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TRANSFER MATRIX STUDY OF FINITE-SIZE CORRECTIONS IN THE 2D ISING MODEL

J. KAUPUŽS

Institute of Mathematics and Computer Science, University of Latvia
29 Rainja Boulevard, LV–1459 Riga, Latvia

Abstract — Effective exact transfer matrix algorithms have been developed to compute the two-point correlation function $G(r)$ of the 2D Ising model on a square finite-size lattice. Systems including up to 800 spins have been considered and corrections to the finite-size scaling at the critical point have been analysed. As a new result, we have found that the correlation function computed at a distance $r \propto L$, where L is the linear size of the lattice, has a nontrivial amplitude correction $\propto L^{-0.25}$ of a very small magnitude.

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1. Introduction

Since the exact solution of the two-dimensional Lenz—Ising (or Ising) model was found by Onsager [28], the study of various phase transition models has been of continuous interest. Remarkable progress has been made in the exact solution of two-dimensional models [6]. The transfer matrix method, applied to analytical calculations on two-dimensional lattices, is well known [6, 28]. The loop counting method [7, 26] appers to be very effective in calculating the partition function, which takes a particularly simple form in the case of a square lattice with Brascamp—Kunz boundary conditions [23]. The asymptotic behavior of the correlation functions can be studied by means of the equations of the conformal field theory [21]. Exact equations for the two-point correlation function of the 2D Ising model on an infinite lattice are known, too [4]. However, no analytical methods for an exact calculation of the correlation function in the 2D Ising model on finite-size lattices exist. This can be done numerically by adopting the conventional transfer matrix method and modifying it to achieve the maximal result (calculation of the largest possible system) with a minimal number of arithmetic operations, as discussed in our paper.

Various modifications of similar enumeration methods, used to calculate the partition function, the coefficients of low-temperature series expansion, the density of states, etc., are well known in the literature. This approach has been often applied to the Ising model on small three-dimensional lattices. The early calculations belong to K. Binder [13], who calculated the partition function (by computing the weight coefficients for states with different energies) and the related internal energy and specific heat for lattices with open boundaries having sizes up to $3 \times 3 \times 6 = 54$ spins. In [8, 12] the enumeration of states has been done for

$5 \times 5 \times 4$ lattice. This method has been widely used to generate the coefficients of the low-temperature series expansion [9–11, 17, 19, 20, 32]. The computation time, which is necessary for such calculations, can be reduced drastically by using some tricks. In particular, the recursive calculations in [10] were performed by adding one spin at a time, which is much faster than adding whole slices, as in earlier calculations [17]. As opposed to the papers cited above, where 3D lattices with open boundaries were considered, we have used such a trick to calculate the correlation function on two-dimensional lattices with periodic boundary conditions. In this case, the use of symmetries is very helpful, too, as discussed in Section 2.1. Another trick that we have used is a special way of growing the lattice by adding slices (each of them being grown spin-by-spin) oriented in the diagonal $\langle 11 \rangle$ crystallographic direction. It allows to enumerate a lattice with a linear size $\sqrt{2}$ times larger than in the usual case of the $\langle 10 \rangle$ direction without dramatical increase in the computation time.

The transfer matrix method was used to enumerate the two-dimensional Ising model on finite-size lattices in [15, 16, 24]. In [24], the universal ratio of the magnetisation (m) moments $U = \langle m^4 \rangle / \langle m^2 \rangle^2$ (which is related to the Binder cumulant $1 - U/3$) at the critical point was examined for square and triangular lattices with periodic boundary conditions and sizes up to $L = 17$ and $L = 16$, respectively. The capability of the transfer matrix method in numerical calculation of the restricted density of the states in the energy-magnetisation space was demonstrated in [16], where strips of width up to $L = 13$ were considered. In [15] the susceptibility at the critical point was calculated for finite-size square lattices with periodic boundary conditions and sizes $L \leqslant 17$. Our improved algorithms allowed us to compute the two-point correlation function at criticality for somewhat larger lattices, consisting of $\leqslant 800$ spins and having a linear size of up to $20\sqrt{2}$ lattice spacings.

Like in many papers (see [1, 2, 4, 5, 15, 18, 23, 27, 29–31] and references therein), our aim is to study the corrections to the scaling in the 2D Ising model. Although it is one of the best investigated models in statistical mechanics, corrections to the scaling is a notoriously difficult problem, and the results are somewhat controversial. It has been well established that corrections to the scaling for free energy, internal energy, specific heat, and zeroes of the partition function are represented by integer correction-to-scaling exponents. It refers both to the finite-size corrections at (or near) criticality and the expansion in powers of the reduced temperature $t = T/T_c - 1 \to 0$ (where T_c is the critical value of temperature T) in the thermodynamical limit.

