Long-range dependence of the two-dimensional Ising model at critical temperature \(^*\)

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In memory of Benoît Mandelbrot

Abstract

The paper gives probabilists who are unfamiliar with the Ising model a coherent, integrated explanation of why the Ising model displays long-range dependence at critical temperature. The Ising model in two dimensions involves spins \(\sigma_{j,k} = \pm 1\) located at every node \((j,k)\) of the lattice, with nearest neighbor interactions. We shall focus on the covariances \(E\sigma_{0,0}\sigma_{0,N}\) and \(E\sigma_{0,0}\sigma_{N,N}\) between the spin at the origin and the spin located either on the axis at \((0,N)\) or located on the diagonal at \((N,N)\), when the temperature equals a critical value. Using a recent formulation of the so-called “Szegő’s theorem”, we explain why these covariances decrease to zero like \(N^{-1/4}\) as \(N \to \infty\), thus at a slow enough rate so as to exhibit long-range dependence.

1 Introduction

Benoît Mandelbrot’s interests extended to Physics as well as to Mathematics. What attracted his attention was behavior, deterministic or stochastic, that can be described by power laws. In particular, he studied stationary phenomena whose covariances at large lags decrease to 0 as a power function, but so slowly that the covariances are not summable. Such behavior is now called long-range dependence, long memory, strong dependence, or 1/f noise. The goal of this paper is to show how it arises in the two-dimensional Ising model at critical temperature.

The literature on the Ising model is large, especially in Mathematical Physics. We shall assume that the reader has no experience with it. We will introduce the Ising model and develop the techniques necessary to achieve our goals. Many of these methods are scattered through the monograph of McCoy and Wu (1973). It is our aim to thread them together in this article\(^1\).

This is in large part an expository effort. One result we obtain is conjectured, in fact, in McCoy and Wu (1973). To prove the conjecture, we use a recently proven extension of the so-called strong Szegő’s limit theorem. Our emphasis, however, is less on Szegő’s theorem than on describing the various steps required to show that the two-dimensional Ising model at critical temperature displays long-range dependence.

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\(^1\)We shall use to the extent possible the same notation as in McCoy and Wu (1973).
We start with the notion of “long-range dependence” which is commonly defined for second-order stationary time series. Recall that a second-order stationary time series \( X = \{ X_n \}_{n \in \mathbb{Z}} \) has a constant mean \( \mu = \mathbb{E} X_n \) and a covariance function
\[
\gamma(n - m) = \mathbb{E} X_n X_m - \mathbb{E} X_n \mathbb{E} X_m = \mathbb{E} X_n X_m - \mu^2,
\]
which depends only on the distance \(|n - m|\). One can characterize the second order properties of the time series \( X \) by specifying its mean \( \mu \) and covariance \( \gamma(n) \), \( n \in \mathbb{Z} \), or one can take a “spectral domain” perspective by focusing on the spectral density \( f(w) \), \( w \in [-\pi, \pi] \), of the time series, if it exists. The spectral density \( f(w) \) is defined as
\[
\int_{-\pi}^{\pi} e^{iwn} f(w) dw = \gamma(n), \quad n \in \mathbb{Z},
\]
that is, it is a function whose Fourier coefficients are the autocovariances \( \gamma(n) \).

We will say that a time series \( X = \{ X_n \}_{n \in \mathbb{Z}} \) exhibits long-range dependence if its covariance function satisfies
\[
\gamma(k) \sim c_1 k^{2d-1}, \quad \text{as } k \to \infty,
\]
where \( c_1 \) is a positive constant and
\[0 < d < 1/2.
\]
The higher \( d \), the stronger the dependence. The bound \( d < 1/2 \) ensures that \( \gamma(k) \to 0 \), as \( k \to \infty \). The bound \( d > 0 \) implies that the covariances are not summable, that is,
\[
\sum_{k=-\infty}^{\infty} \gamma(k) = \infty.
\]

Another consequence of the long-range dependence condition (1.1) is that the variance of the partial sums of \( X_n \) for \( n = 1, \ldots, N \) does not grow like \( N \) as in the case of random walk, but grows faster than \( N \). More precisely,
\[
\text{Var} \left( \sum_{n=1}^{N} X_n \right) = \sum_{j=1}^{N} \sum_{k=1}^{N} \gamma(j - k) \sim c_2 N^{2H}, \quad \text{as } N \to \infty,
\]
where \( c_2 = (d(2d + 1))^{-1}c_1 \) is a constant and
\[
H = d + \frac{1}{2} \in \left( \frac{1}{2}, 1 \right).
\]
The higher the exponent \( H \), the stronger the dependence. If, in fact, the \( X_n \)'s were perfectly correlated, that is, \( \gamma(k) = c_2 \) for all \( k \), then we would get \( \text{Var}(\sum_{n=1}^{N} X_n) = c_2 N^2 \), that is, \( H = 1 \). We do not consider such an extreme case because we suppose that \( \gamma(k) \to 0 \) as \( k \to \infty \).

The exponent \( H \) is often called the Hurst exponent, after Harold Edwin Hurst, the British hydrologist who studied the yearly changes in the level of the Nile through various centuries.

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\( a_n \sim b_n \) means \( \lim_{n \to \infty} a_n / b_n = 1 \).

\( ^3 \)There are also more general definitions of long-range dependence, for example, \( \gamma(k) = k^{2d-1} L(k) \), as \( k \to \infty \), where \( L \) is a slowly varying function at infinity, such as a constant or a logarithm. There is also a definition involving the spectral density, namely, \( f(w) \sim w^{-2d} L_1(w) \), as the frequency \( w \to 0 \), where \( L_1 \) is a slowly varying function at 0. That is, the spectral density blows up as the frequency tends to 0. These definitions are not always equivalent, however (see Taqqu (2003), Samorodnitsky (2006), Pipiras and Taqqu (2012)). For us, here, the definition (1.1) will be sufficient.
Motivated by Hurst’s studies, Benoît Mandelbrot also contributed to Hydrology by suggesting stochastic models to explain the fact that for some rivers, \( H \neq 1/2 \) (see Mandelbrot et al. (1965), Mandelbrot and Van Ness (1968), Mandelbrot and Wallis (1968, 1969)). For an overview, see Montanari (2003).

