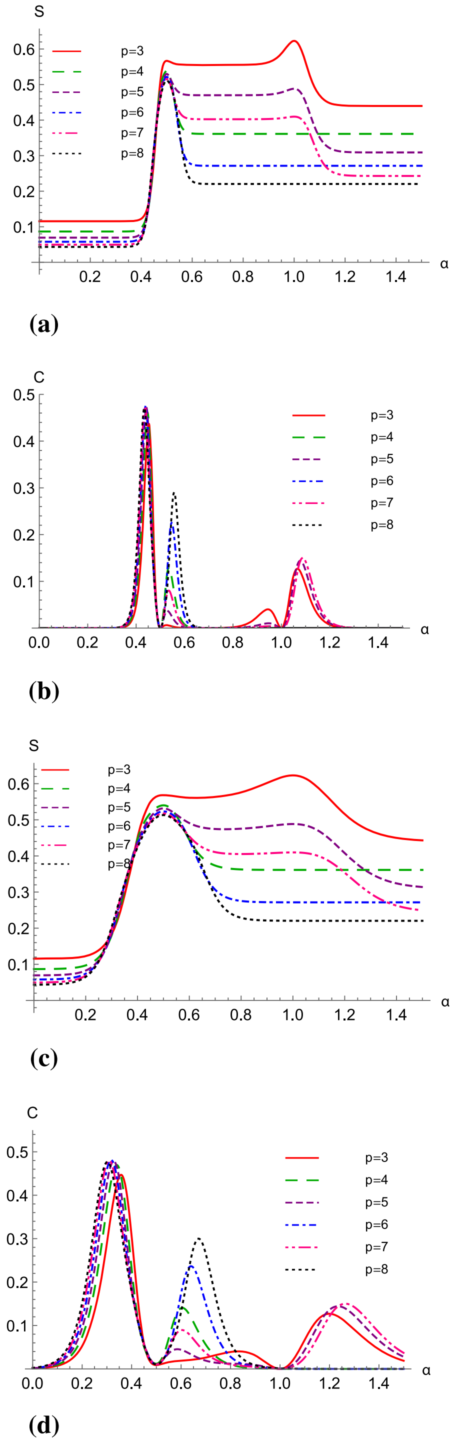


Fig. 3 Plots of entropy and specific heat capacity per spin based on the partition function (6) in the frustration parameter range $0 < \alpha < 1.5$ at the low-temperatures (**a**, **b**) $T = 0.1K$ and (**c**, **d**) $T = 0.3K$. The parameter p of Fig. 1 with the partition function (6) has been chosen as $p = 3, 4, 5, 6, 7, 8$

