Institute of Physics Publishing Journal of Physics A: Mathematical and General

J. Phys. A: Math. Gen. **37** (2004) 1465–1478 PII: S0305-4470(04)67952-2

Probability distribution of magnetization in the one-dimensional Ising model: effects of boundary conditions

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Received 25 August 2003
Published 19 January 2004
Online at stacks.iop.org/JPhysA/37/1465 (DOI: 10.1088/0305-4470/37/5/001)

Abstract
Finite-size scaling functions are investigated both for the mean-square magnetization fluctuations and for the probability distribution of the magnetization in the one-dimensional Ising model. The scaling functions are evaluated in the limit of the temperature going to zero ($T \to 0$), the size of the system going to infinity ($N \to \infty$) while $N[1 - \tanh(J/k_B T)]$ is kept finite (J being the nearest neighbour coupling). Exact calculations using various boundary conditions (periodic, antiperiodic, free, block) demonstrate explicitly how the scaling functions depend on the boundary conditions. We also show that the block (small part of a large system) magnetization distribution results are identical to those obtained for free boundary conditions.

PACS number: 05.50.+q

1. Introduction

Finite-size scaling has been developed intensively during the last few decades [1–4] and it has become a standard tool in the studies of critical systems. An interesting application of the method is using the finite-size scaling of the distribution function of the order-parameter fluctuations as hallmarks of universality classes. The idea goes back to Bruce [5–7] who used it, e.g., to verify that the gas–liquid transition of the two-dimensional Lennard–Jones fluid belongs to the Ising universality class [8]. The list of applications to thermodynamic critical points is long [9] and the idea has re-emerged in non-equilibrium critical (or effectively critical) systems [10–13], as well.

The usefulness of scaling functions as hallmarks of universality classes depends on their availability for comparisons. Indeed, a significant portion of the applications is about the Ising universality class where the scaling functions for the $d = 2, 3, 4,$ dimensional distribution functions are well known from simulations [14, 15] and field-theoretic results in $d = 4-\epsilon$ are also available [16]. The picture gallery of scaling functions is clearly far from complete since these functions have been systematically worked out only for surface growth models [10] and for Gaussian $1/f^{\alpha}$-type noise processes [13].

An important issue concerning the critical distribution functions is their dependence on the boundary conditions (BCs). While theoretical calculations usually address periodic systems, the building of a histogram of a physical quantity (e.g., the magnetization) in an experimental system involves measuring the magnetizations in patches of a given size within the bulk of the system (corresponding to block-spin magnetizations in an Ising model). As has been shown by Binder [14], the block-spin distribution function at criticality depends on the BCs on the block, a finding that is not entirely unexpected since the infinite-range critical correlations feel the boundaries of the system.

The BC dependence of the scaling functions is an interesting problem and, indeed, there has been a series of works where the PDF of the magnetization for the $d = 2$ Ising model at the critical point has been investigated for various BCs [17] including some exotic ones (Möbius strip, Klein bottle). Similar problems have also been studied for the roughness distribution of $1/f^{\alpha}$-type noise processes [13]. Analytical results about BC dependence of the scaling functions are scarce: they are restricted to Gaussian models [13], expansions around $d = 4$ [16] and around the spherical limit [18]. This is why we decided to revisit the $d = 1$ Ising model where the effect of BCs can be seen in analytical detail.

Although the critical temperature of the $d = 1$ Ising model is zero, it displays non-trivial features in its finite-size scaling as the critical point is approached. The particular case of the distribution function of the magnetization in bulk blocks has already been discussed by Bruce [5]. The purpose of this paper is to calculate the scaling function for the case of periodic (PBCs), antiperiodic (APBCs), free (FBCs) and block (BBCs) boundary conditions, and thus gauge the importance of the role played by the BCs.

For pedagogical purposes, we also compute the finite-size scaling of the magnetization fluctuations. The calculation is elementary in this case and one can easily observe that the periodic, antiperiodic and free BCs yield distinct scaling functions. Furthermore, one can also see explicitly how the scaling function associated with the block BCs emerges when a small part of a large system is used for measuring the fluctuations.

The evaluation of the magnetization distribution is somewhat more involved but can be carried out relatively simply by using a combinatorial approach. For the periodic and free BCs, the calculations yield non-trivial functions which are combinations of two delta peaks and a continuum background, with the relative weight of the delta functions reduced for the case of FBCs. The delta functions disappear entirely for antiperiodic BCs. Finally, the combinatorial approach reproduces Bruce's result for the BBCs and it turns out that the block scaling function is identical to that of the FBC case.

2. Model and notation

We consider the one-dimensional Ising chain of N spins ($\sigma_i = \pm 1, i = 1, \ldots, N$) with ferromagnetic ($J > 0$) coupling and with various BCs. The interaction energy of a given configuration of spins $\{\sigma_i\}$ is given by

$$E(\{\sigma_i\}) = -J \sum_{i=1}^{N-1} \sigma_i \sigma_{i+1} - J_{bc} \sigma_N \sigma_1 \tag{1}$$

where $J_{bc} = J, -J, 0$ for periodic, antiperiodic and free BCs respectively. The model is exactly solvable using, e.g., the transfer matrix formalism [19], and the partition functions for periodic BCs (upper signs) and for antiperiodic BCs (lower signs) are

$$Z^{(p),(a)} = 2^N(\cosh^N K \pm \sinh^N K) \tag{2}$$

while the correlations are given by

$$\langle \sigma_i \sigma_{i+n} \rangle^{(p),(a)} = \frac{v^n \pm v^{N-n}}{1 \pm v^N} \tag{3}$$

where $v = \tanh K$ with $K = J/k_B T$ and, furthermore, $1 \leqslant i, i+n \leqslant N$. The above quantities are particularly simple for free BCs

$$Z^{(f)} = 2^N \cosh^{N-1} K \qquad \langle \sigma_i \sigma_{i+n} \rangle^{(f)} = v^n. \tag{4}$$

Note that the correlations only depend on the distance of the two spins and not on their particular positions within the chain. This is true not only in the periodic case but also for APBCs and FBCs. Also note that the (p), (a) and (f) superscripts refer to periodic, antiperiodic and free BCs respectively throughout the paper.