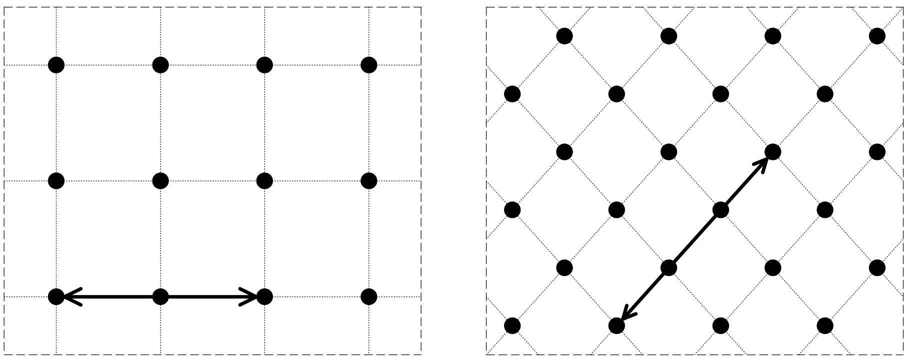
Nevertheless, there are some uncertainties regarding the susceptibility. Aharony and Fisher [1, 2] predicted a scaling amplitude function that is equal above and below T_c, suggesting that the Ising model critical region can be described entirely by two nonlinear scaling fields. The high-temperature (HT) series analysis in [4, 27, 29] revealed a deviation from this law at order t^4 in the expansion of the leading amplitude. It was also confirmed by certain conjectures of the conformal field theory and renormalisation group arguments [15]. The results obtained in [27] are consistent with the leading nontrivial corrections that are (amplitude) modifications of the existing terms of the form $\mid t \mid^{9/4}$ or $t^2 \ln \mid t \mid$. The HT results of [4, 29], however, support the existence of only integer correction-to-scaling exponents, although logarithmic corrections appear, as consistent with [15]. A correction-to-scaling exponent $4/3$ was proposed earlier in [5] for some models of the 2D Ising universality class. It has been found, however, that this correction vanishes in the Ising case [5].

Our results complete the current knowledge about this problem. In particular, we have found that a nontrivial correction to finite-size scaling appears in the two-point correlation function, which is directly related to the susceptibility (cf. Section 4).

2. Exact transfer matrix algorithms for calculation of the correlation function in the 2D Ising model

2.1. Adoption of standard methods

We consider a two-dimensional Ising model where spins are located either on the lattice of dimensions $N \times L$, illustrated in Fig. 1a, or on the lattice of dimensions $\sqrt{2}N \times \sqrt{2}L$ shown in Fig. 1b. The periodic boundaries are indicated by dashed lines. In the case (a), we have L rows and in the case (b) — $2L$ rows, each containing N spins. Figure 1 shows an illustrative example with $N = 4$ and $L = 3$. In our notation nodes are numbered consecutively from left to right, and rows — from bottom to top.



(a) (b)

Figure 1. Illustrative examples of lattices with dimensions $N \times L$ (a) and $\sqrt{2}N \times \sqrt{2}L$ (b) with periodic boundary conditions along the dashed lines. The correlation function has been calculated in the $\langle 10 \rangle$ crystallographic direction, as indicated by the arrows

For convenience, first we consider the use of the transfer matrix method to calculate the partition function

$$Z = \sum_{\{\sigma_k\}} \exp\left(\beta \sum_{\langle i,j \rangle} \sigma_i \sigma_j\right) , \tag{1}$$

where $\sigma_i = \pm 1$ are the spin variables, and the summation runs over all possible spin configurations $\{\sigma_k\}$. The argument of the exponent represents a Hamiltonian of the system including summation over all neighbouring spin pairs $\langle i, j \rangle$ of the given configuration $\{\sigma_k\}$; the parameter β is the coupling constant. We call the factors $\exp(\beta\, \sigma_i \sigma_j)$ contained in (1) the Boltzmann weights of bonds.

Let us consider the lattice (a) in Fig. 1 containing n rows without periodic boundaries along the vertical axis and without interaction between the spins in the upper row. We define the 2^N-component vector $\mathbf{r}_n$ such that the ith component of this vector represents the contribution to the partition function made by the ith spin configuration of the upper row, i. e., the sum over all states of the spin system with a fixed (ith) configuration of this row. Then we have a recurrence relation $\mathbf{r}_{n+1} = T\,\mathbf{r}_n$, where T is the transfer matrix which includes the Boltzmann weights of the newly added bonds. Furthermore, we can write $\mathbf{r}_{n+1}^{(i)} = T\,\mathbf{r}_n^{(i)}$, where $\mathbf{r}_n^{(i)}$ is the partial contribution to $\mathbf{r}_n$ made by the ith configuration of the first row. The components of $\mathbf{r}_1^{(i)}$ are given by $\left(\mathbf{r}_1^{(i)}\right)_j = \delta_{j,i}$. In the case of the periodic boundary conditions, the $(L+1)$-th row must be identical to the first one, which leads to the well-known expression [6, 22]

$$Z = \sum_i \left(\mathbf{r}_{L+1}^{(i)}\right)_i = \text{Trace}\left(T^L\right) = \sum_i \lambda_i^L \,, \tag{2}$$

where λ_i are the eigenvalues of the transfer matrix T. An analogous expression for the lattice in Fig. 1b reads

$$Z = \sum_i \left(\mathbf{r}_{2L+1}^{(i)}\right)_i = \text{Trace}\left([T_2 T_1]^L\right) \,, \tag{3}$$

where the vectors $\mathbf{r}_n^{(i)}$ obey the reccurence relation $\mathbf{r}_{n+1}^{(i)} = T_{1,2}\,\mathbf{r}_n^{(i)}$ with different transfer matrices T_1 and T_2 for odd and even row numbers n, respectively.