The Ising model, which is the focus of this paper, involves a two-dimensional lattice with a random spin \( \sigma_{j,k} = \pm 1 \) at each node \((j,k)\), with nearest neighbor interactions. We will study covariances

\[
E \sigma_{0,0} \sigma_{0,N} \quad \text{and} \quad E \sigma_{0,0} \sigma_{N,N}
\]
as \( N \to \infty \). We will show that at the so-called “critical temperature” these covariances display long-range dependence with \( d = 3/4 \), or equivalently with \( H = 7/8 \). The result for \( E \sigma_{0,0} \sigma_{N,N} \) can be found in McCoy and Wu (2010). The one for \( E \sigma_{0,0} \sigma_{0,N} \) had been conjectured.

The idea is to introduce the notion of bonds in the Ising lattice, then replace this lattice by a larger one, called the counting lattice, to which a number of matrices are associated. The covariances of interest involve these matrices, their inverse and related determinants. Szegö’s limit theorem describes the asymptotic behavior of these determinants.

The Ising model was first studied in the 1920’s by Ernst Ising in his Ph.D. thesis, supervised by Wilhelm Lenz. Ising considered the model in one dimension and found that it does not exhibit a phase transition. Although Ising conjectured that no phase transition occurs in higher dimension, further studies pointed to the contrary, culminating in the seminal work of Onsager (1944) who provided an explicit calculation for the so-called “free energy” of the two-dimensional Ising model. The Ising model has since played a special role in Statistical Mechanics and other areas, as a source of new ideas and as one of few realistic and exactly solvable models. A nice account of the historical developments concerning the Ising model can be found in Niss (2005, 2009).

The paper is structured as follows. In Section 2, we describe the Ising model and state the main theorem and a corollary. The proofs are developed in Sections 3 and 4 where the notions of dimers and Pfaffian are introduced. Szegö’s theorem and its extension are introduced in Section 5. The proofs are completed in Section 6 by applying the extended version of Szegö’s theorem. Section 7 contains some concluding remarks.

## 2 Model formulation and result

We consider the Ising model in two dimensions. The reason is that, in one dimension, the Ising model does not exhibit long-range dependence and, in three dimensions, the Ising model has not been solved exactly yet (in fact, this is still one of the famous open problems in Statistical Mechanics and, more generally, Physics – though see Cipra (2000)). Thus, consider a two-dimensional square lattice (Figure 1), referred to as the Ising lattice, with

\[
2L_v : \text{the number of rows},
\]
\[
2L_h : \text{the number of columns}
\]

(“\(v\)” stands for “vertical”, and “\(h\)” stands for “horizontal”). Denote a general point on the lattice as \((j,k)\), \(-L_v + 1 \leq j \leq L_v, -L_h + 1 \leq k \leq L_h\). Let

\[
\sigma_{j,k} = \pm 1
\]

\(^{4}\text{The model is sometimes referred to as the Lenz–Ising model.}\)
be a variable associated with a lattice point \((j, k)\).\(^5\) We will consider below correlations between \(\sigma_{0,0}\) and \(\sigma_{0,N}\), and \(\sigma_{0,0}\) and \(\sigma_{N,N}\). In fact, we will first let \(L_v, L_h \to \infty\) (the so-called thermodynamic limit), and then investigate these correlations as \(N \to \infty\).

In the Ising model, the collection of variables \(\{\sigma_{j,k} \mid -L_v + 1 \leq j \leq L_v, -L_h + 1 \leq k \leq L_h\}\) is assumed to follow the joint distribution

\[
\frac{1}{Z_{L_v,L_h}} e^{-\beta \mathcal{E}},
\]

where

\[
\mathcal{E} = - \sum_{j=-L_v+1}^{L_v} \sum_{k=-L_h+1}^{L_h} \left( E^h \sigma_{j,k} \sigma_{j,k+1} + E^v \sigma_{j,k} \sigma_{j+1,k} \right)
\]

with some positive constants \(E^h, E^v > 0\), and where

\[
Z_{L_v,L_h} = \sum_{\{\sigma_{j,k}\}} e^{-\beta \mathcal{E}}
\]

is the normalization constant, where the sum is over all possible configurations (outcomes) \(\{\sigma_{j,k}\}\). Since each \(\sigma_{j,k}\) can take 2 values, there are \(2^{(2L_v)(2L_h)}\) configurations. The parameter \(\beta > 0\) is expressed as

\[
\beta = \frac{1}{k_B T},
\]

where \(k_B = 1.38 \times 10^{-23}\) is the Boltzmann's constant and \(T > 0\).

The term \(\mathcal{E}\) in (2.2) is referred to as energy (Hamiltonian) of a configuration \(\{\sigma_{j,k}\}\). Note that the energy is determined only by interactions between neighboring sites, with the contributions \(E^h\) for horizontal interactions and \(E^v\) for vertical interactions. Note also the following effect of individual terms on the overall energy of the system. The energy is lower when neighboring sites

\(^5\)Note that \(j\) and \(k\) in \((j, k)\) refer to row (vertical) and column (horizontal) directions, respectively. This is in accord with the matrix notation where \((j, k)\) is used for a matrix element \(a_{j,k}\). But this is the opposite of the \((x, y)\) convention, where for example \(x\) refers to the horizontal direction.
align as +1 and +1, or as −1 and −1. Lower (negative) energy $E$ translates into higher probability \((2.1)\), that is, as expected in physical terms, the system favors configurations with lower energy.

The parameter $T > 0$ in \((2.4)\) is referred to as temperature (and $\beta$ as inverse temperature). When $T \to \infty$ (high temperature), note that $\beta \to 0$ and hence \((2.1)\) approaches the uniform probability distribution on the lattice. In this case, the variables $\sigma_{j,k}$ tend to be independent and the system is in the disordered state. On the other hand, when $T \to 0$ (low temperature), note that $\beta \to \infty$ and the aligned configurations (all +1 or −1) are more likely. This is because the exponent in \((2.1)\) will be large and positive. In this case, the system is in the ordered state.