3. Finite-size scaling of fluctuations

The mean square fluctuations of the total magnetization $M = \sum_{i=1}^N \sigma_i$ can be calculated via the spin correlations as

$$\langle M^2 \rangle = \sum_{i,j=1}^{N} \langle \sigma_i \sigma_j \rangle. \tag{5}$$

We begin with the discussion of $\langle M^2 \rangle$ for the periodic, free-, and antiperiodic BCs, leaving the case of block BCs for a separate subsection.

3.1. Periodic-, free-, and antiperiodic BC

Substituting the expressions for the spin correlations (3), (4) into equation (5), one easily finds

$$\frac{\langle M^2 \rangle}{N} = \begin{cases} \frac{1+v}{1-v}\frac{1-v^N}{1+v^N} & \text{PBC} \\ \frac{1+v}{1-v}\frac{1+v^N}{1-v^N} - \frac{4v}{N(1-v)^2} & \text{APBC} \\ \frac{1+v}{1-v} - \frac{2v(1-v^N)}{N(1-v)^2} & \text{FBC.} \end{cases} \tag{6}$$

In the thermodynamic limit ($N \to \infty$) all the above expressions reduce to

$$\frac{\langle M^2 \rangle}{N} = \frac{1+v}{1-v}. \tag{7}$$

One can see that the fluctuations diverge as $T \to 0$, and they have a power-law singularity provided $t = 1 - v = 1 - \tanh J/k_B T$ is used as the control parameter. One can also read off (7) the value ($\gamma = 1$) of the susceptibility exponent [20].

The correlation-length exponent, ν, is another exponent needed in finite-size scaling. It is obtained from the spin–spin correlations which decay exponentially in the thermodynamic limit. The correlation length, ξ, defined by the exponential decay is independent of the BC

$$\langle \sigma_i \sigma_{i+n} \rangle_{N\to\infty} = v^n = \mathrm{e}^{-n \ln(1/v)} = \mathrm{e}^{-n/\xi}. \tag{8}$$

and diverges for $T \to 0$ as

$$\xi = -\frac{1}{\ln[1-(1-v)]} \sim (1-v)^{-1} = t^{-1} \tag{9}$$

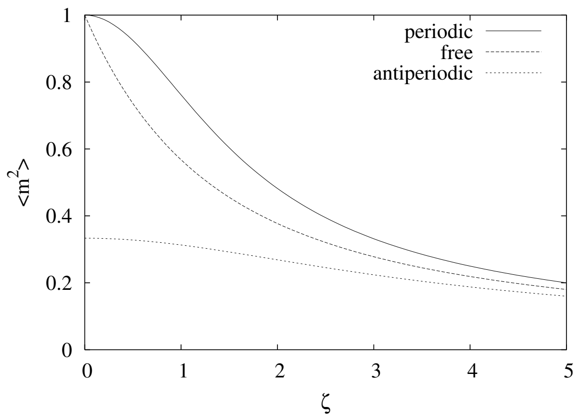

Figure 1. Magnetization fluctuations in the scaling limit for various BCs (see equation (13)). The scaling variable is $\zeta = Nt/2$.

thus providing us with $\nu = 1$. As noted by Chen and Dohm [21], the above definition of the correlation length (rather than that found from the second moment of the correlation function) is the appropriate one to discuss finite-size scaling for this model.

The scaling form one expects in finite-size scaling in dimension d is as follows [1]:

$$\frac{\langle M^2\rangle}{N^{1+\gamma/d\nu}} = \Phi(tN^{1/d\nu}) \tag{10}$$

with N being the number of spins. Putting in the above expression $d = \gamma = \nu = 1$, the finite-size scaling suggestion takes the form

$$\frac{\langle M^2\rangle}{N^2} = \langle m^2\rangle = \Phi(tN) \tag{11}$$

where $m = M/N$ is the magnetization density.

Dividing both sides of equations (6) by N, we indeed find that $\langle M^2\rangle/N^2 = \langle m^2\rangle$ yields well-defined scaling functions in the limit of $t = 1 - v \to 0$ while $tN = 2\zeta$ is kept finite. The scaling variable ζ has a simple meaning since, in the scaling limit

$$2\zeta = Nt = N/\xi, \tag{12}$$

i.e., 2ζ is the average number of domains (or domain walls) in the system. The actual scaling functions are given below

$$\frac{\langle M^2\rangle}{N^2} = \langle m^2\rangle = \begin{cases} \frac{1}{\zeta}\tanh\zeta & \text{PBC} \\ \frac{1}{\zeta}\left(\coth\zeta - \frac{1}{\zeta}\right) & \text{APBC} \\ \frac{1}{\zeta}\left(1 - \frac{1-\mathrm{e}^{-2\zeta}}{2\zeta}\right) & \text{FBC} \end{cases} \tag{13}$$

and they are shown in figure 1. The functions belonging to different BC are clearly distinct thus demonstrating explicitly the BC dependence of the scaling functions.