The actual scheme can be easily adopted to calculate the correlation function $\langle \sigma_i \sigma_j \rangle$ between any two lattice points i and j. Namely, the correlation function $G(x)$ between the points separated by a distance x, as indicated in Fig. 1, is given by the statistical average Z'/Z, where the sum Z' is calculated in the same way as Z, but including the corresponding product of the spin variables. It implies the following replacements:

$$\left(\mathbf{r}_1^{(i)}\right)_j = \delta_{j,i} \Rightarrow \left(\mathbf{r}_1^{(i)}\right)_j = \delta_{j,i}\left(N^{-1}\sum_{\ell=1}^{N} [\sigma(\ell)]_i \, [\sigma(\ell+x)]_i\right) \quad : \text{case (a)} \tag{4}$$

$$\left(\mathbf{r}_{x+1}^{(i)}\right)_j \Rightarrow \left(\mathbf{r}_{x+1}^{(i)}\right)_j \times \left(N^{-1}\sum_{\ell=1}^{N} [\sigma(\ell)]_i \, [\sigma(\ell+\Delta(x))]_j\right) \quad : \text{case (b)} \,, \tag{5}$$

where $\Delta(x) = x/2$ holds for even x, and $\Delta(x) = (x-1)/2$ — for odd x. In our notation, $[\sigma(k)]_i$ is the spin variable in the kth node in a row provided that the whole set of spin variables of this row forms the ith configuration. It is supposed that $\sigma(k+N) \equiv \sigma(k)$ holds according to the periodic boundary conditions. Such a symmetrical form, which includes the averaging over ℓ, allows to reduce the amount of numerical calculations: due to the symmetry we need the summation over only $\approx 2^N/N$ nonequivalent configurations of the first row instead of the total number of 2^N configurations.

2.2. Improved algorithms

The number of the required arithmetic operations can be further reduced if the recurrence relations $\mathbf{r}_{n+1}^{(i)} = T\,\mathbf{r}_n^{(i)}$ and $\mathbf{r}_{n+1}^{(i)} = T_{1,2}\,\mathbf{r}_n^{(i)}$ are split into N steps of adding a single spin. To formulate this in a suitable way, let us first number all the 2^N spin configurations $\{\sigma(1); \sigma(2); \cdots; \sigma(N-1); \sigma(N)\}$ by index i as follows:

$$\begin{array}{lcl} i = 1 & : & \{-1;\ -1;\ \cdots;\ -1;\ -1;\ -1\} \\ i = 2 & : & \{-1;\ -1;\ \cdots;\ -1;\ -1;\ +1\} \\ i = 3 & : & \{-1;\ -1;\ \cdots;\ -1;\ +1;\ -1\} \\ i = 4 & : & \{-1;\ -1;\ \cdots;\ -1;\ +1;\ +1\} \\ \multicolumn{3}{c}{\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots} \\ i = 2^N & : & \{+1;\ +1;\ \cdots;\ +1;\ +1;\ +1\} \end{array} \tag{6}$$

We remind that the sequence of numbers in the ith row corresponds to the spin variables $[\sigma(k)]_i$ with $k = 1, 2, \ldots, N$. They change with i just like the digits of subsequent integer numbers in the binary counting system.

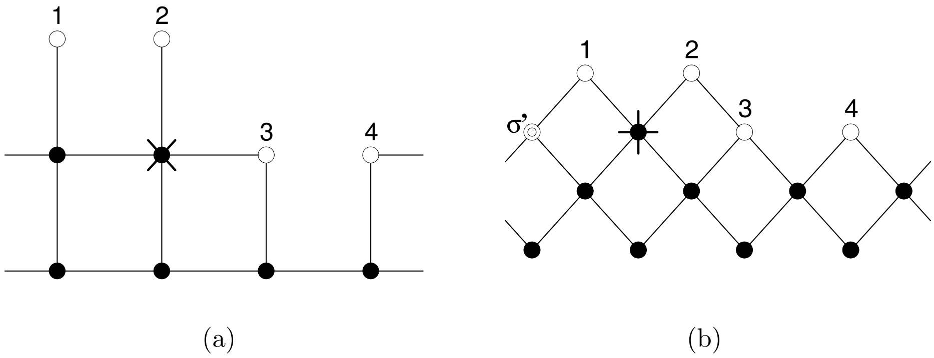


Figure 2. Schematical representation of the algorithms of calculation for the lattices a and b introduced in Fig. 1

Consider now a lattice where n rows are completed, while the $(n+1)$-th row contains only ℓ spins, where $\ell < N$, as illustrated in Fig. 2 in both cases (a) and (b) taking as an example $N = 4$. We consider the partial contribution $(\mathbf{r}_{n+1,\ell})_i$ (i. e., the ith component of vector $\mathbf{r}_{n+1,\ell}$) to the partition function Z (or Z') made by a fixed (ith) configuration of the set of N upper spins. These are the consecutively numbered spins shown in Fig. 2 by open circles. For simplicity, we have dropped the index denoting the configuration of the first row. In the case (b), the spin depicted by a double-circle has a fixed value of σ'. In general, this spin is the nearest bottom-left neighbour of the first spin in the upper row. According to this, one has to distinguish between odd and even n: σ' refers either to the first (for odd n) or to the Nth (for even n) spin of the nth row. It is supposed that the Boltzmann weights are included corresponding to the solid lines in Fig. 2 connecting the spins. In the case (a), the weights responsible for the interaction between the upper numbered spins are not included. Obviously, for a given $\ell > 1$, $\mathbf{r}_{n+1,\ell}$ can be calculeted from $\mathbf{r}_{n+1,\ell-1}$ via summation over one spin variable, marked in Fig. 2 by a cross. In the case (a), it is also true for $\ell = 1$, whereas in the case (b) this variable has a fixed value of σ' at $\ell = 1$. In the latter case, the summation over σ' is performed in the last step when the $(n+1)$-th row is already completed. These manipulations enable us to write for the case (a)

