Domain statistics in a finite Ising chain

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We present a comprehensive study for the statistical properties of random variables that describe the domain structure of a finite Ising chain with nearest-neighbor exchange interactions and free boundary conditions. By use of extensive combinatorics we succeed in obtaining the one-variable probability functions for (i) the number of domain walls, (ii) the number of up domains, and (iii) the number of spins in an up domain. The corresponding averages and variances of these probability distributions are calculated and the limiting case of an infinite chain is considered. Analyzing the averages and the transition time between differing chain states at low temperatures, we also introduce a criterion of the ferromagnetic-like behavior of a finite Ising chain. The results can be used to characterize magnetism in monatomic metal wires and atomic-scale memory devices.

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I. INTRODUCTION

The Ising model, pioneered just 80 years ago [1], has become one of the most popular and useful models of statistical physics. This model system itself and its numerous generalizations found wide application for the investigation of not only physical but also for biological, economical, and social systems, to name only a few. The model has also been widely used to characterize the cooperative behaviors in these and other systems. The salient advantages of the Ising model are that it is generic for systems with phase transitions, it is very convenient to use, and, moreover, for particular cases it can be solved exactly, i.e., its partition function can be calculated, at least in the thermodynamic limit, without approximations. Because exact solutions were found only for a certain one- and two-dimensional versions of the Ising model [2,3], their role for statistical physics is most important.

The ordinary one-dimensional Ising model, which is represented by an infinite chain of Ising spins, i.e., spins that can either be up or down, and which do interact with each other via the nearest-neighbor exchange interaction, does not exhibit the ferromagnetic phase transition at nonzero temperatures [1]. This well-known result corroborates the known argument of Landau and Lifshitz [4], according to which a long-range order in *infinite* one-dimensional systems with *short-range* interactions is absent. The problem of long-range ordering, which can emerge in such systems when these conditions are violated, is of prominent theoretical importance. Its solution for infinite Ising chains with *long-range* interactions between spins has been the subject of a number of remarkable studies (see, e.g., Refs. [5–11]).

A priori, the statistical mechanics of a *finite* Ising chain with only exchange (i.e., short-range) interaction seems not to present an interesting topic. This is so, because it does not exhibit macroscopic ferromagnetic order. A detailed investigation of this model is important, however, by the following motivating reasons. First, the domain statistics in such finite chains, i.e., a probability description of forming domains, domain lengths, and domain walls contains most valuable information on the thermal equilibrium state. To the best of our knowledge, these statistics have not been studied before. The main problem is that the domain characteristics are not ordinary thermodynamic quantities, i.e., they are not readily expressed through the partition function. In short, there are no conventional methods to extract them. Second, a finite Ising chain represents an appropriate phenomenological model for describing magnetism in *monatomic* metal wires deposited on substrates. Indeed, as it has been discovered experimentally [12], a Co chain on Pt substrate is characterized by the exchange coupling (this justifies the nearest-neighbor approximation), very large magnetic anisotropy (this justifies the approximation of atomic magnetic moments by Ising spins), and long-range ferromagnetic order (this justifies the use of finite Ising chains). We do emphasize that in contrast to the case with infinite Ising chains for which ferromagnetic order is forbidden at all nonzero temperatures [13], finite chains can exhibit the ferromagneticlike behavior (see also Sec. IV). Finally, it is very likely that the one-dimensional magnets, which are modeled by finite Ising chains, will have an important implication for magnetic data-storage technology [14].

In this paper, using a variety of combinatorial approaches, we investigate thoroughly the domain statistics in a finite Ising chain. In Sec. II, we describe the model and introduce the main definitions. The joint probability functions that describe the domain structure of a chain are calculated in Sec. III by the combinatorial method. In Sec. IV, we demonstrate that the number of domain walls in a finite Ising chain is binomially distributed. We then introduce a criterion of its ferromagneticlike behavior and consider the limiting case of an infinite chain. In Sec. V, we derive the probability function for the number of up domains and calculate its average

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and its variance. The probability function for the number of spins in an up domain (i.e., domain length) and its numerical characteristics are determined in Sec. VI. We summarize our novel findings in Sec. VII. Some of our technical details and manipulations are deferred to the Appendices.

II. MODEL AND NOTATIONS

We consider a finite Ising chain with free boundary conditions that contains an even number N of Ising spins. We assume that the spins interact through the nearest-neighbor ferromagnetic coupling $J(>0)$ and the spin variables σ_i $(i=1,\ldots,N)$ assume only two values +1 and −1, respectively, corresponding to the up and down spin orientations. For a given spin configuration $\{\sigma_i\}$, the chain energy is written in the form

$$E_N(\{\sigma_i\}) = -J\sum_{i=1}^{N-1} \sigma_i\sigma_{i+1}. \tag{2.1}$$

According to the Gibbs distribution, the probability of this configuration is given by

$$W_N(\{\sigma_i\}) = \frac{1}{Z_N}e^{-\beta E_N(\{\sigma_i\})}, \tag{2.2}$$

where β denotes the inverse temperature measured in energy units, and $Z_N=\Sigma_{\{\sigma_i\}}\exp[-\beta E_N(\{\sigma_i\})]$ is the partition function of a chain. Using, e.g., the transfer matrix method [15], Z_N can be evaluated exactly, yielding the well-known result