Moving from the disordered to ordered state (large $T$ to small $T$), one could expect that the system undergoes a phase transition at some critical temperature $T = T_c > 0$. We shall not define $T_c$ in rigorous terms. Informally, the system exhibits very different characteristics for $T < T_c$ and $T > T_c$. The two-dimensional Ising model turns out to have such phase transition at $T_c > 0$.

Here are few other notes regarding the Ising model. The distribution \((2.1)\) is also known as Boltzmann distribution or Gibbs distribution. The normalization factor

$$Z_{L_v,L_h} = Z_{L_v,L_h}(\beta) = \sum_{\{\sigma_{j,k}\}} e^{-\beta E}$$

\((2.5)\)

in \((2.3)\) is called the partition function. In \((2.5)\), the sum is over every value ±1 of the variables $\sigma_{j,k}$ in the lattice. The energy $E$ in \((2.2)\) is often written more generally as

$$E = -\sum_{j=-L_v+1}^{L_v} \sum_{k=-L_h+1}^{L_h} (E^h \sigma_{j,k} \sigma_{j,k+1} + E^v \sigma_{j,k} \sigma_{j+1,k} + H \sigma_{j,k}),$$

\((2.6)\)

where the terms $H \sigma_{j,k}$ in \((2.6)\) account for the so-called external magnetic field\(^6\) (see the discussion below for the reason of using “magnetic”). With \((2.2)\), we thus focus only on the situation of zero magnetic field $H = 0$. (In fact, the presence of the external magnetic field complicates the matters considerably and the Ising model with a magnetic field $H > 0$ has not been solved explicitly yet. See, for example, McCoy (2010), pp. 277-280.)

Note also that the energy $E$ in \((2.2)\) involves the variables $\sigma_{j,L_h+1}$ and $\sigma_{L_v+1,k}$ “outside” the lattice. What exactly are these variables? This is related to the so-called boundary conditions. The case

$$\sigma_{j,L_h+1} = \sigma_{j,-L_h+1}, \quad \sigma_{L_v+1,k} = \sigma_{-L_v+1,k}$$

\((2.7)\)

is referred to as that of periodic boundary (toroidal or doughnut-shaped) conditions. The case

$$\sigma_{j,L_h+1} = 0, \quad \sigma_{L_v+1,k} = 0$$

\((2.8)\)

is known as that of free boundary conditions. It effectively corresponds to the situation where the terms involving $\sigma_{j,L_h+1}$ and $\sigma_{L_v+1,k}$ are not present in \((2.2)\).

Finally, one of the original applications of the Ising model is to the phenomenon of ferromagnetism. The variables $\sigma_{j,k}$ model a magnetic dipole of atoms of ferromagnetic material (e.g. iron). The variables $\sigma_{j,k}$ are referred to as spins. The critical temperature $T_c$ is known as the Curie temperature. Below this temperature, ferromagnetic materials exhibit spontaneous magnetization.

We are interested here in the behavior of the correlation function of the spin at the origin and the spin at position $(M, N)$, namely

$$C(M, N) = \text{Corr} (\sigma_{0,0}, \sigma_{M,N}) = \frac{\langle E \sigma_{0,0} \sigma_{M,N} \rangle - \langle E \sigma_{0,0} \rangle \langle E \sigma_{M,N} \rangle}{\sqrt{\langle E^2 \sigma_{0,0} \rangle - (\langle E \sigma_{0,0} \rangle)^2} \sqrt{\langle E^2 \sigma_{M,N} \rangle - (\langle E \sigma_{M,N} \rangle)^2}} = \langle E \sigma_{0,0} \sigma_{M,N} \rangle,$$

\(^6\)Do not confuse the magnetic field $H$ in \((2.6)\) with the Hurst parameter in \((1.3)\).
since $\mathbb{E}\sigma_{j,k} = 0$ and $\mathbb{E}\sigma_{j,k}^2 = 1 = \sigma_{j,k}^2$. Thus correlations reduce to covariances. For the sake of simplicity and illustration, we shall only consider row and diagonal covariances

$$C(0,N) = \mathbb{E}\sigma_{0,0}\sigma_{0,N}, \quad C(N,N) = \mathbb{E}\sigma_{0,0}\sigma_{N,N}. \quad (2.9)$$

We shall also work in the case of free boundary conditions (2.8). Our goal is to show the following:

**Theorem 2.1** At the critical temperature $T = T_c$ characterized by

$$1 = \sinh 2\beta E_h \sinh 2\beta E_v \quad (2.10)$$

and as $N \to \infty$,

$$\lim_{L_h \to \infty} \lim_{L_v \to \infty} \mathbb{E}\sigma_{0,0}\sigma_{0,N} \sim \left(\frac{1 + \alpha_1}{1 - \alpha_1}\right)^{1/4} AN^{-1/4}, \quad (2.11)$$

$$\lim_{L_h \to \infty} \lim_{L_v \to \infty} \mathbb{E}\sigma_{0,0}\sigma_{N,N} \sim AN^{-1/4}, \quad (2.12)$$

where $A = 0.645002\ldots$ and

$$\alpha_1 = \frac{z_h(1 - z_v)}{1 + z_v}, \quad z_h = \tanh \beta E_h, \quad z_v = \tanh \beta E_v.$$

The asymptotic behavior of $\mathbb{E}\sigma_{0,0}\sigma_{N,N}$ in (2.12) is stated in McCoy and Wu (1973), (4.43), p. 265, and proved but the asymptotic behavior of $\mathbb{E}\sigma_{0,0}\sigma_{0,N}$ in (2.11), stated in McCoy and Wu (1973), p. 267, is only conjectured (McCoy and Wu (1973), p. 266).

