Physics of the Solid State, 2024, Vol. 66, No. 7

10,05

Markov chains for the analysis of states of one-dimensional spin systems

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Received April 18, 2024
Revised April 18, 2024
Accepted May 8, 2024

We analyze frustrated states of the one-dimensional dilute Ising chain with charged interacting impurities of two types with the mapping of the system to some Markov chain. We perform classification and reveal two types of Markov chains: periodic, with a period of 2, and aperiodic. Frustrated phases with various types of chains have different properties. In phases with periodic Markov chains, long-range order is observed in the sublattice, while another sublattice remains disordered. This results in a conjunction of the non-zero residual entropy and the infinite correlation length. In frustrated phases with aperiodic chains, there is no long-range order, and the correlation length remains finite. It is shown that under the magnetic field the most significant change in the spin chain structure corresponds to the change of the Markov chain type.

Keywords: Markov chains, dilute Ising magnet, frustration, low-dimensional systems, ground state.

DOI: 10.61011/PSS.2024.07.58978.47HH

1. Introduction

The one-dimensional spin models, despite their apparent simplicity compared to the multi-dimensional models, have a set of unique properties. The exact solutions for these models underpin the understanding of a complex behavior of real physical systems and play an important role in studying such phenomena as phase transitions in statistical physics [1]. The absence or complexity of the long-range order formation underlies the unusual behavior of the low-dimensional (pseudo) spin systems. The presence of anisotropy and frustration in the system contribute to a variety of phase diagrams and also to such unusual phenomena as magnetic plateaus [2], quasi-phases and pseudo-transitions [3], as well as the enhancement of the magnetocaloric effect [4]. The disorder also significantly affects the phase, critical and magnetic properties of the systems, and serves as a source of frustration. The frustrated phases, provided that Rojas criterion is fulfilled [5], can be the cause of such subtle pseudo-critical phenomenon as pseudo-transitions expressed as a jump-like change of the system disordered state and are accompanied by sharp features of some thermodynamic functions.

Despite the availability of an exact solution, the analysis of the phase states in one-dimensional systems within the framework of standard formalism presents a non-trivial challenge, especially for states at the boundaries between different phases. An alternative approach in this case could be the construction of a mapping of the one-dimensional model onto a Markov chain, which has previously been utilized to analyze the frustrated phase states of a dilute Ising chain in a magnetic field [6,7], as well as for Potts model on a diamond chain [8]. Such a mapping can be constructed for any model, which partition function can be expressed via the transfer-matrix, that is true, for instance, for various versions of Ising, Potts, Blume−Capel and Blume−Emery−Griffiths models.

One of the sources of frustration in 1D spin systems is the introduction of impurities [7]. In this work, we consider the dilute Ising chain where the charged impurities of two types are introduced. The 2D version of this model was obtained and studied earlier as an atomic limit for a pseudospin model of cuprates [9]. The ground state and thermodynamic properties of the dilute Ising system are influenced by both the frustration due to impurities and the competition of the charge and magnetic orderings [10]. Through numerical simulations on a square lattice, it has been shown that this leads to the presence of non-universal critical behavior [11], first-order phase transitions [12], and reentrant phase transitions [13].

The article is organized as follows. Section 2 includes the constructed and studied phase diagrams of the 1D Ising model with charged impurities in the variables „exchange interaction parameter — chemical potential". Also, concentration dependences are found for the residual entropy of the frustrated phases. Section 3 outlines methodology of mapping the one-dimensional model onto a Markov chain; expressions for the transition matrix, equilibrium state and correlation functions are provided. The Markov chain properties and correlation properties for the frustrated ferromagnetic and antiferromagnetic phases were analyzed. In Section 4, the types of Markov chains are classified according to their symmetry and correlation properties; the influence of the magnetic field on the Markov chains was reviewed. A summary is provided in Section 5.

2. Ground state phase diagrams and residual entropy of the frustrated phases

The ground state phase diagrams, as well as temperature phase diagrams of 2D Ising model with two types of non-magnetic impurities on a square lattice were calculated earlier in works [10,13] by mean field method and computational modeling in zero magnetic field at specified charge density of non-magnetic impurities n, as one of the system parameters.

The Hamiltonian of a 1D dilute Ising model is expressed as follows

$$\mathscr{H}=\sum_{i=1}^{N}\{\Delta S_{z,i}^{2}+VS_{z,i}S_{z,i+1}+JP_{0,i}s_{z,i}s_{z,i+1}P_{0,i+1} - hP_{0,i}s_{z,i}-\mu S_{z,i}\}, \quad (1)$$

where Δ — one-site density-density correlations in the form of a single-ion anisotropy for the pseudospin $S=1$; V — inter-site density-density interaction; J — Ising exchange interaction of spins $s=1/2$; h — external magnetic field; $P_{0,i}=1-S_{z,i}^{2}$ — projection operator for magnetic states. The summation is carried out for N sites of the chain. Using the chemical potential μ, a constraint is imposed on the system in the form of conservation of total charge, which can be expressed as fixing the charge density of non-magnetic impurities: $n=\langle\sum_i S_{z,i}\rangle/N$. A detailed discussion of the density-density interaction within the pseudospin formalism was given in work [12]. Thus, each site of the chain can be in one of the charge states (spinless states of the pseudospin $S_z=\pm1$ for positively and negatively charged impurities, respectively), or in one of the spin states (states of spin $s_z=\pm1/2$, which correspond to projection of the pseudospin $S_z=0$).