$$Z_N = 2^N \cosh^{N-1}(\beta J). \tag{2.3}$$

In order to characterize the domain distribution in a chain, we introduce the number of up spins, s, the number of up domains, p, the number of domain walls, i.e., the number of up-down and down-up spin pairs, k, and the number of spins in the first up domain, l. These numbers satisfy the conditions $0 \leqslant s \leqslant N$, $0 \leqslant p \leqslant N/2$, $0 \leqslant k \leqslant N-1$, $0 \leqslant l \leqslant N$. These numbers are not independent because, for example, if $p=0$ then $s=k=l=0$, and if $p=N/2$ then $s=N/2$, $k=N-1$, and $l=1$. The introduced quantities are random due to thermal agitation, and our main objective is to calculate the one-variable probability functions $P_N(k)$, $P_N(p)$, and $P_N(l)$ that describe in detail domain statistics in a chain of N Ising spins. (Notice that some features of the probability function of magnetization have been studied in [16].) To this end, we also introduce the four-variable probability function $P_N(s,p,k,l)$ representing the joint probability that a chain is characterized by the parameters s, p, k, and l. Taking into account that

$$E_N(\{\sigma_i\}) = E_N(k) = -J(N-1) + 2Jk \tag{2.4}$$

and

$$W_N(\{\sigma_i\}) = W_N(k) = \frac{1}{Z_N}e^{-\beta E_N(k)}, \tag{2.5}$$

this probability function can be written as

$$P_N(s,p,k,l) = W_N(k)K_N(s,p,k,l), \tag{2.6}$$

where $K_N(s,p,k,l)$ is the number of spin configurations possessing the same set of the non-negative integer variables s, p, k, and l. In accordance with the basic laws of probability theory [17], all the one-variable probability functions can be determined by fixing one variable and summing $P_N(s,p,k,l)$ over the admissible values of all remaining variables.

III. JOINT PROBABILITY FUNCTIONS

A. Number of spin configurations

The chain states that we describe in terms of the four variables mentioned above are, in general, degenerate and $K_N(s,p,k,l)$ spin configurations correspond to each of those states. The states with $s=p=k=l=0$ and $s=l=N$, $p=1$, $k=0$ are characterized by only one spin configuration $\{\sigma_i=-1\}$ and $\{\sigma_i=+1\}$ for all i, respectively. Therefore $K_N(0,0,0,0)=K_N(N,1,0,N)=1$. For counting $K_N(s,p,k,l)$ in other cases, when $1 \leqslant s \leqslant N-1$, we use combinatorial methods. Within their framework, we consider an Ising chain with fixed s, p, k, and l as an alternate sequence of p up boxes and $k-p+1$ down boxes in which s up spins and $N-s$ down spins are distributed.

Because the first up box must contain l up spins and in each other up box must be at least one up spin (hence the condition $s-l \geqslant p-1$ must hold), the number $M_\uparrow$ of different distributions of s up spins over p up boxes equals C_{s-l-1}^{p-2}. Here, the binomial coefficients C_n^m with integers n and m are defined as follows: $C_n^m=n!/(n-m)!m!$ if $n \geqslant m \geqslant 0$, $C_n^m=0$ if $m>n\geqslant 0$ or if $n \geqslant 0$ and $m<0$, and $C_n^0=C_n^n=1$ for all integer n. Using these properties, we can represent $M_\uparrow$ in the form $M_\uparrow=C_{s-l-1}^{p-2+\Delta_{spkl}}$ ($\Delta_{spkl}=\delta_{s,0}\delta_{p,0}\delta_{k,0}\delta_{l,0}$, $\delta_{n,m}$ is the Kronecker symbol), which is valid for $0 \leqslant s \leqslant N$.

Similarly, the number $M_\downarrow$ of different distributions of $N-s$ down spins over $k-p+1$ down boxes, each of which contains at least one down spin, is given by $M_\downarrow=C_{N-s-1}^{k-p}$. By the same reason as in the previous case, this formula is also valid for all values of s. It may seem at first glance, due to the multiplication principle of combinatorics, that the representation $K_N(s,p,k,l)=M_\uparrow M_\downarrow$ is valid. This is, however, generally not the case. To obtain the correct formula for $K_N(s,p,k,l)$ we note that for $p \geqslant 1$ the variable k can take only three values: $k=2p$, $k=2p-1$, and $k=2p-2$. If $k=2p$ ($k=2p-2$) then both the first and the last domains in a chain belong to the down (up) type, and the previous formula is valid. However, if $k=2p-1$ then those domains belong to different types and, since the first domain can be either of the up or down type, we find for this case $K_N(s,p,k,l)=2M_\uparrow M_\downarrow$. Collecting the above results, we obtain

$$K_N(s,p,k,l) = (1+\delta_{k,2p-1})C_{s-l-1}^{p-2+\Delta_{spkl}}C_{N-s-1}^{k-p}. \tag{3.1}$$

Note that this representation of the function $K_N(s,p,k,l)$ is valid if the values of its variables are compatible with each other.