The scaling functions coincide for $\zeta \to \infty$. This is understandable since large ζ means large number of domain walls which means that the disordered regime is approached where the effects of the BCs diminish. The differences in $\zeta \to 0$ limit can be accounted for by the number of domain walls in the system. In particular, the ground state is completely aligned

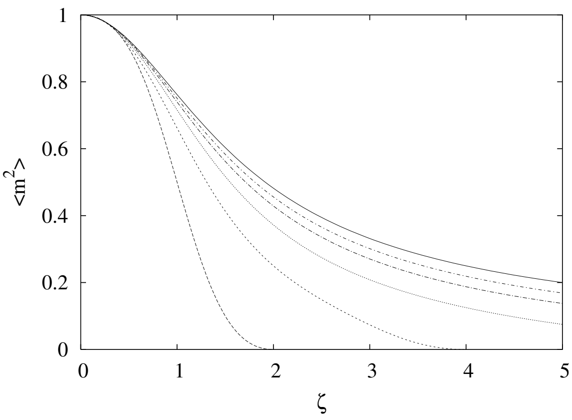

Figure 2. Correction to scaling for magnetization fluctuations for periodic BCs. First equation in (6) is used to calculate $\langle m^2\rangle = \langle M^2\rangle/N^2$ for system with $N = 2, 4, 8, 16, 32$ and ∞. The scaling variable is $\zeta = Nt/2$. The $1/N$ dependence of the correction can be visually observed (note that the distance from the $N = \infty$ curve is halved as N is doubled).

for PBCs and FBCs systems while it contains an arbitrarily positioned single domain wall in the case of APBCs. As a result

$$\langle m^2\rangle^{(p),(f)} = 1 \qquad \langle m^2\rangle^{(a)} = 1/3 \tag{14}$$

explaining the values of the scaling functions at $\zeta = 0$.

The small $\zeta = 0$ behaviour of $\langle m^2\rangle$ can be understood in terms of the smallest energy excitations above the ground states. These excitations are obtained from the ground state by adding a pair domain walls in the case of PBC and APBC, while they consist of a single domain wall for FBC. Their effect is a quadratic (linear) decrease of $\langle m^2\rangle$ near $\zeta = 0$ for PBCs and APBCs (FBCs) systems.

We close this section with a note on the speed of convergence of the scaling function. Looking at equation (6), one can see that $\langle M^2\rangle/N$ converges exponentially to its thermodynamic limit for PBCs, while the convergence is only power law (N^{-1}) for FBCs and APBCs. As to the scaling function, it can be easily shown that the convergence is power law (N^{-1}) even in the PBCs case. More precisely, the correction term is of the form $N^{-1}g(\zeta)$ where $g(\zeta) \leqslant 0$ with $g(\zeta \to 0) = 0$ and $g(\zeta \to \infty) = -1$. Figure 2 displays $\langle m^2\rangle$ calculated from equation (6) for the PBCs case (note that for finite N and using the scaling variable ζ, the results are meaningful only for $\zeta < N$). It should be clear from figure 2 that the convergence is slow although it may appear to be quite good at small ζ due to the particular form of $g(\zeta)$.

3.2. Block (window) boundary conditions

When studying magnetization fluctuations in an experiment, one usually divides the system into blocks and measures the block magnetizations. The corresponding theoretical construction in the $d = 1$ Ising model is to consider a block (window) of length ℓ at a position k in a system of total length N, and study the fluctuations of the block magnetization defined as

$$\left\langle M_\ell^2\right\rangle = \sum_{i,j=k}^{k+\ell-1} \langle \sigma_i\sigma_j\rangle. \tag{15}$$

Provided the full length of the block is within the system (i.e., it does not contain the boundary with the coupling J_{bc}), the correlations entering equation (15) and, consequently, $\langle M_\ell^2\rangle$ does not depend on the location of the block, k, and we can write

$$\langle M_\ell^2\rangle = \ell + 2\sum_{n=1}^{\ell-1}(\ell - n)\langle\sigma_1\sigma_{1+n}\rangle. \tag{16}$$

Substituting now the correlations for PBCs (3), one readily obtains an expression which depends both on the block size ℓ and the system size N

$$\frac{\langle M_\ell^2\rangle^{(p)}}{\ell^2} = \frac{1-v^N}{1+v^N}\frac{1+v}{\ell(1-v)} - \frac{2v(1-v^{N-\ell})}{1+v^N}\frac{1-v^\ell}{\ell^2(1-v)^2} \tag{17}$$

where the superscript (p) denotes the periodic BCs. Introducing the 'aspect ratio' $b = \ell/N$, and using the scaling variable $\zeta = \ell(1-v)/2$, the scaling limit $N \to \infty$, $\ell \to \infty$ with b and ζ finite yields the following scaling function:

$$\begin{aligned}\frac{\langle M_\ell^2\rangle^{(p)}}{\ell^2} &= \langle m_\ell^2\rangle^{(p)}(\zeta, b)\\ &= \frac{1}{\zeta}\left(\tanh\zeta/b - \frac{1-\mathrm{e}^{-2\zeta}}{2\zeta}\frac{1-\mathrm{e}^{-2(1-b)\zeta/b}}{1+\mathrm{e}^{-2\zeta/b}}\right).\end{aligned} \tag{18}$$

As one can see, the scaling function goes over into the FBCs case if $b \to 0$ while it becomes the scaling function for the PBCs case if $b = 1$. The function smoothly interpolates between the limiting cases in $0 < b \leqslant 1$.