Expressions for a grand thermodynamic potential of the system per one site for different phases of the ground state can be written as follows:

$$\omega_{\mathrm{I}}^{\pm}=\Delta+V\pm\mu,\quad \omega_{\mathrm{CO}}=\Delta-V,\quad \omega_{\mathrm{FM}}^{\pm}=J\pm h,$$

$$\omega_{\mathrm{AFM}}=-J,\quad \omega_{\mathrm{PM}}^{\pm\pm}=\frac{\Delta\pm h\pm\mu}{2}. \quad (2)$$

Impurity (I), ferromagnetic (FM), anti-ferromagnetic (AFM), charge-ordered (CO) and paramagnetic (PM) phases correspond to the following configurations of the nearest neighbors for $h>0$: $\mathrm{I}^{\pm}\to(\pm1,\pm1)$, $\mathrm{FM}\to\left(\frac{1}{2},\frac{1}{2}\right)$, $\mathrm{AFM}\to\left(\frac{1}{2},-\frac{1}{2}\right)$, $\mathrm{CO}\to(1,-1)$, $\mathrm{PM}^{\pm}\to(\pm1,\frac{1}{2})$. These „pure“ phases are characterized by the following values of the impurities charge density: $n_{\mathrm{I}^{\pm}}=\pm1$, $n_{\mathrm{FM}}=n_{\mathrm{AFM}}=n_{\mathrm{CO}}=0$, $n_{\mathrm{PM}^{\pm}}=\pm\frac{1}{2}$.

By minimizing the grand potential of the system, new phase diagrams may be built in the variables $(J,\ \mu)$. 2D areas in this case will correspond to the edge values in terms of n for the diagrams built in the representation with the given n. On the contrary, the boundaries between the areas on phase diagrams in variables $(J,\ \mu)$ will correspond to „mixed“ phases with an intermediate value of n, that may have non-zero residual entropy.

In a strong magnetic field $(h\geq 2V)$, the four types of phase diagrams are possible, as shown in Figure 1. Thus, for large negative Δ, the „pure“ phases are (A)FM, COI (true for $n=0$) and $\mathrm{I}^{\pm}$ $(n=\pm1)$. Thus, the intersection of (A)FM-phase with the impurity phase I will give a dilute (anti)ferromagnetically ordered phase (dilute (A)FM) with phase separation into magnetic domains and charged droplets — macroscopic areas with a total volume $|n|$, containing only sites filled with impurities. The number of permutations of charged droplets in a chain that do not change the ground state energy has a power-law asymptotic behavior, and as one approaches the thermodynamic limit $N\to\infty$, the residual entropy of these phases will tend to zero. The intersection of COI with I is the phase of the dilute charge ordering (dilute COI). The charged impurities of one type are randomly distributed against the background of a checkerboard charge ordering. There is an exponentially large number of permutations of „excessive“ impurities without the energy change, which leads to non-zero residual entropy. Thus, dilute COI-phase is frustrated. The charge density of the impurities for both dilute phases can take any value: $0<|n|<1$.

At $\Delta=-h$, a „pure“ paramagnetic phase $\mathrm{PM}^{\pm}$ $\left(n=\pm\frac{1}{2}\right)$ appears, which at the interface with COI causes the charge paramagnetic phase PM-COI that has non-zero residual entropy and exist for $0<|n|<\frac{1}{2}$. PM-COI is a dilute checkerboard charge order with paramagnetic centers as single spins, which are oriented along the field in the ground state. The boundaries of (A)FM with PM provide frustrated (anti) ferromagnetic phase FR-(A)FM with $0<|n|<\frac{1}{2}$. This is a dilute (A)FM-phase with (anti) ferromagnetically ordered clusters (or single spins, aligned with magnetic field) separated by single non-magnetic impurities with the charge density of n. Here, in contrast to the dilute (A)FM-phase, the non-magnetic impurities are not collected into a charged droplet, but are distributed randomly throughout the entire system, resulting in a non-zero residual entropy. At $\frac{2V-h}{2}\leq\Delta\leq0$ an additional boundary between the two paramagnetic phases PM^{+} and PM^{-} appears, which corresponds to the frustrated charge phase FR-COII with sublattice-alternating spins aligned with the field and non-magnetic impurities of both charges. This phase occurs at $0\leq|n|<\frac{1}{2}$.

To obtain the expressions for residual entropy of frustrated phases within the „standard“ transfer-matrix approach, it is necessary to find the maximum eigenvalue of the transfer-matrix, determine the parametrical dependence of the entropy from the charge density using the chemical potential, and find the limit at the zero temperature. This is quite a sophisticated task; however, based on the Markov property of the dilute Ising chain [14], one can analytically define the concentration dependencies of the residual entropy of all frustrated phases of the ground state by an alternative method [6].