B. Three-variable joint probability functions

By using Eqs. (2.6) and (3.1), we next can determine all the three-variable joint probability functions, namely,

$P_N(s,p,k)$, $P_N(p,k,l)$, $P_N(s,p,l)$, and $P_N(s,k,l)$. In view of our purpose, however, i.e., for determining the mentioned above one-variable probability functions, we need only two of them, $P_N(s,p,k)$ and $P_N(p,k,l)$. According to the common rule, to calculate the joint probability function $P_N(s,p,k)$ we need to fix its variables and to perform the summation of $P_N(s,p,k,l)$ over the admissible values of l. Since $l=0$ (and $p=k=0$) if $s=0$, and $l=N$ (and $p=1$, $k=0$) if $s=N$, and $1\leqslant l\leqslant s-p+1$ if $1\leqslant s\leqslant N-1$, we find

$$P_N(s,p,k) = \begin{cases} W_N(0), & s=0,\ s=N, \\ \widetilde{P}_N(s,p,k), & 1\leqslant s\leqslant N-1. \end{cases} \tag{3.2}$$

Here, we have used the conditions that $P_N(0,0,0,0)=W_N(0)$ and $P_N(N,1,0,N)=W_N(0)$, and introduced the notation

$$\widetilde{P}_N(s,p,k) = \sum_{l=1}^{s-p+1} P_N(s,p,k,l). \tag{3.3}$$

In order to evaluate the above sum, we evaluate first the sum $S_1=\sum_{l=1}^{s-p+1}C_{s-l-1}^{p-2}$. If $p=1$ (i.e., $s\geqslant 1$) then, using the properties of binomial coefficients, we obtain $S_1=\sum_{l=1}^{s}C_{s-l-1}^{-1}=C_{-1}^{-1}=1$, and if $p\geqslant 2$ (i.e., $s\geqslant 2$) then, using the relation [18],

$$\sum_{m=0}^{n} C_{c-m}^{b} = C_{c+1}^{b+1} - C_{c-n}^{b+1}, \tag{3.4}$$

being valid when the binomial coefficients exist, we have $S_1=C_{s-1}^{p-1}-C_{p-2}^{p-1}$. Since $C_{p-2}^{p-1}=0$ if $p\geqslant 2$ and $C_{s-1}^{p-1}=1$ if $p=1$, we conclude that the formula $S_1=C_{s-1}^{p-1}$ holds for all $s\geqslant 1$ (we recall that $1\leqslant p\leqslant s$). Therefore, substituting Eq. (3.1) into Eq. (2.6), from Eq. (3.3) we obtain

$$\widetilde{P}_N(s,p,k) = (1+\delta_{k,2p-1})W_N(k)C_{s-1}^{p-1}C_{N-s-1}^{k-p}. \tag{3.5}$$

Although this formula has been derived for $1\leqslant s\leqslant N-1$, its right-hand side exists also for $s=0$ (when $p=k=0$) and $s=N$ (when $p=1$ and $k=0$). Furthermore, since $\widetilde{P}_N(0,0,0)=\widetilde{P}_N(N,1,0)=W_N(0)$, the desired joint probability function (3.2) is given by the same expression, i.e.,

$$P_N(s,p,k) = (1+\delta_{k,2p-1})W_N(k)C_{s-1}^{p-1}C_{N-s-1}^{k-p}. \tag{3.6}$$

To evaluate $P_N(p,k,l)$, we need to find the admissible values of s for fixed p, k, and l. If $p=0$ then $s=0$ (and $p=l=0$), if $p=1$ then $s=l$ for $k=1,2$ and $s=l=N$ for $k=0$, and if $2\leqslant p\leqslant N/2$ then $p+l-1\leqslant s\leqslant N-(k-p+1)$ (recall that $k-p+1$ is the number of down domains in a chain). According to this observation we get

$$P_N(p,k,l) = \begin{cases} W_N(0), & p=0, \\ P_N(l,1,k,l), & p=1, \\ \widetilde{P}_N(p,k,l), & 2\leqslant p\leqslant N/2, \end{cases} \tag{3.7}$$

where

$$P_N(l,1,k,l) = (1+\delta_{k,1})W_N(k)C_{N-l-1}^{k-1} \tag{3.8}$$

and

$$\widetilde{P}_N(p,k,l) = \sum_{s=p+l-1}^{N+p-k-1} P_N(s,p,k,l). \tag{3.9}$$

By use of the relation [18]

$$\sum_{m=0}^{n} C_{c+m}^{c} C_{b-m}^{b-n} = C_{b+c+1}^{n} \tag{3.10}$$

in evaluating

$$\sum_{s=p+l-1}^{N+p-k-1} C_{s-l-1}^{p-2} C_{N-s-1}^{k-p} = C_{N-l-1}^{k-1}, \tag{3.11}$$

from Eq. (3.9) we obtain

$$\widetilde{P}_N(p,k,l) = (1+\delta_{k,2p-1})W_N(k)C_{N-l-1}^{k-1}. \tag{3.12}$$

Comparing this formula with (3.8), we check that, although Eq. (3.12) is derived for $p\geqslant 2$, it remains also valid for $p=1$. Therefore, introducing the notation $\Delta_{pkl}=\delta_{p,0}\delta_{k,0}\delta_{l,0}$, the result in Eq. (3.7) can be represented in the appealing form

$$P_N(p,k,l) = (1+\delta_{k,2p-1})W_N(k)C_{N-l-1}^{k-1+\Delta_{pkl}}. \tag{3.13}$$