If the block is embedded in a FBC system then $\langle M_\ell^2\rangle^{(f)}$ can be deduced from the observation that $\langle\sigma_1\sigma_{1+n}\rangle$ is independent of the system size (see equation (4)). Namely, $\langle M_\ell^2\rangle^{(f)}$ must coincide with $\langle M^2\rangle$ for the FBCs with N replaced by ℓ. Thus we have a scaling function (13) which does not depend on the 'aspect ratio' b

$$\frac{\langle M_\ell^2\rangle^{(f)}}{\ell^2} = \langle m_\ell^2\rangle^{(f)}(\zeta, b) = \langle m^2\rangle^{(f)}(\zeta). \tag{19}$$

Finally, the fluctuations in a block embedded in an antiperiodic chain, can also be calculated and the somewhat more complicated result has a similar structure as in the case of embedding in a periodic chain. Namely, changing the aspect ratio from $b = 1$ to $b = 0$, the result interpolates between the APBCs and the FBCs scaling functions in equation (6).

The common feature of all the above results is that the BCs become irrelevant in the limit $b \to 0$ where the block is much smaller than the system. Furthermore, we find that this bulk behaviour coincides with the FBCs result. Whether this coincidence with the FBCs result is a general feature of bulk fluctuations is not quite clear and should be investigated in more complicated and higher dimensional systems.

4. Magnetization distribution

If at a given temperature, i.e., at a given correlation length, the system size goes to infinity then the magnetization distribution goes to a Gaussian around zero due to the central limit theorem, and goes eventually to a Dirac delta function

$$\lim_{T\to 0}\lim_{N\to\infty} P(m) = \delta(0). \tag{20}$$

On the other hand, at any given system size as the temperature goes to zero, i.e., the correlation length goes to infinity, the magnetization goes to either plus or minus one, and the distribution becomes

$$\lim_{N\to\infty}\lim_{T\to 0} P(m) = \tfrac{1}{2}[\delta(m+1) + \delta(m-1)]. \tag{21}$$

The importance of the $\zeta = Nt/2$ scaling variable is that if $N \to \infty$ and $T \to 0$ in such a way that the correlation length is always proportional to the system size (i.e., ζ is a constant (12)) then a non-tirivial distribution arises even for the $d = 1$ Ising model.

The meaning of ζ suggests the development of a small ζ (small number g of domain walls) expansion. Thus we shall first calculate $P_g(M)$, the probability of a given magnetization in the presence of g domain walls. Once $P_g(M)$ is known, the probability of a given magnetization $P(M)$ can be obtained by summing up $P_g(M)$

$$P(M) = \sum_g P_g(M). \tag{22}$$

The states with g domain walls are degenerate as their energy E_g depends only on the number of walls

$$E_g = \begin{cases} J(2g - N) & \text{PBC} \quad \text{APBC} \\ J(2g - N + 1) & \text{FBC.} \end{cases} \tag{23}$$

Thus, the calculation $P_g(M)$ reduces to counting all possible spin configurations $\Omega_g(M)$ at given g and M values

$$P_g(M) = \frac{\mathrm{e}^{-E_g/k_{\mathrm{B}}T}}{Z}\Omega_g(M). \tag{24}$$

Here Z is the partition function corresponding to a given BC which, in the scaling limit, becomes

$$Z = \begin{cases} 2\,\mathrm{e}^{NK}\cosh\zeta & \text{PBC} \\ 2\,\mathrm{e}^{NK}\sinh\zeta & \text{APBC} \\ 2\,\mathrm{e}^{(N-1)K}\mathrm{e}^{\zeta} & \text{FBC.} \end{cases} \tag{25}$$

For $g = 0$, i.e., if there is no domain wall in the configurations

$$\Omega_0(M) = \delta_{M,N} + \delta_{M,-N}. \tag{26}$$

For $g > 0$, let W_j be the position of the jth wall (say $W_j = i$ when it is just before σ_i) with $j = 1, \ldots, g$, i.e., $W_j < W_{j+1}$ for $j = 1, \ldots, g-1$, and also note that by definition $W_1 > 0$ and $W_g \leqslant N$. Let us denote the magnetization of the domain between W_1 and W_2 by M_1. Now, it is sufficient to obtain the number of configurations with the restriction $M_1 > 0$ and denote it as $\Omega_g^+(M)$,

$$\Omega_g(M) = \Omega_g^+(M) + \Omega_g^+(-M). \tag{27}$$

Note that fixed magnetization also means fixed number of upspins $N_\uparrow = (N+M)/2$ and downspins $N_\downarrow = (N-M)/2$.

4.1. Periodic boundary conditions

PBCs enforce the number of domain walls to be always even $g = 2s$, with $s = 0, \ldots, [N/2]$, where [ ] stands for the integer part. As there is at least one spin after each domain wall, we can imagine those spins as being attached to the walls. A typical configuration looks like

$$\downarrow\downarrow\downarrow\ (W_1 \uparrow)\ \uparrow\uparrow\ (W_2 \downarrow)\ \downarrow\downarrow\downarrow\ \ldots\ \uparrow\uparrow\ (W_{2s} \downarrow)\ \downarrow\downarrow. \tag{28}$$

Now counting all the possible configurations is equivalent to distributing in all possible ways the $N_\uparrow - s$ (not attached) upspins among the s up domains (those domains where the spins are up, i.e., between W_{2j-1} and W_{2j}) and independently distributing the $N_\downarrow - s$ (not attached) downspins among the $s + 1$ down domains (between W_{2j} and W_{2j+1}, also in front of W_1 and behind W_{2s})

$$\Omega^+_{2s}(M) = \binom{N_\uparrow - 1}{s-1}\binom{N_\downarrow}{s}. \tag{29}$$