$$\mathbf{r}_{n+1} = T\,\mathbf{r}_n \equiv \widetilde{W}_N\,\widetilde{W}_{N-1}\cdots\widetilde{W}_2\,\widetilde{W}_1\,\mathbf{r}_n \tag{7}$$

with

$$\widetilde{W}_\ell = \sum_{\sigma=\pm1} W_\ell(\sigma)\ , \tag{8}$$

where the components of the matrices $W_\ell(\sigma)$ are given by

$$\begin{aligned} (W_1(\sigma))_{ij} &= \delta\left(j, j_1(\sigma,1,i)\right)\cdot\exp\left(\beta\,\sigma\left\{[\sigma(1)]_i + [\sigma(2)]_i + [\sigma(N)]_i\right\}\right), \\ (W_\ell(\sigma))_{ij} &= \delta\left(j, j_1(\sigma,\ell,i)\right)\cdot\exp\left(\beta\,\sigma\left\{[\sigma(\ell)]_i + [\sigma(\ell+1)]_i\right\}\right): \quad 1<\ell<N, \\ (W_N(\sigma))_{ij} &= \delta\left(j, j_1(\sigma,N,i)\right)\cdot\exp\left(\beta\,\sigma\,[\sigma(N)]_i\right). \end{aligned} \tag{9}$$

Here $\delta(j,k)$ is the Kronecker symbol and

$$j_1(\sigma,\ell,i) = i + \left(\sigma - [\sigma(\ell)]_i\right)\,2^{N-\ell-1} \tag{10}$$

are the indexes of the old configurations containing $\ell - 1$ spins in the $(n+1)$-th row depending on the value of σ of the spin marked in Fig. 2a by a cross, as well as on the index i of the new configuration with ℓ spins in the $(n+1)$–th row, as consistent with the numbering of (6).

The above equations (7) to (9) refer to the case (a). In the case (b), we have

$$\mathbf{r}_{n+1} = T_{1,2}\,\mathbf{r}_n \equiv \sum_{\sigma'=\pm 1} \widetilde{W}_N^{(1,2)}\,\widetilde{W}_{N-1}^{(1,2)} \cdots \widetilde{W}_2^{(1,2)}\,W_1^{(1,2)}(\sigma')\,\mathbf{r}_n \;, \tag{11}$$

where $\widetilde{W}_\ell^{(1,2)}$ are the matrices

$$\widetilde{W}_\ell^{(1,2)} = \sum_{\sigma=\pm 1} W_\ell^{(1,2)}(\sigma) \;. \tag{12}$$

Here indexes 1 and 2 refer to odd and even row numbers n, respectively, and the components of the matrices $W_\ell^{(1,2)}(\sigma)$ are

$$\left(W_\ell^{(1,2)}(\sigma)\right)_{ij} = \delta\left(j, j_{1,2}(\sigma,\ell,i)\right) \cdot \exp\left(\beta\,[\sigma(\ell)]_i\,\{\sigma + [\sigma(\ell+1)]_i\}\right) \;, \tag{13}$$

where $[\sigma(N+1)]_i \equiv \sigma'$ and the index $j_1(\sigma,\ell,i)$ is given by (10). For the other index we have

$$\begin{aligned} j_2(\sigma,1,i) &= 2i - 2^{N-1}\left([\sigma(1)]_i + 1\right) + \frac{1}{2}(\sigma - 1), \\ j_2(\sigma,\ell,i) &= j_1(\sigma,\ell,i) \quad : \quad \ell \geqslant 2. \end{aligned} \tag{14}$$

Note that the matrices $\widetilde{W}_\ell$ and $\widetilde{W}_\ell^{(1,2)}$ have only two nonzero elements in each row, so that the number of arithmetic operations required for the construction of one row of spins via a subsequent calculation of the vectors $\mathbf{r}_{n+1,\ell}$ increases like $2N \cdot 2^N$ instead of 2^{2N} operations necessary for a straightforward calculation of the vector $T\mathbf{r}_n$. Taking into account the above symmetry of the first row, the computation time is proportional to $2^{2L}L$ for both $L \times L$ (a) and $\sqrt{2}L \times \sqrt{2}L$ (b) lattices in Fig. 1 with periodic boundary conditions.

2.3. Application to different boundary conditions

The developed algorithms can easily be extended to lattices with antiperiodic boundary conditions. The latter implies that $\sigma(N+1) = -\sigma(N)$ holds for each row, and a similar condition is true for each column. We can also consider mixed boundary conditions: periodic along the horizontal axis and antiperiodic along the vertical one, or vice versa. To replace the periodic boundary conditions with antiperiodic ones, we need only to change the sign of the corresponding products of the spin variables on the boundaries. Consider, e. g., the case (a) in Fig. 1. The change of the boundary conditions along the vertical axis means that the first term in the argument of the exponent in each of the Eqs. (9) changes the sign for the last row, i. e., when $n = L$. The same along the horizontal axis implies that the term $[\sigma(N)]_i$ in the equation for $(W_1(\sigma))_{ij}$ changes the sign. In this case, however, the symmetry of the configurations of the first row is partly broken and, therefore, we need summation over a larger number of nonequivalent configurations.