C. Two-variable probability functions

The four-variable joint probability function $P_N(s,p,k,l)$ generates six different two-variable joint probability functions. But keeping in mind the one-variable probability functions, we calculate only two of them, namely $P_N(p,k)$ and $P_N(k,l)$. Because $P_N(p,k)=W_N(0)$ if $k=0$ and the parameter s varies from p to $N+p-k-1$ if $1\leqslant k\leqslant N-1$, the former is given by

$$P_N(p,k) = \begin{cases} W_N(0), & k=0, \\ \widetilde{P}_N(p,k), & 1\leqslant k\leqslant N-1, \end{cases} \tag{3.14}$$

where

$$\widetilde{P}_N(p,k) = \sum_{s=p}^{N+p-k-1} P_N(s,p,k). \tag{3.15}$$

Taking into account that, according to Eq. (3.10), the relation

$$\sum_{s=p}^{N+p-k-1} C_{s-1}^{p-1} C_{N-s-1}^{k-p} = C_{N-1}^{k} \tag{3.16}$$

holds (we used the condition $C_n^{n-m}=C_n^m$), we obtain

$$P_N(p,k) = (1+\delta_{k,2p-1})W_N(k)C_{N-1}^{k}. \tag{3.17}$$

The same expression for $P_N(p,k)$ follows also from the joint probability function (3.13). Indeed, since for $1\leqslant k\leqslant N-1$ the parameter l is varied from 1 to $N-k$ (the maximal value of l corresponds to the case when all the remaining $p-1$ up domains and all $k-p+1$ down domains consist of one spin), we have

$$\tilde{P}_N(p,k) = \sum_{l=1}^{N-k} P_N(s,p,l). \tag{3.18}$$

Substituting Eq. (3.13) into Eq. (3.18), and using the formula $\sum_{l=1}^{N-k} C_{N-l-1}^{k-1} = C_{N-1}^{k} - C_{k-1}^{k}$, which results from Eq. (3.4), and granting the conditions $C_{k-1}^{k}=0$ $(k\neq 0)$ and $C_{N-1}^{0}=1$, we again arrive at Eq. (3.17).

In order to find $P_N(k,l)$ from Eq. (3.13), we first notice that for fixed k the parameter p can take only one or two values. More precisely, if k is odd, i.e., $k=2h+1$ $(0\leqslant h \leqslant N/2-1)$, then the first and the last spins of a chain belong to the different types. In this case, $p=h+1$, $1\leqslant l\leqslant N-2h-1$, and $P_N(k,l)=P_N(h+1,2h+1,l)$. On the contrary, if k is even, i.e., $k=2h$, then the first and the last spins belong to the same type. In accordance with this, at $1\leqslant l\leqslant N-2h$, the parameter p takes two values $p=h$ (if a chain begins and ends by the down spins) and $p=h+1$ (if a chain begins and ends by the up spins), and so $P_N(k,l)=P_N(h,2h,l)+P_N(h+1,2h,l)$. Moreover, if $l=0$ $(p=k=0)$ or $l=N$ $(p=1,\ k=0)$ then $P_N(k,l)=W_N(0)$. Combining these results yields

$$P_N(k,l) = \begin{cases} W_N(0), & l=0,\ l=N, \\ \tilde{P}_N(k,l), & 1\leqslant l\leqslant N-1, \end{cases} \tag{3.19}$$

where

$$\tilde{P}_N(k,l) = \sum_{p=[(k+1)/2]}^{[k/2]+1} P_N(p,k,l) \tag{3.20}$$

wherein $[x]$ denotes the integer part of x. Finally, taking into consideration the following relation:

$$\sum_{p=[(k+1)/2]}^{[k/2]+1} (1+\delta_{k,2p-1}) = 2, \tag{3.21}$$

we find from Eqs. (3.19), (3.20), and (3.13) for the desired probability function the result

$$P_N(k,l) = (2-\delta_{l,0}-\delta_{l,N}) W_N(k) C_{N-l-1}^{k-1+\Delta_{kl}} \tag{3.22}$$

$(\Delta_{kl}=\delta_{k,0}\delta_{l,0})$.

IV. DISTRIBUTION OF DOMAIN WALLS

According to Eqs. (3.17) and (3.21), the one-variable probability function

$$P_N(k) = \sum_{p=[(k+1)/2]}^{[k/2]+1} P_N(p,k), \tag{4.1}$$

which characterizes the distribution of the number of domain walls in a finite chain, is written as

$$P_N(k) = 2W_N(k) C_{N-1}^{k}. \tag{4.2}$$

The last formula reflects the fact that $P_N(k)$ is the overall probability of all $2C_{N-1}^{k}$ spin configurations each of which possesses k domain walls and has the probability $W_N(k)$ (we are grateful to an anonymous referee for this point). By using Eqs. (2.3)–(2.5) and introducing the designation $r=(1+e^{2\beta J})^{-1}$ $(0<r<1/2)$, it can be recast to read as

$$P_N(k) = C_{N-1}^{k} r^k (1-r)^{N-1-k} \tag{4.3}$$

$(0\leqslant k\leqslant N-1)$. This explicitly shows that a binomial distribution for k emerges.