Note that the binomial coefficient $\binom{a}{b} = 0$ for $a < b$, which reflects the fact that there are no configurations with more domain walls than either $2N_\uparrow$ or $2N_\downarrow$, i.e., $s \leqslant \min(N_\uparrow, N_\downarrow)$. With formula (27) one can easily arrive at Ω_{2s} without restriction on the sign of M_1

$$\Omega_{2s}(M) = \binom{N_\uparrow - 1}{s-1}\binom{N_\downarrow}{s} + \binom{N_\downarrow - 1}{s-1}\binom{N_\uparrow}{s}. \tag{30}$$

In the $N \to \infty$ limit, for fix $n_\uparrow = N_\uparrow/N$ and $n_\downarrow = N_\downarrow/N$ the number of configurations becomes

$$\Omega_{2s}(M) = N^{2s-1}\frac{(n_\uparrow n_\downarrow)^{s-1}}{s!(s-1)!}. \tag{31}$$

In this limit we also need to switch from the discrete probabilities $P(M)$ to the probability density $P(m)$, which brings in a factor $N/2$, and substituting equation (31) into equation (24) leads to

$$P_{2s}(m) = \frac{\mathrm{e}^{NK}}{2Z^{(p)}}\,\mathrm{e}^{-4sK}N^{2s}(n_\uparrow n_\downarrow)^{s-1}. \tag{32}$$

Now the scaling limit can be finally taken using (25), and for $s = 0$ one realizes that the expression of equation (26) develops singularities

$$P_0(m) = \frac{1}{2\cosh\zeta}\left[\delta(m+1) + \delta(m-1)\right]. \tag{33}$$

For $s \neq 0$, using $\zeta = N\,\mathrm{e}^{-2K}$ leads to the final result for the magnetization distribution with a fixed $2s$ number of walls

$$P_{2s}(m) = \frac{(\zeta/2)^{2s}(1-m^2)^{s-1}}{s!(s-1)!\cosh\zeta}. \tag{34}$$

It becomes clear at this point that we are doing a small ζ expansion and that a fixed $2s$ number of domain walls belongs to the order $2s$ of the expansion.

The magnetization distribution without restrictions on the number of walls can be obtained from equation (22) which is valid also in the continuum limit

$$P(m) = \sum_{s=0}^{\infty} P_{2s}(m). \tag{35}$$

Using the series form of the modified Bessel functions

$$I_\nu(x) = \sum_{k=0}^{\infty}\frac{(x/2)^{2k+\nu}}{k!(k+\nu)!} \tag{36}$$

leads to the final expression for periodic BCs

$$P^{(p)}(m) = \frac{1}{2\cosh\zeta}\left[\delta(m+1) + \delta(m-1)\right] + \frac{\zeta}{2\sqrt{1-m^2}\cosh\zeta}I_1\big(\zeta\sqrt{1-m^2}\big). \tag{37}$$

The above function is displayed in figure 3.

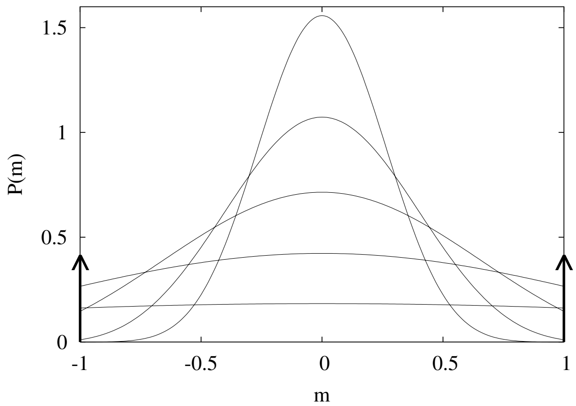

Figure 3. Magnetization distribution $P(m)$ in the $d = 1$ Ising model with periodic BCs in the $T \to 0$ and $N \to \infty$ limit as a function of $m = M/N$ with the scaling variable $\zeta = Nt/2$ fixed at values $\zeta = 1, 2, 4, 8, 16$ (from bottom at origin). The arrows symbolize the singular parts $\sim\delta(m \pm 1)$ of the distributions of equation (37).

One can easily check that $P(m)$ is normalized, i.e., $\int_{-1}^{1} \mathrm{d}m\, P(m) = 1$, by changing the integration variable m to $\theta = \arcsin m$ and using the series form of equation (36). In the same way the expression for the second moment of $P(m)$ in equation (13) can also be obtained.

One can investigate the speed of convergence in N of the magnetization distribution $P(m)$ of equation (37). Instead of making Monte Carlo simulations on the Ising model we calculated numerically the probabilities of possible magnetizations for finite chains, based on equations (24) and (35), and multiplied the results by $(N + 1)/2$ for the sake of comparison with the probability density $P(m)$ in the scaling limit

$$P(m, N) = \frac{N + 1}{2Z} \sum_{s=0}^{[N/2]} \mathrm{e}^{(N-4s)K} \Omega_{2s}(M) \tag{38}$$

where $\Omega_{2s}(M)$ is given by equation (26), (30), and $K = \operatorname{arctanh}(1 - 2\zeta/N)$. Equation (38) can be easily evaluated numerically, as the the computation time increases linearly with N as opposed to the exponentially long time needed to encounter all possible configurations. One observes in figure 4 that the convergence is faster for smaller values of ζ, in agreement with figure 2.