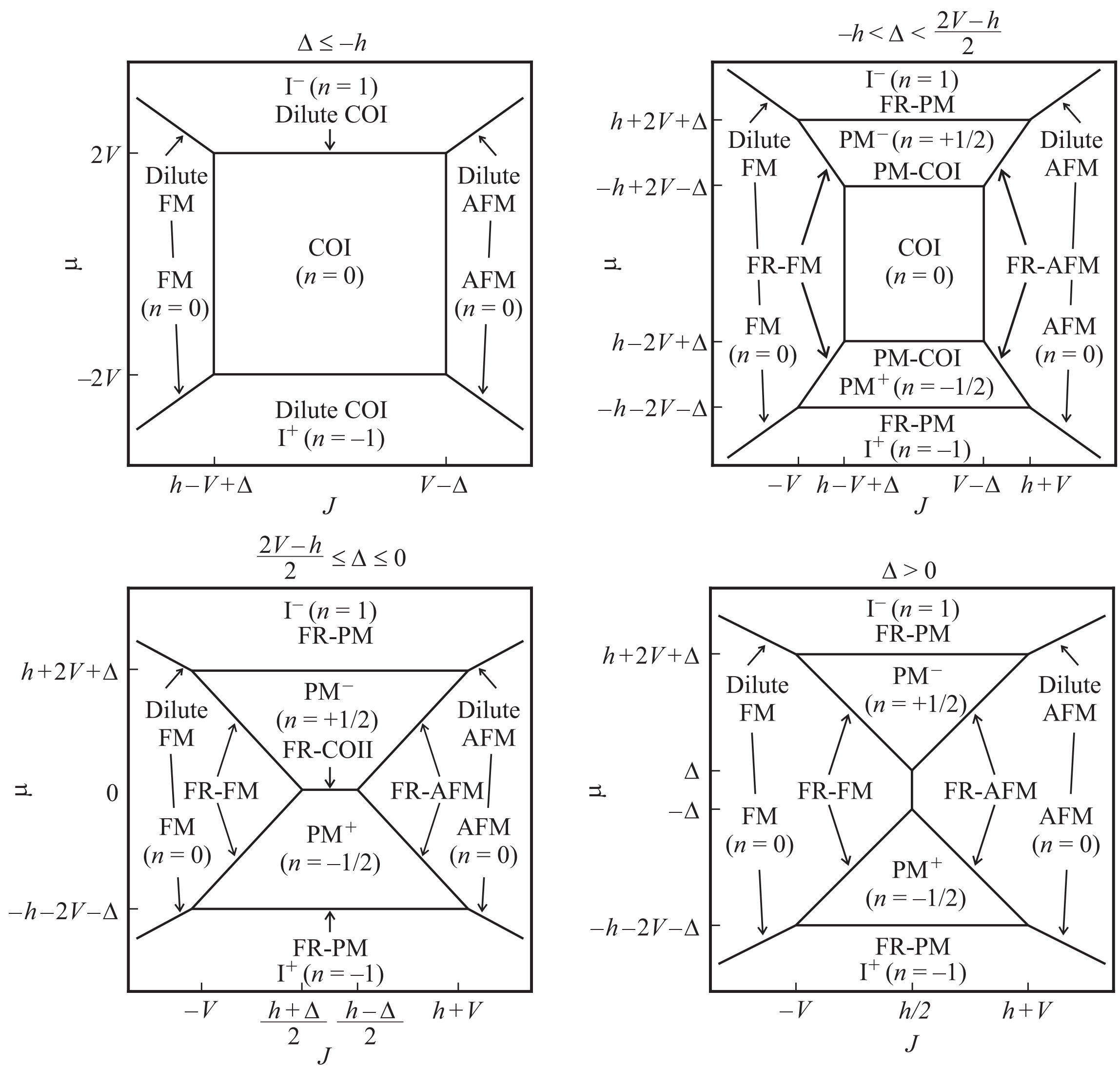


Figure 1. Ground state diagrams for $h \geq 2V$ (strong magnetic field) in variables (J, μ).

The dependences of the residual entropy of the ground state phases on the charge density of impurities n are given in Figure 2 in zero (b) and non-zero (a) magnetic fields. The dilute (A)FM phase has zero residual entropy at all values of the charge density n and is not shown in the Figure. The dilute COI phase has a non-zero entropy for $n \neq 0$, which doesn't depend on magnetic field; it reaches a maximum value of $\frac{1}{2}\ln\frac{\sqrt{5}+1}{\sqrt{5}-1} \approx 0.481$ at $|n| = \frac{1}{\sqrt{5}} \approx 0.447$. The PM-COI and FR-AFM phases in zero field have identical residual entropies, as they are symmetric with respect to the replacement of spin states with pseudospin states. The maximum entropy of these phases is equal to $\frac{\ln 2}{2} \approx 0.347$, and is reached at $|n| = \frac{1}{4}$, while at $h = 0$ maximum values reach $\frac{\ln 3}{2}$ and $\ln 2$ at $|n| = \frac{1}{3}$ for PM-COI and FR-AFM, respectively. The entropies of the FR-FM and FR-PM phases are symmetrical relative to the edge point $|n| = \frac{1}{2}$, and reach their maximum values of $\frac{1}{2}\ln\frac{\sqrt{5}+1}{\sqrt{5}-1} \approx 0.481$ at $|n| = \frac{5\mp\sqrt{5}}{10} \approx \frac{1}{2} \mp 0.224$ for $h \neq 0$ and $\ln 2$ at $|n| = \frac{1}{2} \mp \frac{1}{6}$ at $h = 0$. The FR-COII phase is of particular interest, it arises only in the strong magnetic field $h \geq 2V$. Residual entropy of this phase is non-zero and reaches its maximum value of $\frac{\ln 2}{2} \approx 0.347$ at $n = 0$, which may be caused by re-arrangement of charge states without the change of energy. This is the only phase that remains frustrated at $n = 0$.

It can be noted that the maximum values of the entropy of the frustrated phases FR-COII, PM-COI, FR-AFM are lower than those for dilute COI, FR-FM, FR-PM. Moreover, in zero magnetic field, the entropies of FR-FM, FR-AFM, PM-COI, FR-PM phases increase even more. The reason for this lies in their structure, a detailed analysis of which can also be carried out using a mapping of a 1D system onto a Markov chain [7,8]. Such a mapping may be simulated for any model, the partition function of which allows presentation via the transfer-matrix, that is true, for instance, for various versions of Ising, Potts, Blume–Capel and Blume–Emery–Griffiths models.