Whereas, as expected, the asymptotic behavior of $\mathbb{E}\sigma_{0,0}\sigma_{N,N}$ is invariant under permutation of $h$ and $v$, this is not the case for $\mathbb{E}\sigma_{0,0}\sigma_{0,N}$, for which

$$\frac{1 + \alpha_1}{1 - \alpha_1} = \frac{1 + z_v + z_h - z_hz_v}{1 + z_v - z_h + z_hz_v}. \quad (2.13)$$

Observe that in the special case $E_h = E_v = E$, this ratio simplifies and one has

**Corollary 2.1** If $E_h = E_v$, then at the critical temperature $T = T_c$, one has as $N \to \infty$,

$$\lim_{L_h \to \infty} \lim_{L_v \to \infty} \mathbb{E}\sigma_{0,0}\sigma_{0,N} \sim 2^{1/8} AN^{-1/4}. \quad (2.14)$$

Since, at the critical temperature $T_c$, the covariances behave like $N^{-1/4}$ for large $N$, the Ising model exhibits long-range dependence. By identifying the exponent $2d - 1$ with $-1/4$ and using $H = d + 1/2$, one gets that the Ising model exhibits long-range dependence with

$$d = \frac{3}{8} \quad \text{and} \quad H = \frac{7}{8}. \quad (2.15)$$

Theorem 2.1 and Corollary 2.1 are proved in Section 6.

### 3 Correlations, dimers and Pfaffians

We shall express the correlations $C(0,N)$ and $C(N,N)$ in terms of the determinants of $N \times N$ matrices in the so-called thermodynamic limit $L_v, L_h \to \infty$ first, and then analyze them as $N \to \infty$.

Observe that

$$\mathbb{E}\sigma_{0,0}\sigma_{0,N} = \frac{1}{Z_{L_v,L_h}} \sum_{\sigma_{j,k}} \sigma_{0,0}\sigma_{0,N} e^{-\beta \xi}. \quad (3.1)$$

We shall analyze the two terms $Z_{L_v,L_h}$ and $\sum_{\sigma_{j,k}} \sigma_{0,0}\sigma_{0,N} e^{-\beta \xi}$ separately. The focus will be on the partition function $Z_{L_v,L_h}$, and similar arguments will be outlined for the second term. As for the diagonal correlation $\mathbb{E}\sigma_{0,0}\sigma_{N,N}$, we shall give its corresponding expression without proof.
3.1 Partition function $Z_{L_v,L_h}$

Observe that

$$Z_{L_v,L_h} = \sum_{\{\sigma_{j,k}\}} e^{-\beta E} = \sum_{\{\sigma_{j,k}\}} e^{\beta \sum_{j=-L_v+1}^{L_v} \sum_{k=-L_h+1}^{L_h} (E_h \sigma_{j,k} \sigma_{j,k+1} + E_v \sigma_{j,k} \sigma_{j+1,k})}$$

$$= \sum_{\{\sigma_{j,k}\}} \prod_{j=-L_v+1}^{L_v} \prod_{k=-L_h+1}^{L_h} e^{\beta E_h \sigma_{j,k} \sigma_{j,k+1}} \prod_{j=-L_v+1}^{L_v} \prod_{k=-L_h+1}^{L_h} e^{\beta E_v \sigma_{j,k} \sigma_{j+1,k}}$$

$$= \sum_{\{\sigma_{j,k}\}} \prod_{j=-L_v+1}^{L_v} \prod_{k=-L_h+1}^{L_h} \left( \cosh \beta E_h + \sigma_{j,k} \sigma_{j,k+1} \sinh \beta E_h \right) \times$$

$$\times \prod_{j=-L_v+1}^{L_v} \prod_{k=-L_h+1}^{L_h} \left( \cosh \beta E_v + \sigma_{j,k} \sigma_{j+1,k} \sinh \beta E_v \right), \quad (3.2)$$

since $\cosh a = \frac{1}{2} (e^a + e^{-a})$, $\sinh a = \frac{1}{2} (e^a - e^{-a})$ and thus

$$e^{ax} = \cosh a + x \sinh a, \quad x = \pm 1.$$ 

Under the free boundary conditions, we get further that

$$Z_{L_v,L_h} = (\cosh \beta E_h)^{2L_v(2L_h-1)} (\cosh \beta E_v)^{(2L_v-1)2L_h} \tilde{Z}_{L_v,L_h}, \quad (3.3)$$

where

$$\tilde{Z}_{L_v,L_h} = \sum_{\{\sigma_{j,k}\}} \prod_{j=-L_v+1}^{L_v} \prod_{k=-L_h+1}^{L_h} \left( 1 + \sigma_{j,k} \sigma_{j,k+1} z_h \right) \times$$

$$\times \prod_{j=-L_v+1}^{L_v} \prod_{k=-L_h+1}^{L_h} \left( 1 + \sigma_{j,k} \sigma_{j+1,k} z_v \right) =: \sum_{\{\sigma_{j,k}\}} \tilde{Z}_{L_v,L_h}\{\{\sigma_{j,k}\}\}, \quad (3.4)$$

and

$$z_h = \frac{\sinh \beta E_h}{\cosh \beta E_h} = \tanh \beta E_h, \quad z_v = \tanh \beta E_v. \quad (3.5)$$

Consider now $\tilde{Z}_{L_v,L_h}\{\{\sigma_{j,k}\}\}$ given by (3.4). Expand all the products to express $\tilde{Z}_{L_v,L_h}\{\{\sigma_{j,k}\}\}$ as the sum over a number of terms as

$$\tilde{Z}_{L_v,L_h}\{\{\sigma_{j,k}\}\} = 1 + \sigma_{-L_v+1,-L_h+1} \sigma_{-L_v+1,-L_h+2} z_v + \cdots + \sigma_{L_v-1,L_h} \sigma_{L_v,L_h} z_v$$

$$+ \cdots + \prod_{j=-L_v+1}^{L_v} \prod_{k=-L_h+1}^{L_h} \sigma_{j,k} \sigma_{j,k+1} z_h \prod_{j=-L_v+1}^{L_v} \prod_{k=-L_h+1}^{L_h} \sigma_{j,k} \sigma_{j+1,k} z_v. \quad (3.6)$$