3. Transfer matrix study of the critical correlation function and corrections to the scaling in the 2D Ising model

3.1. General scaling arguments

It is well known [3] that in the thermodynamic limit the correlation function of the Ising model behaves like $G(r) \propto r^{2-d-\eta}$ at large distances $r \to \infty$ at the critical (i. e., phase transition) point $\beta = \beta_c$, where η is the critical exponent having the value $\eta = 1/4$ in two dimensions ($d = 2$). Based on our transfer matrix algorithms developed in Section 2, here we test the corrections to the scaling in the 2D Ising model at the critical point [6] $\beta = \beta_c = \frac{1}{2} \ln \left(1 + \sqrt{2}\right)$.

According to the general arguments of the finite-size scaling theory [14], the expected finite-size scaling relation for the critical correlation function, i. e., for $G(r)$ at the critical point $\beta = \beta_c$, reads

$$G(r) \simeq r^{2-d-\eta} f(r/L) : \quad r \to \infty, \quad L \to \infty \; , \tag{15}$$

where the scaling function $f(z)$ depends also on the crystallographic orientation of the line connecting the correlating spins, as well as on the orientation of the periodic boundaries. A natural extension of (15), including the corrections to the scaling, is

$$G(r) = \sum_{\ell \geqslant 0} r^{-\lambda_\ell} f_\ell(r/L) \; , \tag{16}$$

where the term with $\lambda_0 \equiv d - 2 + \eta$ is the leading one, whereas those with the subsequently increasing exponents λ_1, λ_2, etc., represent the corrections to the scaling. The substitution $f_\ell(z) = z^{\lambda_\ell} f'(z)$ transforms the asymptotic expansion (16) to

$$G(r) = f'_0(r/L) \, L^{-\lambda_0} \left(1 + \sum_{\ell \geqslant 1} L^{-\omega_\ell} \, \tilde{f}_\ell(r/L) \right) \; , \tag{17}$$

where $\tilde{f}_\ell(z) = f'_\ell(z)/f_0(z)$ and $\omega_\ell = \lambda_\ell - \lambda_0$ are the correction-to-scaling exponents. To get some idea about the exponents ω_ℓ, it is useful to consider first the thermodynamic limit $L \to \infty$ or $r/L \to 0$. In particular, the critical correlation function $G(r)$ of the 2D Ising model in $\langle 11 \rangle$ crystallographic direction on an infinite lattice can be calculated easily based on the known exact formulae [4], and it yields $G(r) \propto r^{-1/4} \left[1 + \mathcal{O}\left(r^{-2}\right)\right]$ at large distances $r \to \infty$. The structure of the asymptotic expansion is consistent with $\omega_\ell = 2\ell$ in this case. Nevertheless, our calculations in the 2D Ising model discussed in Section 3.2 indicate the existence of a nontrivial finite-size correction of the kind of $L^{-1/4}$. The thermodynamic limit is a particular case of the finite-size scaling with the scaling argument $r/L \to 0$, therefore it is possible that the nontrivial corrections to the correlation function in the 2D Ising model vanish in this special case, but not in general.

3.2. Correction-to-scaling analysis for the $\sqrt{2}L \times \sqrt{2}L$ lattice

Based on the scaling analysis in Section 3.1, here we discuss the corrections to the scaling for the $\sqrt{2}L \times \sqrt{2}L$ lattice in Fig. 1b. We have calculated the correlation function $G(r)$ at $r = L$ in the $\langle 10 \rangle$ direction with the aim to identify the correction exponents ω_ℓ in (17). Further we use the notation $\omega_1 \equiv \omega$.

Let us define the effective correction-to-scaling exponent $\omega_{\mathrm{eff}}(L)$ via the solution of the equations

$$\tilde{L}^{1/4} G(r=\tilde{L}) = a + b\,\tilde{L}^{-\omega_{\mathrm{eff}}} \tag{18}$$

at $\tilde{L} = L$, $L+\Delta L$, $L+2\Delta L$ for three unknown quantities ω_{eff}, a, and b. According to (17), where $\lambda_0 = \eta = 1/4$, such a definition gives us the leading correction-to-scaling exponent ω at $L \to \infty$, i. e., $\lim_{L\to\infty} \omega_{\mathrm{eff}}(L) = \omega$.

The calculated values of $G(r)$ at $r = L$ and the corresponding effective exponents $\omega_{\mathrm{eff}}(L)$, determined at $\Delta L = 1$, are given in Table 1. Within the considered range of sizes L, the effective exponent $\omega_{\mathrm{eff}}(L)$ converges to a value of about 2. The obtained sequence of $\omega_{\mathrm{eff}}(L)$ can be extrapolated to $L = \infty$. For this purpose we have considered the ratio of the following two increments in ω_{eff},

$$\rho(L) = \frac{\omega_{\mathrm{eff}}(L+\Delta L) - \omega_{\mathrm{eff}}(L)}{\omega_{\mathrm{eff}}(L) - \omega_{\mathrm{eff}}(L-\Delta L)}\ . \tag{19}$$