4.2. Antiperiodic boundary conditions

The main difference from the periodic case is that the number of domain walls is odd $g = 2s-1$, with $s = 1, \ldots, [(N+1)/2]$. As there has to be at least one domain wall in each configuration there are no Dirac delta peaks at $m = \pm 1$ in the distribution. A typical configuration looks like

$$\downarrow\downarrow (W_1 \uparrow) \uparrow\uparrow\uparrow (W_2 \downarrow) \downarrow\downarrow \ldots \downarrow\downarrow (W_{2s-1} \uparrow) \uparrow\uparrow\uparrow . \tag{39}$$

The number of configurations with the restriction of $M_1 > 0$ is

$$\Omega^{+}_{2s-1}(M) = \binom{N_\uparrow - 1}{s - 1}\binom{N_\downarrow}{s - 1} \tag{40}$$

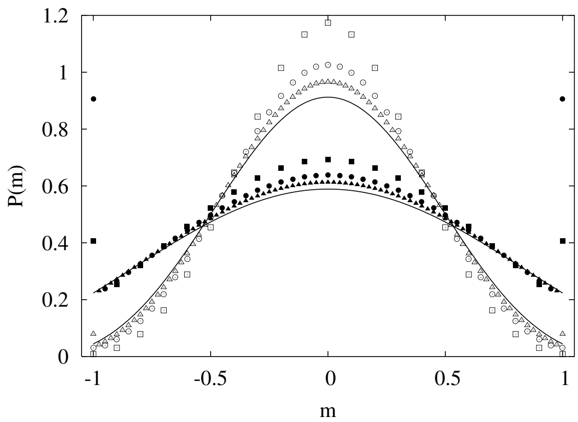

Figure 4. Magnetization distribution $P(m)$ for periodic BCs in the $N \to \infty$ limit (only the regular part of equation (37) is depicted) compared to its finite $N = 20$ (square), 40 (circle), and 80 (triangle) forms of equation (38) with the scaling variable being $\zeta = 3$ (closed symbols), and 6 (open symbols). Observe the evolving singularities at $m = \pm 1$ for finite systems (closed triangles are out of range).

as we have $N_\uparrow - s$ free upspins to distribute into s up domains and $N_\downarrow - s + 1$ free downspins for s down domains. In the continuum limit the number of configurations becomes

$$\Omega_{2s-1}(M) = 2N^{2s-2} \frac{(n_\uparrow n_\downarrow)^{s-1}}{(s-1)!^2} \tag{41}$$

and the magnetization distribution with fixed number of walls (24) reads

$$P_{2s-1}(m) = \frac{(\zeta/2)^{2s-1}(1-m^2)^{s-1}}{(s-1)!^2 \sinh\zeta}. \tag{42}$$

Summing this expression up over the possible number of walls (22) leads to the final result

$$P^{(a)}(m) = \frac{\zeta}{2\sinh\zeta} I_0\big(\zeta\sqrt{1-m^2}\big). \tag{43}$$

4.3. Free boundary conditions

In the case of free BCs the number of domain walls can be both even $g = 2s$ and odd $g = 2s-1$ with $s = 1, \ldots, [N/2]$. The only difference in counting all possible configurations, with a given g, M, and the condition $M_1 > 0$, is the supplementary restriction that there always has to be a down spin before the first wall for obvious reasons, which can be visualized as ($\downarrow W_1 \uparrow$) in example (28). Now the number of configurations can be easily obtained

$$\begin{aligned} \Omega^+_{2s-1}(M) &= \binom{N_\uparrow - 1}{s-1}\binom{N_\downarrow - 1}{s-1} \\ \Omega^+_{2s}(M) &= \binom{N_\uparrow - 1}{s-1}\binom{N_\downarrow - 1}{s} \end{aligned} \tag{44}$$

and one observes that in the scaling limit they are equal to the corresponding periodic (31) or antiperiodic (41) result, i.e., $\Omega^{(f)}_{2s}(M) = \Omega^{(p)}_{2s}(M)$ and $\Omega^{(f)}_{2s-1}(M) = \Omega^{(a)}_{2s-1}(M)$. The energies of both the even and odd states are greater than the energies of the corresponding periodic and

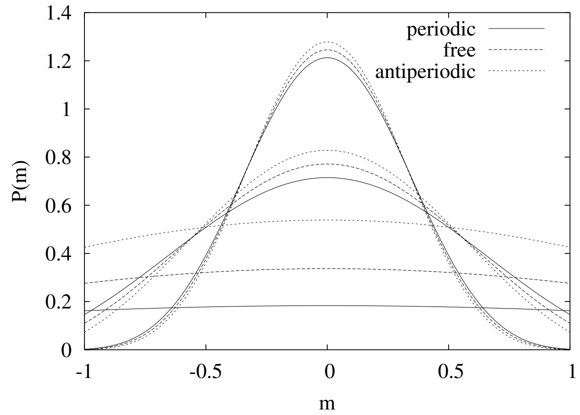

Figure 5. Comparison of the regular parts of the magnetization distribution $P(m)$ for periodic, antiperiodic, and free BCs in the scaling limit, with the scaling variable being $\zeta = 1$, 4, and 10 (from bottom at origin). Note that the Dirac deltas at $m = \pm 1$ of the periodic and the free case are not displayed.