The fact that the number of domain walls in an Ising chain is binomially distributed has a simple interpretation. To demonstrate this we first remind ourselves that the binomial distribution gives the probability $C_n^m q^m (1-q)^{n-m}$ of m successes in a sequence of n independent trials, called Bernoulli trials, each of which has only one outcome, i.e., success with probability q or failure with probability $1-q$. In our case, we consider a chain as a result of one-by-one addition of $N-1$ spins to the seed one. We treat each addition as a trial whose outcome is either along or opposite the direction of the added spin with respect to the direction of the nearest spin. If the added spin has the opposite direction then the domain wall is formed and we call such an outcome a success. Hence, a chain of N Ising spins with k domain walls is equivalent, in the above sense, to a sequence of $N-1$ Bernoulli trials that have k successes. Due to the exchange interaction, the probability q of success equals $e^{-\beta J}/(e^{-\beta J}+e^{\beta J})=r$, and so the probability that a chain has exactly k domain walls is indeed given by Eq. (4.3).

The probability function (4.3) is properly normalized, i.e., $\sum_{k=0}^{N-1} P_N(k)=1$, and, in accordance with well-known properties of the binomial distribution [17], the average $\langle k\rangle = \sum_{k=1}^{N-1} k P_N(k)$ and the variance $\sigma_k^2 \equiv \langle k^2\rangle - \langle k\rangle^2 = \sum_{k=1}^{N-1} k^2 P_N(k) - \langle k\rangle^2$ of the number of domain walls in a chain assume the form

$$\langle k\rangle = (N-1)r, \quad \sigma_k^2 = (N-1)(1-r)r. \tag{4.4}$$

For $\beta J \ll 1$, we obtain $\langle k\rangle=(N-1)(1-\beta J)/2$ and $\sigma_k^2=(N-1)(1-\beta^2 J^2)/4$ with linear and quadratic accuracy in βJ, respectively. The relation $\lim_{\beta J\to 0}\langle k\rangle=(N-1)/2$ makes explicit that in the high-temperature case, which is characterized by the condition $r=1/2$, approximately one domain wall falls on two spins, implying that each domain contains, on average, two spins (see also Sec. VI).

The increase of βJ leads to the decrease of r and Eq. (4.4) yields $\langle k\rangle \approx \sigma_k^2 \approx (N-1)e^{-2\beta J}$ for large enough values of βJ. If $2\beta J \gg \ln N$ then the condition $\langle k\rangle \ll 1$ holds, which indicates that in this case the spin configurations $\{\sigma_i=1\}$ and $\{\sigma_i=-1\}$ play the main role in determining the chain properties. Let τ_{tr} and τ_m be the transition time between these states, i.e., the average time during which a chain passes from the state $\{\sigma_i=1\}$ to the state $\{\sigma_i=-1\}$, and the measurement time, i.e., the total time necessary to perform a measurement of the magnetization, respectively. Then, if $2\beta J \gg \ln N$ and $\tau_{tr} \gg \tau_m$, a chain possesses a spontaneous magnetization. In other words, these conditions form a criterion of the ferromagneticlike behavior of a finite Ising chain. Notice that in the thermodynamic limit $(N\to\infty)$ the second condition holds always, see just below, while the first condition holds only if $T=0$. Therefore, in full agreement with [1], the long-range ferromagnetic order in an infinite chain occurs only at zero temperature.

In order to estimate the dependence of τ_{tr} on N, it is necessary to go beyond the Ising model. To this end, we consider the Ising spins as the classical Heisenberg spins with large uniaxial anisotropy and use the Arrhenius-Neel law [19,20]. According to it, the average time τ between the spin reversals can be evaluated as $\tau \sim \tau_0 e^{\beta \Delta U}$, where τ_0 is the spin precession time, and $\Delta U(\gg \beta^{-1})$ is the height of the potential barrier between two equilibrium directions of each spin. Since a chain in a state with $\langle k\rangle \ll 1$ can be associated with a single enlarged spin for which the potential barrier height is given by $N\,\Delta U$, we find that the transition time τ_{tr} exponentially grows with N: $\tau_{tr} \sim \tau e^{(N-1)\beta \Delta U}$. Note also that because $\beta J \to \infty$ and $\tau_{tr} \to \infty$ as $T \to 0$, there is always a temperature interval where a finite Ising chain exhibits the ferromagneticlike behavior.

We briefly discuss here also the problem of domain walls distribution in an infinite chain. As is well known [21], the binomial distribution has no unique asymptotic as the number of Bernoulli trials tends to infinity. However, since in our case the parameter r does not depend on N, the probability function $P_N(k)$ does have it. To characterize $P_N(k)$ as $N \to \infty$, we assume in Eq. (4.3) that $k = \langle k\rangle + \sigma_k z$ and define the probability function $P_k(z) = \lim_{N\to\infty} \sigma_k P_N(\langle k\rangle + \sigma_k z)$ of the parameter z. Applying a local limit theorem [21], we immediately find that $P_k(z)$ has the standard Gaussian distribution: $P_k(z) = (2\pi)^{-1/2} e^{-z^2/2}$.