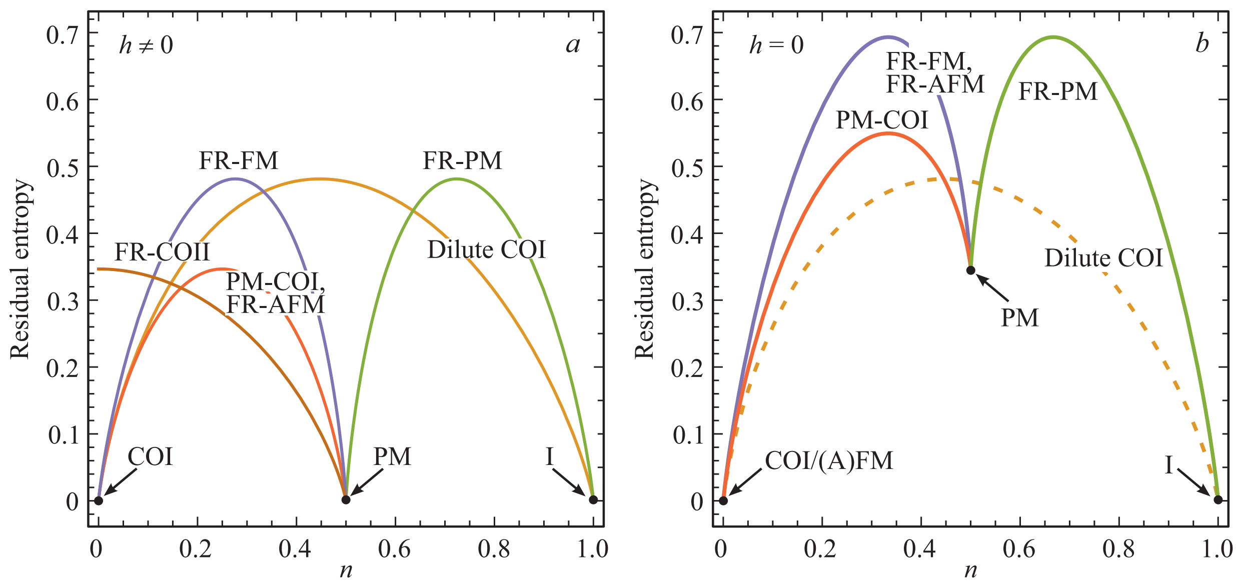


Figure 2. Concentration dependencies of the residual entropy of various ground state phases at (a) $h \neq 0$; (b) $h = 0$.

3. Mapping a 1D spin model onto a Markov chain

1D system transfer-matrix with Hamiltonian (1) in the local basis of states

$$\Phi = \{|S_z, s_z\rangle\} = \left\{|+1,0\rangle, |-1,0\rangle, \left|0,+\frac{1}{2}\right\rangle, \left|0,-\frac{1}{2}\right\rangle\right\}$$
$$\equiv \left\{+1,-1,+\frac{1}{2},-\frac{1}{2}\right\}$$

has a structure

$$\hat{T} = \begin{pmatrix} e^{-\beta\omega_{\mathrm{I}}^{-}} & e^{-\beta\omega_{\mathrm{CO}}} & e^{-\beta\omega_{\mathrm{PM}}^{--}} & e^{-\beta\omega_{\mathrm{PM}}^{+-}} \\ e^{-\beta\omega_{\mathrm{CO}}} & e^{-\beta\omega_{\mathrm{I}}^{+}} & e^{-\beta\omega_{\mathrm{PM}}^{-+}} & e^{-\beta\omega_{\mathrm{PM}}^{++}} \\ e^{-\beta\omega_{\mathrm{PM}}^{--}} & e^{-\beta\omega_{\mathrm{PM}}^{-+}} & e^{-\beta\omega_{\mathrm{FM}}^{-}} & e^{-\beta\omega_{\mathrm{AFM}}} \\ e^{-\beta\omega_{\mathrm{PM}}^{+-}} & e^{-\beta\omega_{\mathrm{PM}}^{++}} & e^{-\beta\omega_{\mathrm{AFM}}} & e^{-\beta\omega_{\mathrm{FM}}^{+}} \end{pmatrix}, \quad (3)$$

where the notations (2) are used for grand thermodynamic potentials of the ground state phases.

As elements of the transition matrix of the Markov chain, one can take the conditional probabilities $P(b|a)$ of realizing state b at the $(i+1)$-site given that the i-site is in state a. The conditional probabilities can be defined by Bayes formula $P(ab) = P(a)P(b|a)$, where $P(a) = \langle P_{a,i}\rangle$ — probability of implementation of a state At the i-site, $P(ab) = \langle P_{a,i}P_{b,i+1}\rangle$ — probability of joint implementation of a and b states on i- and $(i+1)$-sites, respectively, $P_{a,i}$ — projector on a state for site i.

By using the transfer matrix (3) built on the states a, one can find the correlators [8]

$$\langle P_{a,i}\rangle = \langle a|\lambda_1\rangle\langle\lambda_1|a\rangle, \quad (4)$$

$$\langle P_{a,i}P_{b,i+l}\rangle = \langle a|\lambda_1\rangle \frac{T_{ab}^{l}}{\lambda_1^{l}} \langle\lambda_1|b\rangle, \quad (5)$$

where λ_1 — the largest eigenvalue of the transfer-matrix, $\langle a|\lambda_1\rangle = \upsilon_a$ — the element of the eigenvector of the transfer-matrix for state a corresponding to the largest eigenvalue λ_1.