antiperiodic states (23) by J and thus we can write the scaling limit of the probability of a given M as

$$P_g^{(f)}(M) = \frac{\mathrm{e}^{-E_g^{(f)}/k_\mathrm{B}T}}{Z^{(f)}}\Omega_g^{(f)}(M) = \begin{cases} \frac{\mathrm{e}^{-K}Z^{(p)}}{Z^{(f)}}P_g^{(p)}(M) & g = 2s \\ \frac{\mathrm{e}^{-K}Z^{(a)}}{Z^{(f)}}P_g^{(a)}(M) & g = 2s-1. \end{cases} \tag{45}$$

Using equations (25), one finds that the prefactors of the distributions depend only on ζ, thus collecting the contributions with different number of domain walls (22), we obtain an expression for $P^{(f)}(m)$ through $P^{(p),(a)}(m)$

$$P^{(f)}(m) = \mathrm{e}^{-\zeta}[\cosh\zeta\, P^{(p)}(m) + \sinh\zeta\, P^{(a)}(m)] \tag{46}$$

which leads to

$$P^{(f)}(m) = \frac{\mathrm{e}^{-\zeta}}{2}[\delta(m+1) + \delta(m-1)] + \frac{\zeta\,\mathrm{e}^{-\zeta}}{2\sqrt{1-m^2}}I_1\big(\zeta\sqrt{1-m^2}\big) + \frac{\zeta\,\mathrm{e}^{-\zeta}}{2}I_0\big(\zeta\sqrt{1-m^2}\big). \tag{47}$$

As we shall see in the following section, the above expression applies for bulk BC as well. The bulk result was obtained previously by Bruce (see [5] equation (3.20)). Note also that the relationship established between the distributions for different BCs (46) is certainly valid for the fluctuations of the magnetization (13) as well.

One should note that the coefficient of the singular part is larger for the periodic case, i.e., a periodic system is more likely to be in the completely ordered steady state. This is expected due to the lower energy of the states with $2s - 1$ domain walls than that with $2s$ domain walls. In figure 5 we display the non-singular part of the distributions. This non-singular part also shows the expected sequence from PBCs resulting in the most ordered state to APBCs yielding the most disordered state.

4.4. Block boundary conditions

We start with the simplest case, i.e., impose free BCs on the chain and investigate the magnetization of a finite segment (block) of length ℓ. As we shall show the distribution of M_ℓ is identical to the free end result for any ℓ. In order to see this, consider the Boltzmann weight of a configuration of the spins for the segment of spins between σ_k and $\sigma_{n=k+\ell}$

$$P(\{\sigma_k,\ldots,\sigma_n\}) = \frac{\sum_{\{\sigma\}_{1,k-1},\{\sigma\}_{n+1,N}} \exp\left(K\sum_{j=1}^{N-1}\sigma_j\sigma_{j+1}\right)}{\sum_{\{\sigma\}_{1,N}} \exp\left(K\sum_{j=1}^{N-1}\sigma_j\sigma_{j+1}\right)} \tag{48}$$

where $\sum_{\{\sigma\}_{i,j}}$ denotes summing over possible values of the spins between sites i and j. One can 'integrate out' the end spin $\sigma_1 = \pm 1$ in both the numerator and the denominator yielding cancelling factors $e^K + e^{-K}$. This can be repeated till the spin σ_k is reached and then the same can be done starting from the other end (σ_N) of the chain. As a result one obtains

$$P(\{\sigma_k,\ldots,\sigma_n\}) = \frac{\exp\left(K\sum_{j=k}^{n-1}\sigma_j\sigma_{j+1}\right)}{\sum_{\{\sigma\}_{k,n}} \exp\left(K\sum_{j=k}^{n-1}\sigma_j\sigma_{j+1}\right)}. \tag{49}$$

This is the free end probability distribution for the spins in the segment $[k, k+\ell]$, thus the magnetization distribution $P(m_\ell)$, with $m_\ell = M_\ell/\ell$, is identical to the FBCs case given by equation (47), i.e., $P^{(f)}(m_\ell) = P^{(f)}(m)$.

The above derivation does not hold for chains with PBCs and APBCs and one expects that the $P(M_\ell)$ depends on the aspect ratio $b = \ell/N$. In the $b \to 0$ limit, i.e., when the window size is relatively small, however, $P(M_\ell)$ becomes independent from the BCs imposed on the whole chain. More precisely, this happens in the scaling limit $\ell, N \to \infty$, $t \to 0$ with $\zeta = \ell t/2$ and $b = \ell/N$ kept constant, a limit where the correlation length $\xi \sim \ell \ll N$ and the effects of the boundaries of the chain can be neglected.

4.5. Asymptotic regimes

The small ζ expansion is already given by equation (22). For sufficiently small ζ the distribution $P(m)$ can be approximated by the first few terms, e.g., the Dirac delta functions (except for the antiperiodic case) plus a constant probability density for all BCs.

For large values of ζ a Gaussian approximation can be obtained using only the first term of the large x asymptotic of the Bessel functions

$$I_1(x) \approx I_0(x) \approx \frac{e^x}{\sqrt{2\pi x}} \tag{50}$$

and using also the condition $m \ll 1$, where $P(m)$ significantly differs from zero, due to the factor $\exp(\zeta\sqrt{1-m^2})$

$$P(m) \approx \frac{1}{\sqrt{2\pi\zeta}}\, e^{-m^2\zeta/2}. \tag{51}$$

$P(m)$ eventually evolves to a Dirac delta function $\delta(m)$ for $\zeta \to \infty$.

5. Final remarks

The fluctuations of the magnetization in the one-dimensional Ising model have been investigated near its critical point in the limit of $T \to 0$ and $N \to \infty$ with the average number of domain walls ($2\zeta = Nt$) kept constant. A simple combinatorial derivation has been presented for the magnetization distributions and it was shown that in this limit these distributions are non-trivial well-defined functions of the magnetization and the control parameter ζ.