V. DISTRIBUTION OF UP DOMAINS

To derive the one-variable probability function $P_N(p)$ that describes the distribution of the number of up domains in a finite chain, we again proceed from the joint probability function $P_N(p,k)$. A simple consideration shows that $k=0$ if $p=0$, $k=2p-i$ $(i=0,1,2)$ if $1 \leq p \leq N/2-1$, and $k=2p-i$ $(i=1,2)$ if $p=N/2$. Hence, for fixed p the parameter k is varied from $2p-2+2\delta_{p,0}$ to $2p-\delta_{p,N/2}$, and $P_N(p)$ is given by

$$P_N(p) = \sum_{k=2p-2+2\delta_{p,0}}^{2p-\delta_{p,N/2}} P_N(p,k). \tag{5.1}$$

Substituting Eq. (3.17) into this formula and taking into account the properties of binomial coefficients, this probability distribution is obtained as

$$P_N(p) = \sum_{n=0}^{2} (1+\delta_{1,n}) W_N(2p-n) C_{N-1}^{2p-n}. \tag{5.2}$$

Finally, using Eqs. (2.3)–(2.5), from Eq. (5.2) we find the desired probability function in the form

$$P_N(p) = \frac{1}{2}\sum_{n=0}^{2} (1+\delta_{1,n}) C_{N-1}^{2p-n} r^{2p-n}(1-r)^{N-1-2p+n} \tag{5.3}$$

$(0 \leq p \leq N/2)$. This distribution, due to its formal closeness to the ordinary binomial distribution, will be termed the *modified binomial distribution.*

Taking into consideration the results for the finite series [18],

$$\sum_{k=0}^{[n/2]} C_n^{2k} x^k = \frac{(1+\sqrt{x})^n + (1-\sqrt{x})^n}{2}, \tag{5.4}$$

$$\sum_{k=0}^{[(n-1)/2]} C_n^{2k+1} x^k = \frac{(1+\sqrt{x})^n - (1-\sqrt{x})^n}{2\sqrt{x}}, \tag{5.5}$$

and the properties of the binomial coefficients, one readily finds that the quantities

$$I_n^m = \sum_{p=0}^{N/2} C_{N-1-m}^{2p-n-m} r^{2p-n}(1-r)^{N-1-2p+n} \tag{5.6}$$

$(n,m=0,1,2)$ can be represented in the form

$$I_n^m = \frac{r^m}{2}[1+(-1)^{n+m}(1-2r)^{N-1-m}]. \tag{5.7}$$

With these results, it follows that the modified binomial distribution is also properly normalized, namely,

$$\sum_{p=0}^{N/2} P_N(p) = \frac{1}{2}\sum_{n=0}^{2} (1+\delta_{1,n}) I_n^0 = 1. \tag{5.8}$$

The average of the number of up domains in a chain is defined as $\langle p\rangle = \sum_{p=0}^{N/2} p P_N(p)$. Using the probability function (5.3) and the identity

$$2pC_{N-1}^{2p-n} = nC_{N-1}^{2p-n} + (N-1)C_{N-2}^{2p-n-1}, \tag{5.9}$$

which can be verified directly, we find

$$\langle p\rangle = \frac{1}{4}\sum_{n=0}^{2} (1+\delta_{1,n})[nI_n^0 + (N-1)I_n^1], \tag{5.10}$$

and substituting Eq. (5.7) into Eq. (5.10) we obtain

$$\langle p\rangle = \frac{1}{2} + \frac{1}{2}(N-1)r. \tag{5.11}$$

It may seem strange at first glance that $\langle p\rangle = 1/2$ in the low-temperature limit $(r \to 0)$, but in compliance with Eq. (5.3) at $r \to 0$ only two states of a chain, namely $\{\sigma_i = -1\}$ $(p=0)$ and $\{\sigma_i = 1\}$ $(p=1)$, have nonzero probabilities and they are equal to $1/2$. Notice also that, according to Eqs. (4.4) and (5.11), the general condition $2\langle p\rangle = 1 + \langle k\rangle$ always holds.

To find the variance $\sigma_p^2 = \langle p^2\rangle - \langle p\rangle^2$ of the number of up domains in a chain, we first calculate the second moment $\langle p^2\rangle = \sum_{p=0}^{N/2} p^2 P_N(p)$. By applying the identity

$$4p^2 C_{N-1}^{2p-n} = n^2 C_{N-1}^{2p-n} + (2n+1)(N-1)C_{N-2}^{2p-n-1} + (N-1)(N-2)C_{N-3}^{2p-n-2} \tag{5.12}$$

(note that last term equals zero at $N=2$) and the notation (5.6), this quantity can be expressed as

$$\langle p^2\rangle = \frac{1}{8}\sum_{n=0}^{2}(1+\delta_{1,n})[n^2I_n^0 + (2n+1)(N-1)I_n^1 + (N-1)(N-2)I_n^2]. \quad (5.13)$$

Inserting Eq. (5.7) into this formula and performing straightforward calculations yields

$$\langle p^2\rangle = \frac{3}{8} + \frac{3}{4}(N-1)r + \frac{1}{4}(N-1)(N-2)r^2 + \frac{1}{8}(1-2r)^{N-1}. \quad (5.14)$$

Therefore, using the definition of the variance σ_p^2, we find

$$\sigma_p^2 = \frac{1}{8} + \frac{1}{4}(N-1)(1-r)r + \frac{1}{8}(1-2r)^{N-1}. \quad (5.15)$$

The fact that $\langle p^2\rangle \to 1/2$ ($\sigma_p^2 \to 1/4$) as $r\to 0$ has the same interpretation as the low-temperature behavior of $\langle p\rangle$ given above.

In conclusion, we note that if $p=\langle p\rangle + \sigma_p z$ as $N\to\infty$ then the parameter z again possesses a standard Gaussian distribution (see Appendix A).