Each term in the sum (3.6) can be thought as containing a factor for every pair of nearest-neighbor sites $(j,k)$ and $(j',k')$ on the lattice. This factor is either 1, when 1 from $1 + \sigma_{j,k} \sigma_{j',k'} z$ is selected in the product, or $\sigma_{j,k} \sigma_{j',k'} z$, when $\sigma_{j,k} \sigma_{j',k'} z$ is selected from the product ($z$ denotes $z_h$ or $z_v$). For example, the first term in (3.6) occurs when each pair of nearest-neighbor sites contributes 1, and the last term in (3.6) occurs when each contributes $\sigma_{j,k} \sigma_{j',k'} z$. Each term in the sum (3.6) will therefore include either 1, $\sigma_{j,k}$, $\sigma_{j,k}^2$, or $\sigma_{j,k}^2$ and hence one of the five quantities can be
associated with each site \((j, k)\). Note now that the terms in the sum \(\tilde{Z}_{L_v, L_h}(\{\sigma_{j,k}\})\) with sites having \(\sigma_{j,k}\) or \(\sigma_{j,k}^3\) will vanish in the total sum \(\sum_{\{\sigma_{j,k}\}}\) in (3.4) because

\[
\sum_{\sigma_{j,k}=\pm 1} \sigma_{j,k} = \sum_{\sigma_{j,k}=\pm 1} \sigma_{j,k}^3 = 0.
\]

Thus only

\[
\text{the terms having } 1, \sigma_{j,k}^2 \equiv 1 \text{ or } \sigma_{j,k}^4 \equiv 1 \quad (3.7)
\]

will not vanish in the total sum \(\sum_{\{\sigma_{j,k}\}}\).

The presence of a term \(\sigma_{j,k}\sigma_{j,k+1}z_h\) in (3.6) can be interpreted as indicating the presence of a horizontal bond \(z_h\) connecting the sites \((j, k)\) and \((j, k + 1)\). A corresponding interpretation holds for \(\sigma_{j,k}\sigma_{j+1,k}z_v\). From a different perspective, when \(1, \sigma_{j,k}^2\) or \(\sigma_{j,k}^4\) is associated with the site \((j, k)\), then zero, two or four bonds traverse the site \((j, k)\). Therefore, the terms in the sum (3.6) where the conditions (3.7) hold can be regarded as depicting a figure on a lattice with the following properties:

(i) each bond between nearest neighbors may be used, at most, once;

(ii) an even number of bonds terminate at each site.

Figure 2 depicts one such figure. Observe that such figure would contribute a term

\[
z_h^p z_v^q
\]

to the total sum \(\sum_{\{\sigma_{j,k}\}}\), where \(p\) is the number of horizontal bonds in the figure \((p = 16\) in Figure 2) and \(q\) is the number of vertical bonds in the figure \((q = 16\) in Figure 2). Statement (ii) above implies that \(p\) and \(q\) are even. Since there are

\[
\sum_{\{\sigma_{j,k}\}} 1 = 2^{2L_v 2L_h}
\]
different configurations, one gets that

\[
\tilde{Z}_{L_v, L_h} = 2^{2L_v 2L_h} \sum_{p,q} N_{p,q} z_h^p z_v^q =: 2^{2L_v 2L_h} g(z_h, z_v),
\]

where \(N_{p,q}\) is the number of figures on the lattice with the properties (i) and (ii) above, and where \(p, q\) are the numbers of horizontal and vertical bonds of the figure. By convention, \(N_{0,0} = 1\). The next step is to compute the “generating function”

\[
g(z_1, z_2) = \sum_{p,q} N_{p,q} z_1^p z_2^q \quad (3.9)
\]

associated with counting of the figures as in Figure 2. Observe that \(g(z_1, z_2) \geq 0\) since \(p\) and \(q\) are even.

3.2 Dimers

There is an ingenious way to turn the problem of computing (3.9) into the so-called “problem of counting closest-packed dimer coverings” on a suitable lattice as explained in McCoy and Wu
We will see later that the latter problem has a solution involving a matrix determinant which can then be studied more easily.

The first step is to replace the Ising lattice by a larger lattice, which we will call the counting lattice. More specifically, replace each site of the Ising lattice, as on the left side of Figure 3, by a six-site cluster depicted on the right side of Figure 3. Note that, as in the Ising lattice, the six-site cluster has four connecting lines. The difference is that one site is now replaced by six sites. The new, counting lattice has then $2K = 6(2L_v)(2L_h)$ sites and is formed by connecting six-site clusters and is depicted in Figure 4.

In the next step, the idea is to replace each of eight possible Ising site configuration bonds with a suitable configuration of bonds on the counting lattice. The replacement is done according to Figure 5. With this replacement, each figure counted in (3.9) is replaced by another figure in the counting lattice. In the Ising lattice, two adjacent sites may be either unconnected or connected by a bond. In the counting lattice, each site has exactly one bond with one of its neighbors indicated by a double line in Figure 5. Each such bond is called a dimer. The figure one gets in the counting lattice is called a closest-packed dimer configuration. Then, the problem of counting in (3.9) can be replaced by counting dimer configurations in the counting lattice.

To make this connection more precise, three classes of bonds need to be distinguished in the counting lattice: (1) horizontal bonds between clusters, (2) vertical bonds between clusters, and (3) bonds within a cluster. Let

$$G(z_1, z_2, z_3) = \sum_{p,q,r} N_{p,q,r} z_1^p z_2^q z_3^r$$

be the corresponding generating function, where $N_{p,q,r}$ is the number of dimer configurations on the counting lattice with $p$ bonds of type (1), $q$ bonds of type (2) and $r$ bonds of type (3). In particular, one can think that bonds of types (1), (2) and (3) carry weights of sizes $z_1$, $z_2$ and $z_3$.