Thus, the conditional probabilities are equal to the correlators ratio

$$P(b|a) = \frac{\langle P_{a,i}P_{b,i+1}\rangle}{\langle P_{a,i}\rangle} = \frac{T_{ab}\upsilon_b}{\lambda_1\upsilon_a} = \pi_{ab}. \quad (6)$$

Equilibrium (stationary) state of the system can be expressed as a limiting distribution p of the Markov chain, which remains unchanged as a result of the transition matrix action. Respectively, for p_a components of the limiting distribution the following is true

$$\sum_a p_a\pi_{ab} = p_b, \ \sum_a p_a = 1, \ p_a = P(a) = \langle P_{a,i}\rangle. \quad (7)$$

Given (4), for symmetric transfer-matrices the limiting distribution is associated with the normalized eigenvector corresponding to the largest eigenvalue

$$p_a = \upsilon_a^2. \quad (8)$$

Pair distribution functions can also be expressed using the transition matrix, if we use the conclusion of Kolmogorov–Chapman theorem:

$$\langle P_{a,i}P_{b,i+l}\rangle = \sum_{s_1,\ldots,s_{l-1}} P(a)P(a|s_1)P(s_1|s_2)\ldots P(s_{l-1}|b)$$
$$= p_a\pi_{ab}^{l} = \pi_{ba}^{l}p_b. \quad (9)$$

The correlation function for the states a and b, thus, can be expressed as follows:

$$K_{ab}(l) = \langle P_{a,i}P_{b,i+l}\rangle - \langle P_{a,i}\rangle\langle P_{b,i}\rangle = p_a\pi^l_{ab} - p_a p_b$$
$$= p_b\pi^l_{ba} - p_a p_b. \qquad (10)$$

Taking into account $\sigma_{z,i} = P_{0,i}s_{z,i}/s = P_{\frac{1}{2},i} - P_{-\frac{1}{2},i}$, one can calculate the spin correlation function:

$$C(l) = \langle\sigma_{z,i}\sigma_{z,i+l}\rangle - \langle\sigma_{z,i}\rangle^2. \qquad (11)$$

To construct the transition matrix and the corresponding Markov chain for a specific frustrated ground state phases, one can leave only the leading order elements in the transfer matrix, and neglect the remaining elements due to their exponentially small contributions at low temperatures. We will do it for the frustrated magnetic phases FR-AFM and FR-FM.

Let's consider the system in the external magnetic field: $h > 0$. For convenience, we will examine the cases of positive impurities charge: $n > 0$. Since FR-AFM phase arises on the intersection of AFM and PM phases on (J, μ)-diagram (see Figure 1), in the transfer-matrix we'll keep only the members corresponding to the necessary configurations of the neighboring states:

$$\hat{T} = \begin{pmatrix} 0 & e^{-\beta\omega_{\mathrm{PM}}^{--}} & 0 \\ e^{-\beta\omega_{\mathrm{PM}}^{--}} & 0 & e^{-\beta\omega_{\mathrm{AFM}}} \\ 0 & e^{-\beta\omega_{\mathrm{AFM}}} & 0 \end{pmatrix} = \begin{pmatrix} 0 & e & 0 \\ e & 0 & d \\ 0 & d & 0 \end{pmatrix}.$$

-1 state is absent, the system states space will be reduced to $\Phi = \{+1, +\frac{1}{2}, -\frac{1}{2}\}$. The largest eigenvalue of the transfer-matrix is equal to $\lambda_1 = \sqrt{d^2 + e^2}$ with the eigenvector $\boldsymbol{v} = \left(\frac{e}{\sqrt{2}\lambda_1}, 0, \frac{1}{\sqrt{2}}, \frac{d}{\sqrt{2}\lambda_1}\right)^T$.

According to expressions (6), (8) let's define the form of the transition matrix and limiting distribution for this phase:

$$\pi = \begin{pmatrix} 0 & 1 & 0 \\ \frac{e^2}{\lambda_1^2} & 0 & \frac{d^2}{\lambda_1^2} \\ 0 & 1 & 0 \end{pmatrix}, \quad \boldsymbol{p} = \frac{1}{2\lambda_1^2}\begin{pmatrix} e^2 \\ \lambda_1^2 \\ d^2 \end{pmatrix}. \qquad (12)$$

The condition of constant charge density of impurities can be written as

$$n = P(1) - P(-1) = p_1 - p_{-1}. \qquad (13)$$

Then, the elements of the transition matrix and limiting distribution can be expressed through n:

$$\pi = \begin{pmatrix} 0 & 1 & 0 \\ 2n & 0 & 1-2n \\ 0 & 1 & 0 \end{pmatrix}, \quad \boldsymbol{p} = \begin{pmatrix} n \\ \frac{1}{2} \\ \frac{1}{2} - n \end{pmatrix}. \qquad (14)$$

For the FR-AFM phase, the equilibrium state is the state when the half of the chain is filled with spins $+\frac{1}{2}$, while

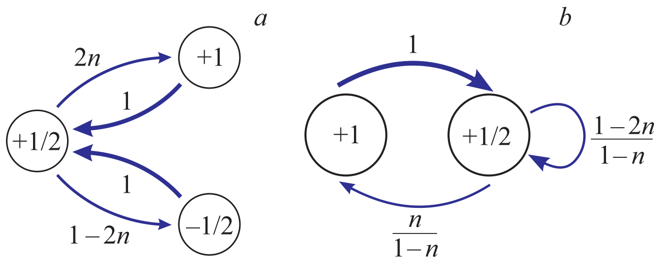


Figure 3. Transition graphs between the states of Markov chain for the transition matrix of phases *a*) FR-AFM; *b*) FR-FM.

the remaining part of the system is a mixture of positively charged impurities with density of n (with pseudospin $+1$) and spins $-\frac{1}{2}$ with density of $\frac{1}{2} - n$. Based on the type of transition matrix it is convenient to built the graph of possible transitions. The vertices of the graph designate possible states of the system, the links from one vertex to another show possible transitions between the states. It is presented in Figure 3, *a* for the FR-AFM phase. Thicker lines correspond to larger conditional probabilities of the transition. Transitions to the $+\frac{1}{2}$ state from others occur with probability 1, this state fully fills one sublattice, while the second sublattice is chaotically filled with $+1$ and $-\frac{1}{2}$ states in accordance with a fixed value of n.