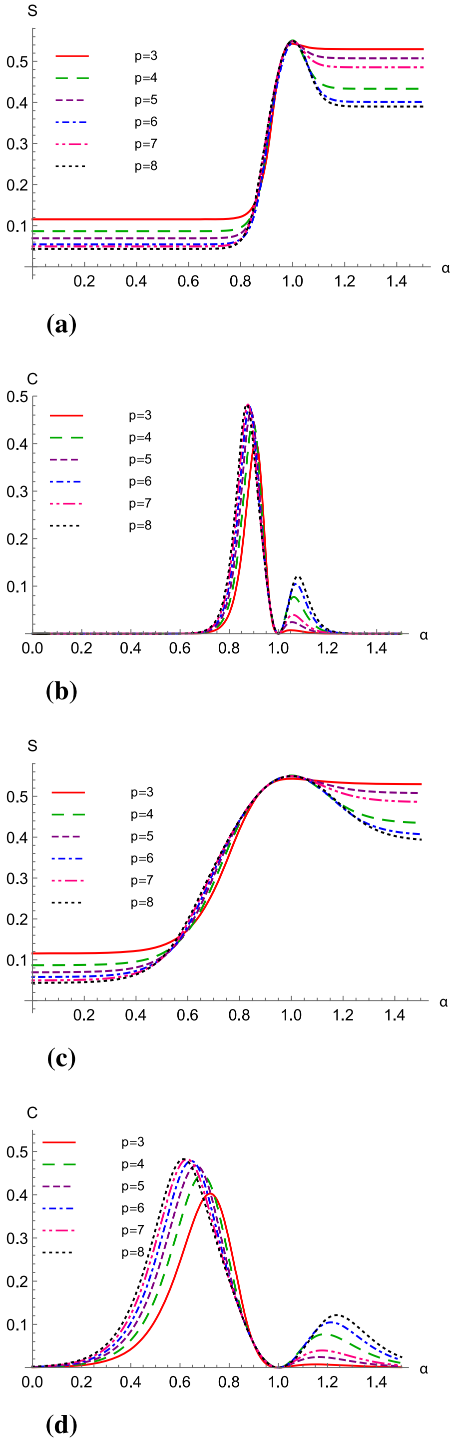


Fig. 4 Plots of entropy and specific heat capacity per spin based on the partition function (12) in the frustration parameter range $0 < \alpha < 1.5$ at the low-temperatures (**a**, **b**) $T = 0.1K$ and (**c**, **d**) $T = 0.3K$. The parameter p of Fig. 2 with the partition function (12) has been chosen as $p = 3, 4, 5, 6, 7, 8$

factor $(2p+1)(2+\frac{1}{3}p(p+1))$ in case only p odd, at $\alpha = 1$. The frustration effect in the case of the two-ring Ising spin-$\frac{1}{2}$ chain corresponding to Fig. 2 is simpler as we deal with two ground levels whether p is even or odd. For $\alpha < 1$, the ground level of Fig. 2, with arbitrary $p \geq 2$, whether even or odd, is $E^{2p}_{0,0}(1,-\alpha) = p(\alpha-2)$ with the degeneracy factor 2. Besides, for $\alpha > 1$, the ground levels are $E^{2p}_{\frac{p}{2},\frac{p}{2}}(1,-\alpha) = -p\alpha$ and $E^{2p}_{\frac{p-1}{2},\frac{p-1}{2}}(1,-\alpha) = -2-(p-2)\alpha$ with the degeneracy factors 2^{p+1} $2^p p$, respectively. Consequently, for energy $-p$ corresponding to $\alpha = 1$, we obtain the degeneracy factors $2(1+2^p)$ and $2(1+2^{p-1}p)$ in cases p even and odd, respectively. Therefore, the two-ring Ising chains in Fig. 2 for energy $-p$ find maximal frustration due to competing ferromagnetic and antiferromagnetic interactions. In Figs. 3 and 4, we have depicted plots of the entropy and specific heat capacity per spin as the functions of the frustration parameter at the low-temperatures $T = 0.1K$ and $0.3K$ for $p = 3, 4, 5, 6, 7, 8$ of the two-ring Ising chains in Figs. 1 and 2. These curves verify the analysis above. The entropy and specific heat capacity per spin for the Ising chains in Fig. 1 take the maximum and minimum values in the vicinity of $\alpha = \frac{1}{2}$ ($\alpha = 1$), in both cases even and odd p (only for odd p). The plots of the entropy and specific heat capacity per spin for the Ising chains in Fig. 2 involve the maximum and minimum values, respectively, in the vicinity of only $\alpha = 1$, in both cases even and odd p.

Data Availability Statement This manuscript is a theoretical research and has no associated data.