---

7In Chemistry, a dimer is a structure formed by two sub-units.
8One uses this term whenever each site has exactly one bond with one of its neighbors.
respectively. The generating functions (3.9) and (3.10) are then related as follows:

\[ g(z_1, z_2) = G(z_1, z_2, 1), \]

(3.11)

by assigning the weight \( z_3 = 1 \) to bonds within clusters. This is because a horizontal (resp. vertical) bond in the Ising lattice is associated with a horizontal (resp. vertical) bond between clusters (see Figure 5).

The advantage of the formulation (3.10) or (3.11) is that it can be related to the determinant of a matrix. We shall do this in two steps. In the first step, we shall express (3.11) as

\[ g(z_1, z_2) = G(z_1, z_2, 1) = \sum_p \bar{b}_{p_1, p_2} \bar{b}_{p_3, p_4} \cdots \bar{b}_{p_2K-1, p_2K}, \]

(3.12)

where \( \bar{B} = (\bar{b}_{pq})_{1 \leq p, q \leq 2^K} \) is a suitable \( 2^K \times 2^K \) matrix (the bar does not refer here to the complex conjugate) and \( \sum_p' \) is the sum over all permutations \( p_1, p_2, \ldots, p_{2^K} \) of \( 1, 2, \ldots, 2^K \) satisfying

\[ p_{2m-1} < p_{2m}, \ 1 \leq m < K, \quad p_{2m-1} < p_{2m+1}, \ 1 \leq m < K - 1. \]

(3.13)

For example, if \( 2^K = 4 \), the sum is over the permutations 1234, 1324 and 1423 of 1234. Relation (3.13) is satisfied since these permutations are such that \( p_1 < p_2, \ p_1 < p_3 \) and \( p_3 < p_4 \), where, in the permutation 1324, for example, \( p_1 = 1, \ p_2 = 3, \ p_3 = 2, \ p_4 = 4 \). In the second step, the expression (3.12) will be written as the so-called Pfaffian of a matrix. As stated below, the Pfaffian of a matrix is the square root of its determinant. We shall now detail these two steps.

In the first step, the expression (3.12) and the permutations (3.13) above are naturally related to closest-packed dimer configurations on any lattice. Suppose a lattice (that is, any lattice) consists of \( 2K \) sites and enumerate these sites by \( 1, 2, \ldots, 2^K \). Observe that there is a one-to-one correspondence between closest-packed dimer configurations on the lattice and permutations satisfying (3.13): the permutation

\[ p_1 p_2 \mid p_3 p_4 \mid \cdots \mid p_{2K-1} p_{2K} \]

is associated with the closest-packed dimer configuration where dimers connect the sites \( p_1 \) and \( p_2 \), \( p_3 \) and \( p_4 \), \ldots, \( p_{2K-1} \) and \( p_{2K} \).
with a lattice of $2K = 4$ sites, there are 3 closest-packed dimer configurations associated with

$$12\,|\,34, \quad 13\,|\,24 \quad \text{and} \quad 14\,|\,23,$$

as illustrated in Figure 6. Suppose, in addition, that a dimer connecting sites $p$ and $q$ carries a weight $\overline{b}_{p,q}$. Then, we define the weight of the closest-packed dimer configuration associated with the permutation $p_1 p_2 \mid p_3 p_4 \mid \cdots \mid p_{2K-1} p_{2K}$ as

$$\overline{b}_{p_1,p_2} \overline{b}_{p_3,p_4} \cdots \overline{b}_{p_{2K-1},p_{2K}}.$$

Therefore,

$$\sum_{p} \overline{b}_{p_1,p_2} \overline{b}_{p_3,p_4} \cdots \overline{b}_{p_{2K-1},p_{2K}}$$

is exactly the sum of the weights of all closest-packed dimer configurations.

With the latter fact in mind, we now turn to the relation (3.12). The function $G(z_1, z_2, 1)$ can then be written as

$$G(z_1, z_2, 1) = \sum_{p} \overline{b}_{p_1,p_2} \overline{b}_{p_3,p_4} \cdots \overline{b}_{p_{2K-1},p_{2K}},$$

where

$$2K = 6(2L_v)(2L_h)$$

is the number of sites in the counting lattice, the sum $\sum_{p} \overline{b}_{p,q}$ can be viewed as over all closest-packed dimer configurations, and the weights $\overline{b}_{p,q}$ are such that

$$\overline{b}_{p,q} = \begin{cases} 
1, & \text{if } p \text{ and } q \text{ are neighboring sites within the same six-site cluster}, \\
13, & \text{if sites } p \text{ and } q \text{ connect two six-site clusters in the vertical direction}, \\
14, & \text{if sites } p \text{ and } q \text{ connect two six-site clusters in the horizontal direction}, \\
0, & \text{otherwise}.
\end{cases}$$

(3.15)
Figure 5: Replacement of eight possible Ising site configuration bonds by suitable configuration bonds on the counting lattice. The connecting bonds are indicated by double lines. Observe that a horizontal (resp. vertical) bond at an Ising site is associated with a horizontal (resp. vertical) bond connecting clusters.

Figure 7 illustrates this. The weight 0 in $b_{pq}$ ensures that only closest-packed dimer configurations with dimers connecting neighboring sites count for the function $G(z_1, z_2, 1)$. This means, in particular, that most of the elements $\overline{b}_{pq}$ are actually zero.

A matrix $\overline{B} = (\overline{b}_{pq})$ satisfying (3.15) can be constructed as follows. Consider first $6 \times 6$ matrices $\overline{B}(j, k; j', k')$ labeled by the Ising lattice sites $(j, k)$ and $(j', k')$, where $-L_v + 1 \leq j, j' \leq L_v$, $-L_h + 1 \leq k, k' \leq L_h$. They are zero matrices except in the following cases, where they are defined as:

$$
\overline{B}(j, k; j, k) = 
\begin{pmatrix}
R & L & U & D & 1 & 2 \\
0 & 0 & 1 & 0 & 0 & 1 \\
0 & 0 & 0 & 1 & 1 & 0 \\
1 & 0 & 0 & 0 & 0 & 1 \\
0 & 1 & 0 & 0 & 1 & 0 \\
0 & 1 & 0 & 1 & 0 & 1 \\
1 & 0 & 1 & 0 & 1 & 0
\end{pmatrix}
$$