VI. DISTRIBUTION OF DOMAIN LENGTHS

To find the probability function of domain lengths, $P_N(l)$, we proceed from the joint probability function (3.22). Since for $1\leqslant l\leqslant N-1$ the number of domain walls k can vary from 1 to $N-l$ and $k=0$ if $l=0$ or $l=N$, this probability function can be written as

$$P_N(l) = \begin{cases} W_N(0), & l=0,\ l=N, \\ \widetilde{P}_N(l), & 1\leqslant l\leqslant N-1, \end{cases} \quad (6.1)$$

where

$$\widetilde{P}_N(l) = \sum_{k=1}^{N-l} P_N(k,l). \quad (6.2)$$

In virtue of this, taking into account that $W_N(0)=(1-r)^{N-1}/2$ and using the standard series $\Sigma_{k=0}^{n} C_n^k x^k = (1+x)^n$ which permits us to reduce Eq. (6.2) into the form $\widetilde{P}_N(l)=r(1-r)^{l-1}$, we obtain

$$P_N(l) = \begin{cases} (1-r)^{N-1}/2, & l=0,\ l=N, \\ r(1-r)^{l-1}, & 1\leqslant l\leqslant N-1. \end{cases} \quad (6.3)$$

It is not difficult to verify, using the well-known relation $\Sigma_{k=0}^{n} x^k = (1-x^{n+1})/(1-x)$, that this distribution, which we term the *finite geometric distribution*, is normalized, i.e., $\Sigma_{l=0}^{N} P_N(l)=1$. Note also that in the limit of an infinite chain the domain lengths distribution (6.3) is reduced to the geometric distribution, $P_\infty(l)=r(1-r)^{l-1}$ $(l=1,2,\ldots)$, whose mean and variance are $1/r$ and $(1-r)/r^2$, respectively.

By applying the standard series, $\Sigma_{k=0}^{n} kx^k = [x+(nx-n-1)x^{n+1}]/(1-x)^2$, the average length of an up domain, $\langle l\rangle = \Sigma_{l=0}^{N} lP_N(l)$, can be represented in the form

$$\langle l\rangle = \frac{2-Nr(1-r)^{N-1}-2(1-r)^N}{2r}. \quad (6.4)$$

An alternative derivation of this result is presented in Appendix B. According to this expression, we find $\lim_{N\to\infty}\langle l\rangle = 1/r$, $\lim_{r\to 0}\langle l\rangle = N/2$, and $\lim_{r\to 1/2}\langle l\rangle = 2-(N+2)2^{-N}$. The last condition shows that in the high-temperature limit the average number of spins that form one up domain in a long chain is approximately equal to 2.

All other moments of the finite geometric distribution (6.3) are also calculated exactly. In particular, the variance of domain lengths, $\sigma_l^2 = \langle l^2\rangle - \langle l\rangle^2$, is given by

$$\sigma_l^2 = (1-r)/r^2 - (N/2)^2[2+(1-r)^{N-1}](1-r)^{N-1} - N[1-2r + (1-r)^N](1-r)^{N-1}/r + [r-(1-r)^N](1-r)^N/r^2. \quad (6.5)$$

With this result we immediately obtain $\sigma_l^2 \to (1-r)/r^2$ as $N\to\infty$, $\sigma_l^2\to N^2/4$ as $r\to 0$, and $\sigma_l^2 \to 2-(N^2-2)2^{-N}-(N+2)^2 2^{-2N}$ as $r\to 1/2$.

To gain more insight into the domain statistics, we also introduce the probability function $P_N^+(l)$ that describes the domain lengths distribution in assemblies of Ising chains, each of which contains at least one up domain of nonzero length. In other words, we assume that the parameter l can vary from 1 to N. In this case, in contrast with Eq. (3.22), the joint probability function $P_N^+(k,l)$ that a chain contains k domain walls and the first up domain contains l spins is written as

$$P_N^+(k,l) = (2-\delta_{l,N})W_N^+(k)C_{N-l-1}^{k-1}, \quad (6.6)$$

where $W_N^+(k)=e^{-\beta E_N(k)}/Z_N^+$ and $Z_N^+ = Z_N - e^{\beta J(N-1)}$ is the partition function for such a chain. Therefore, the probability function $P_N^+(l)$, which is defined as $P_N^+(l)=\Sigma_{k=1-\delta_{l,N}}^{N-l} P_N^+(k,l)$, assumes the form

$$P_N^+(l) = \frac{2}{2-(1-r)^{N-1}}\begin{cases} (1-r)^{N-1}/2, & l=N, \\ r(1-r)^{l-1}, & 1\leqslant l\leqslant N-1. \end{cases} \quad (6.7)$$

One can again verify that the normalization condition $\Sigma_{l=1}^{N} P_N^+(l)=1$ holds, and that the average length of an up domain, $\langle l\rangle^+ = \Sigma_{l=1}^{N} lP_N^+(l)$, can be represented as

$$\langle l\rangle^+ = \frac{2-Nr(1-r)^{N-1}-2(1-r)^N}{2r-r(1-r)^{N-1}}. \quad (6.8)$$

As $N\to\infty$, the averages $\langle l\rangle^+$ and $\langle l\rangle$ tend to the same limit, but their low- and high-temperature limits are different: $\lim_{r\to 0}\langle l\rangle^+ = N$ and $\lim_{r\to 1/2}\langle l\rangle^+ = 2-N/(2^N-1)$. The former confirms the possibility of the existence of the ferromagneticlike state in a finite Ising chain at low temperatures. We note in this context that the condition $2\beta J \gg \ln N$, which we introduced in Sec. IV is equivalent to the condition $\xi\gg N$, where ξ is the spin-spin correlation length. According to [22], in the case of Ising chains with only exchange interaction and free boundary conditions the correlation length is given by the exact formula $\xi = -\ln^{-1}(1-2r)$. Since at low temperatures the asymptotic relations $\xi\sim 1/2r$ and $r\sim e^{-2\beta J}$ hold, the condition $\xi\gg N$ is actually reduced to $2\beta J\gg \ln N$.