The impurity and spin correlation functions are equal, correspondingly

$$K_{+1,+1}(l) = (-1)^l n^2, \quad C(l) = (-1)^l(1-n)^2. \qquad (15)$$

Both correlation functions are characterized by the infinite correlation length: $\xi = \infty$.

Thus, the chain is divided into two sublattices. One of them is fully ordered — filled with $+\frac{1}{2}$ spins, which gives an infinite correlation length. In the second sublattice, the spins $-\frac{1}{2}$ are replaced by $+1$ impurities with increasing n and are arranged chaotically. The state of this sublattice is frustrated and is characterized by the correlation functions equal to zero. Because of this, the FR-AFM phase combines ordering on one sublattice and chaotic character on the other, which gives infinite correlation length and non-zero entropy. It is clearly seen when analyzing the two-step transition matrix

$$\pi^2 = \begin{pmatrix} 2n & 0 & 1-2n \\ 0 & 1 & 0 \\ 2n & 0 & 1-2n \end{pmatrix}. \qquad (16)$$

The state space of the two-step Markov chain splits into two independent sub-spaces: $\Phi = \{+\frac{1}{2}\} \cup \{+1, -\frac{1}{2}\}$, which describe two sublattices of the spin chain.

As a result, FR-AFM phase may be represented as a set of AFM-clusters separated by single impurities. In this case, AFM clusters always contain an odd number of spins and have states $+\frac{1}{2}$ at the edges, aligned with the external magnetic field $h > 0$.

Let's consider an equivalent frustrated ferromagnetic phase FR-FM in the field $h > 0$. It corresponds to the boundary between phases FM and PM on (J, μ)-diagram (see Figure 1). The transfer-matrix, transition matrix and equilibrium system state in this phase will be expressed as follows:

$$\hat{T} = \begin{pmatrix} 0 & e^{-\beta\omega_{\rm PM}^{--}} \\ e^{-\beta\omega_{\rm PM}^{--}} & e^{-\beta\omega_{\rm FM}^{+}} \end{pmatrix},$$

$$\pi = \begin{pmatrix} 0 & 1 \\ \frac{n}{1-n} & \frac{1-2n}{1-n} \end{pmatrix}, \quad \boldsymbol{p} = \begin{pmatrix} n \\ 1-n \end{pmatrix}. \quad (17)$$

Now the states space is reduced to $\Phi = \{+1, +\frac{1}{2}\}$. The system equilibrium state is itself the ferromagnetic clusters separated by single non-magnetic impurities. The transition graph is shown in Figure 3, *b*.

The impurity and spin correlation functions are equal to:

$$K_{+1+1}(l) = K_{+\frac{1}{2}+\frac{1}{2}}(l) = C(l) = (-1)^l n(1-n)e^{-l/\xi}, \quad (18)$$

where the correlation length ξ is finite and depends on the charge density:

$$\xi = \left[\ln\left(\frac{1-n}{n}\right)\right]^{-1}. \quad (19)$$

This means, that at $h \neq 0$ there are no critical fluctuations, and the state remains frustrated and disordered even at $T = 0$. The correlation length is equal to zero at $n = 0$, when the FR-FM phase transits into the ordered FM-phase with entropy equal to zero.

In the absence of external magnetic field the properties of FR-AFM and FR-FM phases will slightly change. For the FR-AFM phase the mutual relations between the impurities state $+1$ and spin state $-\frac{1}{2}$ will be added into Markov chain. For the FR-FM phase the spin state $-\frac{1}{2}$, having the same relation with impurities, as $+\frac{1}{2}$ state, will appear. Now the spin states $\pm\frac{1}{2}$ are included in Markov chain symmetrically. The correlation functions in the zero field decrease exponentially for both phases,

$$K_{+1+1}^{\text{FR-AFM}}(l) = K_{+1+1}^{\text{FR-FM}} = (-1)^l(1-n)ne^{-l/\xi_c}, \quad (20)$$

$$C^{\text{FR-AFM}}(l) = (-1)^l C^{\text{FR-FM}}(l) = (-1)^l(1-n)e^{-l/\xi_s}, \quad (21)$$

where charge and spin correlation lengths are equal, correspondingly

$$\xi_c = \left[\ln\left(\frac{1-n}{n}\right)\right]^{-1}, \quad \xi_s = \left[\ln\left(\frac{1-n}{1-2n}\right)\right]^{-1}. \quad (22)$$

As a result, the application of an external magnetic field may induce a subtle rearrangement of states, leading to the emergence of long-range order characterized by an infinite correlation length within one of the sublattices. In contrast, in the ferromagnetic phase FR-FM the response to the magnetic field is primarily characterized by the flipping of spin clusters in the direction of the applied field.