12
Figure 6: All possible closest-packed dimer configurations in a lattice of 4 sites.

Figure 7: The connecting bonds between sites are indicated by double lines. The weight $b_{pq}$ connecting two sites $p$ and $q$ is indicated. It is 1, $z_1$ or $z_2$ according to whether $p$ and $q$ are within the same six-site cluster, connect two six-site clusters in the vertical direction or connect two six-site clusters in the horizontal direction. All other bonds have weight 0.

for $-L_v + 1 \leq j \leq L_v$, $-L_h + 1 \leq k \leq L_h$,

$$\overline{B}(j, k; j, k + 1) = \overline{B}(j, k + 1; j, k)^T = \begin{pmatrix} R & L & U & D \end{pmatrix} = \begin{pmatrix} R & L & U & D \end{pmatrix}$$

for $-L_v + 1 \leq j \leq L_v$, $-L_h + 1 \leq k \leq L_h - 1$,

$$\overline{B}(j, k; j + 1, k) = \overline{B}(j + 1, k; j, k)^T = \begin{pmatrix} R & L & U & D \end{pmatrix} = \begin{pmatrix} R & L & U & D \end{pmatrix}$$
for \(-L_v + 1 \leq j \leq L_v - 1, -L_h + 1 \leq k \leq L_h\). Each site \((j, k)\) of the Ising lattice corresponds to a six-site cluster in the counting lattice. Think now of \(\overline{B}(j, k; j', k')\) as containing weights \(\overline{b}_{pq}\) between sites in six-site clusters denoted \((j, k)\) and \((j', k')\) (within the same cluster if \((j, k) = (j', k')\)). The labels \(R, L, U, D, 1, 2\) correspond to the six sites in a cluster, depicted in Figure 8. (\(R\) stands for “Right”, \(L\) for “Left”, \(U\) for “Up” and \(D\) for “Down”.) Note that these matrices are exactly such that their elements \(\overline{b}_{pq}\) satisfy (3.15). For example, within a cluster, a site \(R\) can only connect to \(U\) or \(2\) with the weight of 1.

Finally, the matrix \(\overline{B} = (\overline{b}_{pq})_{1 \leq p, q \leq 2K}\) is made of the \(6 \times 6\) blocks or submatrices \(\overline{B}(j, k; j', k')\), \(-L_v + 1 \leq j, j' \leq L_v, -L_h + 1 \leq k, k' \leq L_h\), we just defined. The exact placement of the blocks inside of the matrix \(\overline{B}\) is as follows. Order the \(d = (2L_v)(2L_h)\) sites \((j, k)\) along the rows for increasing columns \(k\), that is,

\[
(-L_v + 1, -L_h + 1), \ldots, (-L_v + 1, L_h),
\]
\[
(-L_v + 2, -L_h + 1), \ldots, (-L_v + 2, L_h),
\]
\[
\ldots
\]
\[
(L_v, -L_h + 1), \ldots, (L_v, L_h)
\]

and renumber the sites \(1 \leq m \leq d\). This renumbering associates then to each pair \((j, k), (j', k')\) a pair \((m, n)\), \(1 \leq m, n \leq d\). In the matrix \(\overline{B}\), its \((m, n)\) block of size 6 is then defined as \(\overline{B}(j, k; j', k')\).

### 3.3 Pfaffians

We now turn to the second step described in the discussion around (3.12), namely, to express (3.12) as the Pfaffian of a matrix. We first define the Pfaffian.

**Definition 3.1** Consider a \(2K \times 2K\) antisymmetric real-valued matrix \(A = (a_{jk})_{1 \leq j, k \leq 2K}\), that is, with elements \(a_{jk} = -a_{kj}\) and \(a_{jj} = 0\). Its Pfaffian is defined as

\[
\text{Pf}A = \sum_p' \delta_p a_{p_1 p_2} a_{p_3 p_4} \ldots a_{p_{2K-1} p_{2K}},
\]

where, as in (3.13), \(\sum_p'\) is the sum over all permutations \(p_1, p_2, \ldots, p_{2K}\) of \(1, 2, \ldots, 2K\) satisfying

\[
p_{2m-1} < p_{2m}, 1 \leq m < K, \quad p_{2m-1} < p_{2m+1}, 1 \leq m < K - 1
\]
and where $\delta_p$, the parity of the permutation $p$, is 1 if the permutation $p$ is made up of an even number of transpositions and $-1$ if $p$ is made of an odd number of transpositions.

For example, if $2K = 4$, and

$$A = \begin{pmatrix}
0 & a_{12} & a_{13} & a_{14} \\
-a_{12} & 0 & a_{23} & a_{24} \\
-a_{13} & -a_{23} & 0 & a_{34} \\
-a_{14} & -a_{24} & -a_{34} & 0
\end{pmatrix},$$

then by (3.14),

$$\text{Pf}A = a_{12}a_{34} - a_{13}a_{24} + a_{14}a_{23}.$$

This is because 1234, 1324, 1423 involve respectively 0, 1 and 2 transpositions.

The usefulness of the Pfaffian comes from the following formula: for an antisymmetric matrix $A$,

$$(\text{Pf}A)^2 = \det(A) \quad (3.18)$$

(see, for example, pp. 47-51 in McCoy and Wu (1973) for a proof). For example, if $2K = 2$ and

$$A = \begin{pmatrix}
0 & a_{12} \\
-a_{12} & 0
\end{pmatrix},$$

then one sees immediately that $(\text{Pf}A)^2 = \det(A)$ because $\text{Pf}A = a_{12}$ and $\det(A) = a_{12}^2$.

The relation (3.12) is not exactly the Pfaffian of the matrix $B$ in that it does not include the parity factor $\delta_p$. In fact, the parity factor can be introduced by suitably altering the signs of the elements of the matrix $B$. We shall describe but not prove the assignment for doing so. See, for example, pp. 51-67 in McCoy and Wu (1973) for more details.