References

1. C.N. Yang, C.P. Yang, Phys. Rev. **147**, 303 (1966)
2. U. Brandt, J. Stolze, Z Phys. B: Condensed Matter. **64**, 481 (1986)
3. J.M. Dixon, J.A. Tuszynski, M.L.A. Nip, Physica A: Stat. Mech. Appl. **289**, 137 (2001)
4. S. Redner, J. Stat. Phys. **25**, 15 (1981)
5. A.K. Murtazaev, ZhG Ibaev, J. Exp. Theor. Phys. **113**, 106 (2011)
6. A.V. Zarubin, F.A. Kassan-Ogly, A.I. Proshkin, A.E. Shestakov, J. Exp. Theor. Phys. **128**, 778 (2019)
7. A.V. Zarubin, F.A. Kassan-Ogly, A.I. Proshkin, J. Magn. Magn. Mater. **514**, 167144 (2020)
8. A. Bühler, N. Elstner, G. Uhrig, Eur. Phys. J. B **16**, 475 (2000)
9. J.R.L. de Almeida, Eur. Phys. J. B **13**, 289 (2000)
10. A.K. Murtazaev, I.K. Kamilov, A.B. Babaev, J. Exp. Theor. Phys. **99**, 1201 (2004)
11. A.K. Murtazaev, A. Babaev, J. Magn. Magn. Mater. **321**, 2630 (2009)
12. C. Herrero, Eur. Phys. J. B **70**, 435 (2009)
13. F.A. Kassan-Ogly, A.K. Murtazaev, A.K. Zhuravlev, M.K. Ramazanov, A.I. Proshkin, J. Magn. Magn. Mater. **384**, 247 (2015)
14. M.K. Badiev, A.K. Murtazaev, M.K. Ramazanov, J. Exp. Theor. Phys. **123**, 623 (2016)
15. L. Pan, D. Zhang, H.-H. Hung, Y.-J. Liu, Eur. Phys. J. B **90**, 105 (2017)
16. M. Kumar, F. Corberi, E. Lippiello, S. Puri, Eur. Phys. J. B **93**, 88 (2020)
17. Z. Wang, A. Marandi, K. Wen, R.L. Byer, Y. Yamamoto, Phys. Rev. A. **88**, 063853 (2013)
18. A. Marandi, Z. Wang, K. Takata, R.L. Byer, Y. Yamamoto, Nat. Photonics **8**, 937 (2014)
19. T. Inagaki et al., Science **354**(6312), 603 (2016)
20. P.L. McMahon et al., Science **354**(6312), 614 (2016)
21. K. Takata et al., Sci. Rep. **6**, 34089 (2016)
22. T. Balcerzak, K. Szalowski, M. Jascur, J. Magn. Magn. Mater. **507**, 166825 (2020)
23. J. Majewski, H. Li, J. Ott, Am. J. Hum. Genet. **69**, 853 (2001)
24. Y.J. Choi, H.T. Yi, S. Lee, Q. Huang, V. Kiryukhin, S.W. Cheong, Phys. Rev. Lett. **100**, 047601 (2008)
25. Y. Qi, A. Du, Physica A: Stat. Mech. Appl. **390**, 1064 (2011)
26. G. Yun-Jun, W. Ke-Feng, L. Jun-Ming, Chin. Phys. B **18**, 2557 (2009)
27. M. Böhme, W. Plass, Chem. Sci. **10**, 9155 (2019)
28. J.F. Dobson, J. Math. Phys. **10**, 40 (1969)
29. J. Stephenson, Can. J. Phys. **48**, 1724 (1970)
30. J. Stephenson, J. Appl. Phys. **42**, 1278 (1971)

31. M. Inoue, M. Kubo, J. Magn. Res. **4**, 175 (1971)
32. L. Kalok, L.C. de Menezes, Z. Phys, B **20**, 223 (1975)
33. A.J. Fedro, Phys. Rev. B **14**, 2983 (1976)
34. R. Liebmann, *Statistical Mechanics of Periodic Frustrated Ising Systems*, Lecture Notes in Physics, vol. 251. (Springer, Berlin, 1986)
35. T. Yokota, Phys. Rev. B **39**, 12312 (1989)
36. M.A. Yurischev, JETP **104**, 461 (2007)
37. R. Q. Wei, An exact solution to the partition function of the finite-size Ising model, arXiv:1805.01366
38. M.G. Pini, A. Rettori, Phys. Rev. B **48**, 3240 (1993)
39. H. Fakhri, S.B. Seyedein Ardebili, Physica A: Stat. Mech. Appl. **523**, 557 (2019)
40. H. Fakhri, S.B. Seyedein Ardebili, J. Stat. Mech.: Theory Exp. 083201 (2019)