A simple analysis shows that $\rho(L)$ behaves like

$$\rho(L) = 1 - \Delta L \cdot (\omega' + 1) L^{-1} + \mathcal{O}\left(L^{-2}\right) \tag{20}$$

at $L \to \infty$ if $\omega_{\mathrm{eff}}(L) = \omega + \mathcal{O}\left(L^{-\omega'}\right)$ holds with an exponent $\omega' > 1$. Let the values of $\omega_{\mathrm{eff}}(L)$ be known up to $L = L_{\mathrm{max}}$. Then we can calculate from (19) the $\rho(L)$ values up to $L = L_{\mathrm{max}} - \Delta L$ and make a suitable ansatz like

$$\rho(L) = 1 - 3\Delta L \cdot L^{-1} + b\,L^{-2} \quad \text{at} \quad L \geqslant L_{\mathrm{max}} \tag{21}$$

for a formal extrapolation of $\omega_{\mathrm{eff}}(L)$ to $L = \infty$. This is consistent with (20) where $\omega' = 2$. The coefficient b is found by matching the result to the precisely calculated value at $L = L_{\mathrm{max}} - \Delta L$. The subsequent values of $\omega_{\mathrm{eff}}(L)$, calculated from (19) and (21) at $L > L_{\mathrm{max}}$, converge to some value $\widetilde{\omega}(L_{\mathrm{max}})$ at $L \to \infty$. If the leading correction-to-scaling exponent ω is 2, then the extrapolation result $\widetilde{\omega}(L_{\mathrm{max}})$ will tend to 2 at $L_{\mathrm{max}} \to \infty$ irrespective of the precise value of ω'. It is evident from Table 1 that the extrapolated values of the effective correction exponent, i. e., $\widetilde{\omega}(L)$, come surprisingly close to 2 at certain L values. Besides, the ratio of increments $\rho(L)$ in this case is well approximated by (21), as consistent with the existence of a correction term in (17) with exponent 4. These observations coincide with the idea that $\omega_\ell = 2\ell$ holds, like in the case of an infinite lattice.

On the other hand, we can see from Table 1 that $\Delta\widetilde{\omega}(L) = \widetilde{\omega}(L) - 2$ tends to increase in magnitude at $L > 13$. We have illustrated this systematic and smooth deviation in Fig. 3. The only reasonable explanation of this behavior is that expansion (17) necessarily contains exponent 2 and, likely, also exponent 4, and at the same time it contains also a correction of a very small amplitude with $\omega < 2$. The latter explains the increase in $\Delta\widetilde{\omega}(L)$. Namely, the correction to the scaling for $L^{1/4}G(L)$ behaves like $\mathrm{const} \cdot L^{-2}\left[1 + \mathcal{O}\left(L^{-2}\right) + \varepsilon\, L^{2-\omega}\right]$ with $\varepsilon \ll 1$, which implies a slow crossover of the effective exponent $\omega_{\mathrm{eff}}(L)$ from values of about 2 to the asymptotic value ω. Besides, in the region where $\varepsilon\, L^{2-\omega} \ll 1$ holds, the effective exponent behaves like

$$\omega_{\mathrm{eff}}(L) \simeq 2 + b_1 L^{2-\omega} + b_2 L^{-2}\ , \tag{22}$$

where $b_1 \ll 1$ and b_2 are constants. Note that the trivial corrections $\propto L^{-n}$ with an integer $n \geqslant 2$ appear in the expansion of $\omega_{\mathrm{eff}}(L)$ according to (17) and (18), taking into account that (17) contains correction exponents 2, 4, 6, etc., in general (since otherwise they could not have shown up at $r/L \to 0$). By using the extrapolation of ω_{eff} with $\omega' = 2$ in (20) and (21),

Table 1. The critical correlation function $G(r = L)$ in the $\langle 10 \rangle$ crystallographic direction and the effective exponents $\omega_{\text{eff}}(L)$ and $\widetilde{\omega}(L)$ vs the linear size L of the lattice (b) in Fig. 1

L	$G(L)$	$\omega_{\text{eff}}(L)$	$\widetilde{\omega}(L)$
2	0.8000000000000000		
3	0.7203484812087670		
4	0.6690636562097066		
5	0.6321925914229602		
6	0.6037455936471098		
7	0.5807668304926868		
8	0.5616046762441826	2.066235298	
9	0.5452468033693456	2.043461090	
10	0.5310294874153481	2.030235674	1.996772124
11	0.5184950262041604	2.022130104	1.999333324
12	0.5073151480587211	2.016864947	1.999941357
13	0.4972468711401118	2.013265826	2.000036957
14	0.4881056192765374	2.010701166	2.000040498
15	0.4797481011874659	2.008811505	2.000044005
16	0.4720609977942179	2.007380630	2.000053415
17	0.4649532511721054	2.006272191	2.000063984
18	0.4583506666254706	2.005396785	2.000073711
19	0.4521920457268738		
20	0.4464263594840965		

we have compensated the effect of the correction term $b_2 L^{-2}$. Besides, by matching the amplitude b in (21) we have compensated also the next trivial correction term $\sim L^{-3}$ in the expansion of $\omega_{\text{eff}}(L)$. It means that the extrapolated exponent $\widetilde{\omega}(L)$ does not contain these expansion terms, i. e., we have

$$\widetilde{\omega}(L) = 2 + b_1 L^{2-\omega} + \delta\widetilde{\omega}(L) , \tag{23}$$

where $\delta\widetilde{\omega}(L)$ represents a remainder term. It includes trivial corrections like L^{-4}, L^{-5}, etc., and also subleading nontrivial corrections, as well as corrections of order $(\varepsilon\, L^{2-\omega})^2$, $(\varepsilon\, L^{2-\omega})^3$, etc., neglected in (22). According to the latter, Eq. (23) is meaningless in the thermodynamic limit $L \to \infty$, but it can be used to evaluate the correction-to-scaling exponent ω from the transient behavior at large, but not too large values of L where $b_1 L^{2-\omega} \ll 1$ holds. In our example the latter condition is well satisfied, indeed.