Thus, the analysis of the ground state phases using Markov chains facilitates the identification of the features of the phases structure and reveals the hidden sublattice ordering. This method also allows for the analytical determination of correlation functions and correlation lengths, as well as the calculation of residual entropy.

4. Types of Markov chains of the 1D dilute Ising model

Now we classify the types of Markov chains and determine their form for the existing phases. The results for the frustrated ground state phases are presented in the Table, where for each phase we provide the transition matrix π, the form of the equilibrium state $\boldsymbol{p}$, the transition graph between states in the space Φ, as well as the form of the correlation functions and correlation lengths.

In the presence of a magnetic field, we can distinguish two types of Markov chains; they are given in the first two parts of the Table. The FR-AFM, FR-COII and PM-COI phases have Markov chains with a period of 2 and an infinite correlation length due to the ordered sublattice. As a result, the residual entropy for these phases is lower than that of the second class of frustrated phases. The second class phases, FR-FM, dilute COI, and FR-PM, are characterized by a Markov chain consisting of two states and a finite correlation length that depends on n.

The rearrangements of Markov chains at $h = 0$ also occur in other phases sensitive to a magnetic field. The characteristics of Markov chains for such phases in the absence of a magnetic field are given in the last part of the Table. The Markov chain for the paramagnetic charge phase PM-COI in the absence of a magnetic field retains a period of 2; however, now, in addition to the state $+\frac{1}{2}$, the opposite spin state $-\frac{1}{2}$ emerges. While the long-range ordering of impurities in the sublattice remains stable at any magnetic field, the spin states become uncorrelated in the absence of a magnetic field. Markov chain of the frustrated paramagnetic phase FR-PM in zero field contains an additional state $-\frac{1}{2}$, which is symmetric to $+\frac{1}{2}$. The charge correlation length remains unchanged; however, the spin correlation function becomes zero, which increases the residual entropy of this phase.

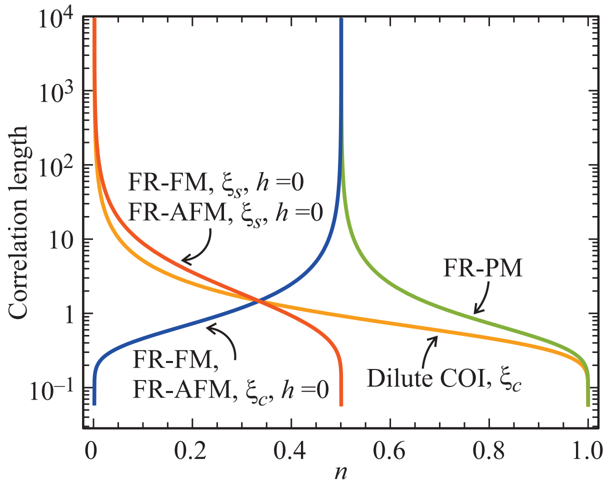
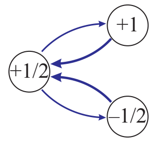
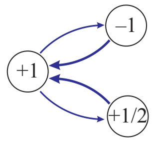
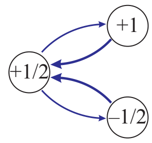
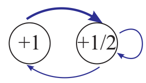
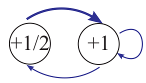
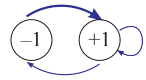
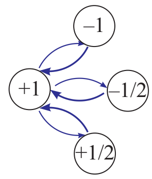
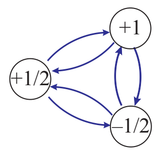
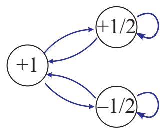
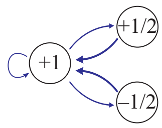


Figure 4. Correlation length of ground state phases as a function of charge density of non-magnetic impurities n in a logarithmic scale.

Table of frustrated phases mapping on Markov chains ($n > 0$)