The ζ dependence of the magnetization distribution should be emphasized, as it means that the order parameter distribution of a system can, in general, depend on the way the critical point is approached and the thermodynamic limit is taken.

We focused our attention on the effect of boundary conditions, namely we imposed periodic, antiperiodic and free BCs on the chain. The magnetization distributions are shown to be sensitive to the BCs and well distinguishable for all values of ζ. For antiperiodic BCs the distributions differ fundamentally from the periodic and free BCs case (lack of Dirac delta peaks for APBCs).

We also showed that the distribution of the magnetization of a segment (BBCs) of the whole chain with FBCs coincide with the distribution of the total magnetization, independently of the size of the segment. For PBCs or APBCs chains the above statement is true only if the relative segment size b goes to zero.

It is worth mentioning the analogies to a simple random walk. The corresponding quantity is the distribution of the width of the walk (mean square deviation of the position of the walker), and for that two distinct functions have been exactly derived for periodic and free BCs [13]. The qualitative behaviour of BBCs is also the same as that of the Ising model discussed above.

It would be very interesting to see similar calculations for the order parameter distribution in other equilibrium one-dimensional models, e.g., the classical and quantum XY and Heisenberg models, or non-equilibrium ones, e.g., absorbing state phase transitions.

Acknowledgments

We would like to thank Z Bajnok, G Györgyi and M Plischke for useful discussions. This research has been partially supported by the Hungarian Academy of Sciences (grant no OTKA T029792 and T043734) and by the Swiss National Science Foundation.

References

[1] Fisher M E 1971 Critical Phenomena *Proc. 1970 International School of Physics Enrico Fermi* ed M S Green (New York: Academic) Course 51

[2] Barber M N 1983 *Phase Transitions and Critical Phenomena* ed C Domb and J L Lebowitz vol 8 (New York: Academic)

[3] Cardy J L 1988 *Finite Size Scaling* (Amsterdam: North-Holland)

[4] Privman V (ed) 1990 *Finite Size Scaling and Numerical Simulation of Statistical Physics* (Singapore: World Scientific)

[5] Bruce A D 1981 *J. Phys. C: Solid State Physics* **14** 3667

[6] Bruce A D 1985 *J. Phys. A: Math. Gen.* **18** L873

[7] Nicolaides D and Bruce A D 1988 *J. Phys. A: Math. Gen.* **21** 233

[8] Bruce A D and Wilding N B 1992 *Phys. Rev. Lett.* **68** 193

[9] Nicolaides D and Ewans R 1989 *Phys. Rev. Lett.* **63** 778
Wilding N B and Niebala P 1996 *Phys. Rev.* E **53** 926
Müller M and Wilding N B 1995 *Phys. Rev.* E **51** 2079

de Queiroz S L A and Stinchcomb R B 2001 *Phys. Rev.* E **64** 036117
Tsypin M M 1994 *Phys. Rev. Lett.* **73** 2015
[10] Foltin G, Oerding K, Rácz Z, Workman R L and Zia R K P 1994 *Phys. Rev.* E R639
Plischke M, Rácz Z and Zia R K P 1994 *Phys. Rev.* E **50** 3589
Rácz Z and Plischke M 1994 *Phys. Rev.* E **50** 3530
Antal T and Rácz Z 1996 *Phys. Rev.* E **54** 2256
Marinari E, Pagnani A, Parisi G and Rácz Z 2002 *Phys. Rev.* E **65** 026136
[11] Bramwell S T, Holdsworth P C W and Pinton J-F 1998 *Nature* **396** 552
Bramwell S T *et al* 2000 *Phys. Rev. Lett.* **84** 3744
Aji V and Goldenfeld N 2001 *Phys. Rev. Lett.* **86** 1007
[12] Korniss G, Toroczkai Z, Novotny M A and Rikvold P A 2000 *Phys. Rev. Lett.* **84** 1351
Korniss G, White C J, Rikvold P A and Novotny M A 2000 *Phys. Rev.* E **63** 016120
Tripathy G and van Saarloos W 2000 *Phys. Rev. Lett.* **85** 3556
Lubeck S and Heger P C 2003 *Phys. Rev. Lett.* **90** 230601
[13] Antal T, Droz M, Györgyi G and Rácz Z 2001 *Phys. Rev. Lett.* **87** 240601
Antal T, Droz M, Györgyi G and Rácz Z 2002 *Phys. Rev.* E **65** 046140
[14] Binder K 1981 *Z. Phys.* B **43** 119
[15] Tsypin M M and Blöte H W J 2000 *Phys. Rev.* E **62** 73
[16] Eisenriegler E and Tomaschitz R 1987 *Phys. Rev.* B **35** 4876
[17] McCoy B M and Wu T T 1973 *The Two-Dimensional Ising Model* (Cambridge, MA: Harvard University Press)
Hu C-K, Lin C-Y and Chen J-A 1995 *Phys. Rev. Lett.* **75** 193
Lu W T and Wu F Y 2001 *Phys. Rev.* E **63** 026107
Kaneda K and Okabe Y 2001 *Phys. Rev. Lett.* **86** 2134
[18] Brezin E 1982 *J. Physique* **43** 15
[19] Kramers H A and Wannier G H 1941 *Phys. Rev.* **60** 252
[20] Baxter R J 1982 *Exactly Solvable Models in Statistical Physics* (London: Academic)
[21] Chen X S and Dohm V 2000 *Eur. Phys.* B **15** 283