Based on (23), we have estimated the nontrivial correction-to-scaling exponent ω by using the data of $\widetilde{\omega}(L)$ in Table 1. We have used two different ansatzs

$$2 - \omega_1(L) = \ln\left[\Delta\widetilde{\omega}(L)/\Delta\widetilde{\omega}(L-1)\right] / \ln[L/(L-1)] \tag{24}$$

and

$$2 - \omega_2(L) = L\,\left[\Delta\widetilde{\omega}(L) - \Delta\widetilde{\omega}(L-1)\right] / \Delta\widetilde{\omega}(L) , \tag{25}$$

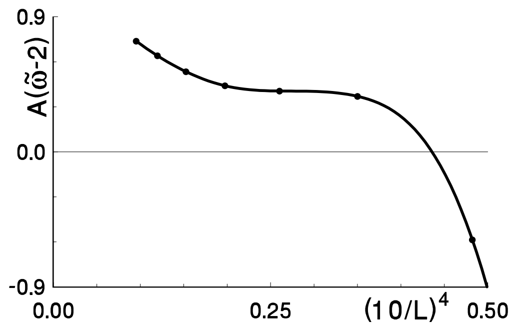


Figure 3. The deviation of the extrapolated effective exponent $\Delta\widetilde{\omega}(L) = \widetilde{\omega}(L) - 2$, scaled by a factor $A = 10^4$, as a function of L^{-4}. The extrapolation has been made by using the calculated $G(r)$ values in Table 1 up to the size $L+2$. A linear convergence to zero would be expected in the absence of any nontrivial correction terms

as well as the linear combination of them

$$\omega(L) = (1-\alpha)\,\omega_1(L) + \alpha\,\omega_2(L) \tag{26}$$

containing a free parameter α. We have $\omega(L) = \omega_1(L)$ at $\alpha = 0$ and $\omega(L) = \omega_2(L)$ at $\alpha = 1$. In general, the effective exponent $\omega(L)$ converges to the same result ω at an arbitrary value of α, but at certain values the convergence is better. The results for $2 - \omega(L)$ vs $L^{\omega-6}$ at different α values are presented in Fig. 4 by a set of curves. In this scale the convergence to the asymptotic value would be linear (within the actual region where $L \gg 1$ and $b_1\,L^{2-\omega} \ll 1$ hold) for $\alpha = 0$ under the condition $\delta\widetilde{\omega}(L) \propto L^{-4}$. We have chosen the scale of $L^{-5.75}$, as it is consistent with our result $\omega = 1/4$. Nothing is changed if we use a slightly different scale, e. g., L^{-4} consistent with $\omega = 2$ or $L^{-14/3}$ consistent with the correction-to-scaling exponent $\omega = 4/3$ proposed for some models of the 2D Ising universality class in [5]. As we

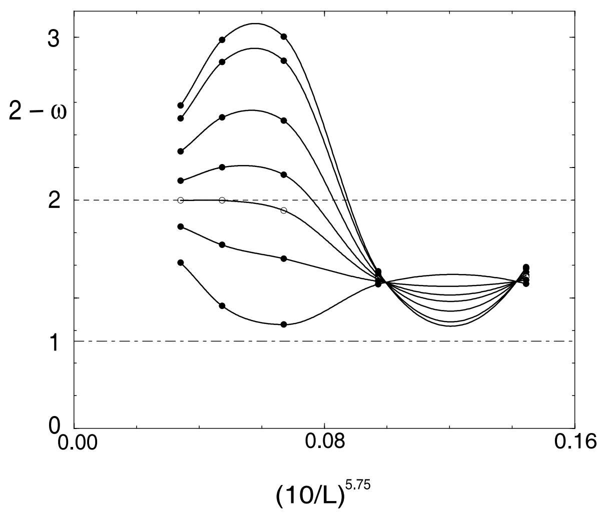


Figure 4. The exponent $2-\omega$ estimated from (26) at different system sizes. From top to bottom (if viewed from the left): $\alpha = 0, 1, 3.5, 5.75, 7.243, 9.25, 12$. The results for the optimal α value 7.243 are shown by open circles. The dashed line indicates our estimated asymptotic value $2 - \omega = 1.75$, whereas the dash dot line — the value 2/3 which would be expected according to [5]

see from Fig. 4, all curves tend to merge at an asymptotic value of about $2-\omega = 1.75$ shown by a dashed line, which corresponds to $\omega = 1/4$. The optimal value of α is defined by the condition that the last two estimates $\omega(17)$ and $\omega(18)$ agree with each other. It occurs at $\alpha = 7.243$, and the last two points lie just on the dashed line.

3.3. Comparison to the known exact results and estimation of numerical errors

We have carefully checked our algorithms comparing the results with those obtained via a straightforward counting of all spin configurations for small lattices, as well as comparing the obtained values of the partition function to those calculated from the known exact analytical expressions [7]. The relative discrepancies were extremely small (e. g., 10^{-15}), obviously, due to the purely numerical inaccuracy.

We have used the double-precision FORTRAN programs. The numerical errors in Table 1 have been estimated by repeating some calculations with a twice larger number of digits (REAL*16 option). Thus, the errors in the $G(L)$ values for $L = 10$ to $L = 17$ are $4.7 \cdot 10^{-17}$, $4.06{\cdot}10^{-16}$, $-3.52{\cdot}10^{-16}$, $-5.65{\cdot}10^{-16}$, $1.03{\cdot}10^{-15}$, $1.41{\cdot}10^{-15}$, $-1.71{\cdot}10^{-16}$, and $3.09{\cdot}10^{-16}$. To eliminate the summation error for the largest lattice $L = 20$, we have split the summation over the configurations of the first row into several parts in such a way that a relatively small part, including only the first 10 000 configurations from the total number of 52 487 nonequivalent ones, makes the main contribution to Z and Z'. The same trick with splitting into two approximately equal parts has been used at $L = 19$. As a result, the numerical errors at $L = 18, 19, 20$ are not much larger than the above listed values for $10 \leqslant L \leqslant 17$. The resulting numerical errors in Fig. 4 are comparable to 0.03 (they are larger on the periphery and smaller in the middle part around $2 - \omega \sim 1.75$), i. e., about the symbol size. In Fig. 3, the errors are practically not seen.