Type of Markov chain	Phase	Transition matrix π	Equilibrium state $\boldsymbol{p}$	Transition graph	Correlation functions $K_{+1+1}(l), C(l)$ and correlation lengths
Periodic with a period of 2	FR-AFM ($h > 0$)	$\begin{pmatrix} 0 & 1 & 0 \\ 2n & 0 & 1-2n \\ 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} n \\ \frac{1}{2} \\ \frac{1}{2}-n \end{pmatrix}$		$C(l) = (-1)^l(1-n)^2$, $K_{+1+1}(l) = (-1)^l n^2$, $\xi = \infty$
	PM-COI ($h > 0$)	$\begin{pmatrix} 0 & 1-2n & 2n \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{2} \\ \frac{1}{2}-n \\ n \end{pmatrix}$		$K_{+1+1}(l) = \frac{(-1)^l}{4}$, $C(l) = (-1)^l n^2$, $\xi = \infty$
	FR-COII	$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ \frac{1}{2}+n & \frac{1}{2}-n & 0 \end{pmatrix}$	$\begin{pmatrix} \frac{1+2n}{4} \\ \frac{1-2n}{4} \\ \frac{1}{2} \end{pmatrix}$		$K_{+1+1}(l) = \frac{(-1)^l(1+2n)^2}{16}$, $C(l) = \frac{(-1)^l}{4}$, $\xi = \infty$
Aperiodic	FR-FM ($h > 0$)	$\begin{pmatrix} 0 & 1 \\ \frac{n}{1-n} & \frac{1-2n}{1-n} \end{pmatrix}$	$\begin{pmatrix} n \\ 1-n \end{pmatrix}$		$K_{+1+1}(l) = C(l) = (-1)^l n(1-n)e^{-l/\xi}$, $\xi = \left[\ln\left(\frac{1-n}{n}\right)\right]^{-1}$
	FR-PM ($h > 0$)	$\begin{pmatrix} \frac{2n-1}{n} & \frac{1-n}{n} \\ 1 & 0 \end{pmatrix}$			$K_{+1+1}(l) = C(l) = (-1)^l n(1-n)e^{-l/\xi}$, $\xi = \left[\ln\left(\frac{n}{1-n}\right)\right]^{-1}$
	dilute COI	$\begin{pmatrix} \frac{2n}{1+n} & \frac{1-n}{1+n} \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} \frac{1+n}{2} \\ \frac{1-n}{2} \end{pmatrix}$		$K_{+1+1}(l) = \frac{(-1)^l}{4}(1-n^2)e^{-l/\xi}$, $\xi = \left[\ln\left(\frac{1+n}{1-n}\right)\right]^{-1}$
Periodic with a period of 2	PM-COI ($h = 0$)	$\begin{pmatrix} 0 & 1-2n & n & n \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{2} \\ \frac{1}{2}-n \\ \frac{n}{2} \\ \frac{n}{2} \end{pmatrix}$		$K_{+1,+1}(l) = \frac{(-1)^l}{4}$, $C(l) = 0, \xi_c = \infty$
Aperiodic	FR-AFM ($h = 0$)	$\begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{n}{1-n} & 0 & \frac{1-2n}{1-n} \\ \frac{n}{1-n} & \frac{1-2n}{1-n} & 0 \end{pmatrix}$	$\begin{pmatrix} n \\ \frac{1-n}{2} \\ \frac{1-n}{2} \end{pmatrix}$		$K_{+1,+1} = (-1)^l(1-n)ne^{-l/\xi_c}$, $\xi_c = \left[\ln\left(\frac{1-n}{n}\right)\right]^{-1}$, $C(l) = (\mp 1)^l(1-n)e^{-l/\xi_s}$, $\xi_s = \left[\ln\left(\frac{1-n}{1-2n}\right)\right]^{-1}$
	FR-FM ($h = 0$)	$\begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{n}{1-n} & \frac{1-2n}{1-n} & 0 \\ \frac{n}{1-n} & 0 & \frac{1-2n}{1-n} \end{pmatrix}$			
	FR-PM ($h = 0$)	$\begin{pmatrix} \frac{2n-1}{n} & \frac{1-n}{2n} & \frac{1-n}{2n} \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}$			$K_{+1,+1} = (-1)^l ne^{-l/\xi}$, $\xi_c = \left[\ln\left(\frac{n}{1-n}\right)\right]^{-1}$, $C(l) = 0$

The Figure 4 illustrates the concentration dependencies of the correlation lengths of various frustrated phases in a logarithmic scale, both in the presence and absence of a magnetic field h. The correlation lengths of phases with periodic Markov chains are not depicted, since they are infinite for any n.

The impurity correlation length ξ_c for the phases FR-(A)FM at $h = 0$ is the same as that for the FR-FM phase at $h \neq 0$. It becomes zero at $n = 0$, when frustrated phases transition into „pure“ (A)FM phases. In that case, the spin correlation length ξ_s goes to infinity. This indicates a magnetic phase transition at $T = 0$, when the (A)FM-state becomes fully ordered. Another boundary point is $n = \frac{1}{2}$, corresponding to „pure“ paramagnetic ordering PM. In this point the impurity correlation length is divergent, while the spin correlation length tends to zero. In the FR-PM phase, compared to the FR-FM, the roles of impurity and spin states are interchanged, resulting in symmetrical properties of these phases relative to the $n = \frac{1}{2}$ point; absence of the spin correlation in the FR-PM phase in zero magnetic field is an exclusion. In the dilute COI phase the long-range checkerboard charge ordering at $T = 0$ occurs only in „pure“ COI limit, at $n = 0$, when the charge correlation length becomes divergent.

5. Conclusion

Using a method based on Markov chains analysis, the properties of frustrated phases of the Ising chain with two types of charged impurities have been studied.

The considered model exhibits a wide variety of ground state phases, most of which have non-zero residual entropy, and tend to be frustrated in this context. In zero magnetic field each frustrated phase has its own type of Markov chain. In an external field, the system has only 2 types of Markov chains, each of which is typical for three different frustrated phases of the ground state. The properties of these 2 Markov chains differ significantly. Thus, the frustrated antiferromagnetic FR-AFM phase, the paramagnetic charge phase PM-COI and a mixture of impurity paramagnetic phases FR-COII have periodic Markov chains with a period of 2 and three states. This indicates the presence of ordering on one of the spin chain sublattices, while the second sublattice remains completely disordered. Due to this hidden ordering, the correlation length of the system is infinite, while the residual entropy is relatively small. The frustrated ferromagnetic FR-FM, checkerboard charge dilute COI and paramagnetic FR-PM phases can be effectively described by aperiodic Markov chains with two states. This is in line with a spin chain composed of clusters of one state type, which are separated by single sites of the second state type. In this case, no long-range order is established in the system, resulting in a finite correlation length that depends on the charge density. Consequently, the residual entropy is higher than that of the first-type phases.

The performed analysis shows that when a magnetic field is included, the most significant change in the structure of the spin chain corresponds to a change in the type of the Markov chain: for the frustrated antiferromagnetic phase FR-AFM, the aperiodic Markov chain becomes periodic, which indicates the emergence of a long-range order in the system.

Funding

This study was supported financially by grant No. 24-22-00196 from the Russian Science Foundation.

Conflict of interest

The authors declare that they have no conflict of interest.

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Translated by T.Zorina

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