VII. CONCLUSIONS

We have determined the domain statistics in a finite chain of Ising spins that interact only through the exchange interaction. For a chain with an even number of spins and free boundary conditions, we have calculated, via a combinatorial approach, the joint probability function of four random variables (namely, the number of up spins, the number of up domains, the number of domain walls, and the number of spins in the first up-domain) that thoroughly describe the domain statistics in a chain. Starting out from this result, we derived the probability distribution functions for the number of domain walls, number of up domains, and number of spins in an up domain. The first corresponds to the binomial distribution, the second to the modified binomial distribution, and the third to the finite geometric distribution. For each of them, we have calculated the corresponding thermal average and variance, have analyzed the cases of low and high temperatures, and, as well, have considered the thermodynamic limit.

In addition, we have derived a criterion that a finite Ising chain exhibits the ferromagneticlike behavior. According to it, the transition time between the fully magnetized chain states must exceed the measuring time, and the average number of domain walls must be much less than 1. These conditions hold, i.e., a finite Ising chain does display a ferromagneticlike order on the measuring time scale, if the temperature is sufficiently small.

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APPENDIX A: DISTRIBUTION OF DOMAINS IN AN INFINITE CHAIN

To find the probability function of the parameter z, $P_p(z)=\lim_{N\to\infty}\sigma_p P_N(\langle p\rangle+\sigma_p z)$, first we represent the binomial coefficients in Eq. (5.3) as

$$C_a^b=\frac{\Gamma(a+1)}{\Gamma(b+1)\Gamma(a-b+1)} \tag{A1}$$

($\Gamma(x)$ is the gamma function) and use the Stirling formula [23]

$$\Gamma(x)\sim\sqrt{2\pi}e^{-x}x^{x-1/2}\quad(x\to\infty). \tag{A2}$$

This yields

$$C_{N-1}^{2\langle p\rangle+2\sigma_p z-n}\sim\frac{eR_n}{\sqrt{2\pi N}(1-r)^N}\left(\frac{1-r}{r}\right)^{Nr+2\sigma_p z+3/2-r-n} \tag{A3}$$

and

$$R_n\sim\left(1-\frac{2\sigma_p z+1-r-n}{N(1-r)}\right)^{-N(1-r)+2\sigma_p z+3/2-r-n}\times\left(1+\frac{2\sigma_p z+2-r-n}{Nr}\right)^{-Nr-2\sigma_p z-3/2+r+n} \tag{A4}$$

as $N\to\infty$, and so

$$P_p(z)=\lim_{N\to\infty}\frac{e\sigma_p}{2\sqrt{2\pi r(1-r)N}}\sum_{n=0}^{2}(1+\delta_{1,n})R_n. \tag{A5}$$

Finally, taking into account that $\sigma_p^2/N\to r(1-r)/4$ and $\ln R_n\to -z^2/2-1$ as $N\to\infty$, we indeed find that $P_p(z)=(2\pi)^{-1/2}e^{-z^2/2}$.

APPENDIX B: ALTERNATIVE DERIVATION OF EQ. (6.4)

Using the joint probability function (3.6), we can also represent $\langle l\rangle$ in the following form:

$$\langle l\rangle=\sum_{p=1}^{N/2}\frac{1}{p}\sum_{k=2p-2}^{2p-\delta_{p,N/2}}\sum_{s=p}^{N+p-k-1}sP_N(s,p,k). \tag{B1}$$

Since $sC_{s-1}^{p-1}=pC_s^p$, $W_N(k)=r^k(1-r)^{N-k-1}/2$, and according to the result for the series (3.10),

$$\sum_{s=p}^{N+p-k-1}sC_{s-1}^{p-1}C_{N-s-1}^{k-p}=pC_N^{k+1}, \tag{B2}$$

Eq. (B1) can be rewritten as

$$\langle l\rangle=\frac{(1-r)^{N-1}}{2}\sum_{n=0}^{2}(1+\delta_{1,n})Y_n, \tag{B3}$$

where

$$Y_n=\sum_{p=1}^{N/2}\left(\frac{r}{1-r}\right)^{2p-n}C_N^{2p+1-n}. \tag{B4}$$

Upon calculating these quantities with the help of the series (5.4) and (5.5),

$$Y_n=\frac{1-r}{2r}\left[\left(\frac{1}{1-r}\right)^N-(-1)^n\left(\frac{1-2r}{1-r}\right)^N-2\delta_{1,n}\right]-N\delta_{0,n} \tag{B5}$$

($n=0,1,2$), and substituting the corresponding expressions into Eq. (B3), we again obtain Eq. (6.4).

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