4. Discussion

Using our method of effective exponents, we have also analysed the corrections to the scaling for the correlation function $G(r)$ on an infinite lattice computed by the exact formulae given in [4]. In this case, the effective exponents depend on finite distances r used in the estimations based on (16), where $r/L = 0$. We have found that $\widetilde{\omega}_{\text{eff}}(r)$ for the correlation function in different crystallographic directions converges to 2 in complete agreement with $\omega_\ell = 2\ell$. It is consistent with the analytical solution for the $\langle 11 \rangle$ direction. The latter shows that our method is not misleading, and the nontrivial correction we have found before is a real finite-size effect. This is an essentially new result, since the known results (see [18, 30, 31] and references therein) for the thermodynamic functions (free energy, internal energy, specific heat) show only “trivial” corrections with integer correction-to-scaling exponents. Besides, it was proved in [23] for the case of the Brascamp—Kunz boundary conditions that no nontrivial corrections to the finite-size scaling show up in zeroes of the partition function and in related quantities like specific heat. There is no contradiction with our result, since the correlation function cannot be calculated from the zeroes of the partition function and contains more detailed information about the model than the partition function depending on the temperature and the system size.

It is interesting to compare our results with those of the high temperature series analysis in [4, 27, 29]. An evidence was provided in [27] for the existence of a correction term with the correction-to-scaling exponent $\theta = 9/4$ in the asymptotic expansion of the susceptibility χ approaching the critical point $t = |\beta - \beta_c|/\beta_c \to 0$. According to the known finite-size scaling arguments [14], θ is related to the finite-size correction exponent ω by $\theta = \nu\omega$, where ν is the critical exponent describing the divergence of the correlation length $\xi \sim t^{-\nu}$ at $t \to 0$. If a correction with $\theta = 9/4$ exists in the susceptibility, then it must be present also in the correlation function due to the relation $\chi = \sum_{\mathbf{x}} G(\mathbf{x}_1 - \mathbf{x})$, where the summation runs over the set of vectors $\mathbf{x}$ pointing from the origin to all possible lattice sites. The inverse statement is not true: a nontrivial correction term existing in the correlation function can vanish in χ due to the summation of contributions with opposite signs. Our calculations by exact algorithms have not revealed the finite-size correction $\propto L^{-9/4}$ corresponding to $\theta = 9/4$ at the critical point. Hence, either it has a too small amplitude or is absent. The latter would be consistent with the idea that the statement of [4, 29] about the presence of only integer correction-to-scaling exponents in the susceptibility can be extended to the finite-size scaling. Our analysis at the critical point $\beta = \beta_c$, however, does not exclude the possibility that nontrivial corrections appear in the susceptibility away from β_c at $\xi \propto L$. Besides, nontrivial corrections to the scaling can easily be overseen in a numerical analysis, if they have very small amplitudes (e. g. 10^{-6} or smaller), as in our case of the $L^{-1/4}$ correction.

The correction with $\omega = 1/4$, as well as that with $\omega = 9/4$ can be, in principle, expected in view of the theory developed in [25]. According to [25], the singular structure of the correlation function in the thermodynamic limit at $t \to 0$ is represented by the correction-to-scaling exponents $\theta_\ell = \ell\eta$ (with $\ell = 1, 2, 3, \ldots$), which correspond to the exponents $\omega_\ell = \theta_\ell/\nu$ in the finite-size scaling. In the 2D Ising model, where $\nu = 1$ and $\eta = 1/4$ [6], we have $\theta_\ell = \omega_\ell$, so that $\omega = 1/4$ correponds to $\ell = 1$ and $\omega = 9/4$ — to $\ell = 9$. Besides, some of the expansion coefficients can be zero [25], therefore it is possible that only a subset of the whole set of exponents $\omega_\ell = \ell\eta/\nu$ appears. From this point of view, it is possible that nontrivial corrections to the scaling show up only in the correlation function and are canceled in the susceptibility due to the summation.

It was conjectured in [15] that all corrections to the scaling in the 2D Ising model arise from the breaking of rotational symmetry within framework of the conformal field theory. This conjecture is based solely on the fact that it explains all known and established corrections to the scaling. The question arises whether or not the $L^{-1/4}$ correction proposed by our analysis can also be explained in this way. The negative answer would mean that possibly other sources of finite-size corrections exist. In this aspect, it was mentioned in [15] (see p. 30, top) that the lattice Ising model shows also features that are not predicted by the conformal field theory and the renormalisation group.

5. Conclusions

The two-point correlation function of the 2D Ising model at the critical point has been calculated numerically by the exact transfer matrix algorithms developed in this paper. The results for finite lattices including up to 800 spins point to existence of a nontrivial correction to the finite-size scaling with a very small amplitude and an exponent of about 1/4. It is in contrast to the case of the infinite lattice, where no nontrivial corrections to the scaling have been observed. Our results agree with the theory developed in [25].

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