For the sum (3.12) to have the parity factor $\delta_p$, the blocks of the matrix $B$ have to be replaced by the blocks:

$$\bar{A}(j; k; j, k) = \begin{pmatrix}
R & L & U & D & 1 & 2 \\
R & 0 & 0 & -1 & 0 & 0 & 1 \\
L & 0 & 0 & 0 & -1 & 1 & 0 \\
U & 1 & 0 & 0 & 0 & 0 & -1 \\
D & 0 & 1 & 0 & 0 & -1 & 0 \\
1 & 0 & -1 & 0 & 1 & 0 & 1 \\
2 & -1 & 0 & 1 & 0 & -1 & 0
\end{pmatrix}, \quad (3.19)$$

for $-L_v + 1 \leq j \leq L_v$, $-L_h + 1 \leq k \leq L_h$,

$$\bar{A}(j, k; j, k + 1) = -\bar{A}(j, k + 1; j, k)^T = \begin{pmatrix}
R & L & U & D & 1 & 2 \\
R & 0 & z_1 & 0 & 0 & 0 & 0 \\
L & 0 & 0 & 0 & 0 & 0 & 0 \\
U & 0 & 0 & 0 & 0 & 0 & 0 \\
D & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 \\
2 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}, \quad (3.20)$$
for \(-L_v + 1 \leq j \leq L_v, -L_h + 1 \leq k \leq L_h - 1,

\[ \overline{A}(j, k; j + 1, k) = -\overline{A}(j + 1, k; j, k)^T = \begin{pmatrix} R & L & U & D & 1 & 2 \\ R & 0 & 0 & 0 & 0 & 0 \\ L & 0 & 0 & 0 & 0 & 0 \\ U & 0 & 0 & z_2 & 0 & 0 \\ D & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 2 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \tag{3.21} \]

for \(-L_v + 1 \leq j \leq L_v - 1, -L_h + 1 \leq k \leq L_h\). Denote the corresponding matrix by \(\overline{A}\) and its elements by \(a_{p,q}\). (The \(2K \times 2K\) matrix \(\overline{A}\) is defined in the same way as \(\overline{B}\) but using blocks \(\overline{A}(j, k; j', k')\) instead of \(\overline{B}(j, k; j', k')\).) Note that the only difference between the elements of \(A\) and \(B\) is that some of the entries have different signs. It is convenient to think of the sign assignment graphically as depicted in Figure 9. Each bond between sites of the counting lattice now not only carries a weight \((z_1, z_2, 1 \text{ or } 0)\) but also a direction. The sign of the elements of the matrix blocks \(\overline{A}(j, k; j', k')\) now corresponds to this direction. For example, the sign is positive if the connecting bond is in the forward direction, as indicated by the arrows in Figure 10. Thus, one can show (McCoy and Wu (1973), pp. 81, 51-58) that

\[ g(z_1, z_2) = \sum_p' \delta_p \pi_{p1} \pi_{p2} \pi_{p3} \pi_{p4} \cdots \pi_{p5} \pi_{p6} = \text{Pf} \overline{A} = (\det(\overline{A}))^{1/2}, \tag{3.22} \]

where the sum is as in (3.12), \(\delta_p\) is the parity factor and \(\text{Pf} \overline{A}\) is the Pfaffian in Definition 3.1. The sign at the square root in (3.22) is positive since \(g(z_1, z_2)\) is defined in (3.9) with even exponents.

Let \(c_R, c_L, c_U, c_D, c_1, c_2\) denote the columns of any \(6 \times 6\) block \(\overline{A}(j, k; j', k')\), and let us perform the following operations:

\[ c_R - c_1, c_U + c_1, c_L + c_2, c_D - c_2. \]

After these operations, the block \(\overline{A}(j, k; j, k)\) becomes

\[ R \begin{pmatrix} R & L & U & D & 1 & 2 \\ R & 0 & 1 & -1 & -1 & 0 \\ L & -1 & 0 & 1 & -1 & 1 \\ U & 1 & -1 & 0 & 1 & 0 \\ D & 1 & 1 & -1 & 0 & -1 \\ 1 & 0 & 0 & 0 & 0 & 1 \\ 2 & 0 & 0 & 0 & 0 & -1 \end{pmatrix} \tag{3.23} \]

and the other blocks \(\overline{A}(j, k; j', k')\) remain the same. Note that the last two rows of the block (3.23) are zero except the \(2 \times 2\) submatrix

\[ \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{3.24} \]

in the bottom-right corner. Since the determinant of the submatrix (3.24) equals 1, the rows and columns of the matrix \(\overline{A}\) corresponding to the submatrix can be eliminated without affecting the determinant of \(\overline{A}\). We thus have

\[ \det(\overline{A}) = \det(A), \tag{3.25} \]
Figure 9: The counting lattice with directions between sites.

where

$$A(j, k; j', k') =\begin{pmatrix} R & L & U & D \\ 0 & 1 & -1 & -1 \\ -1 & 0 & 1 & -1 \\ 1 & -1 & 0 & 1 \\ 1 & 1 & -1 & 0 \end{pmatrix}$$  \hspace{1cm} (3.26)$$

and all other $A(j, k; j', k')$ are identical to $A(j, k; j', k')$ with the rows and columns labeled 1 and 2 removed. Thus, we also have

$$g(z_1, z_2) = (\det(A))^{1/2},$$  \hspace{1cm} (3.27)$$

where $A$ is now a $2K \times 2K$ matrix with

$$2K = 4(2L_v)(2L_h).$$

Combining (3.3), (3.8) and (3.27), we obtain that

$$Z_{L_v,L_h} = (\cosh \beta E_h)^{2L_v(2L_h-1)}(\cosh \beta E_v)^{2L_v(2L_v-1)}2L_v2L_h(\det(A))^{1/2},$$  \hspace{1cm} (3.28)$$

where $z_1, z_2$ in $A$ are replaced by $z_h$ and $z_v$.

The right-hand side of (3.28) provides an expression for the denominator (partition function) of (3.1). One can derive similarly an expression for the numerator of (3.1). Proceeding as in (3.2) and (3.3), we have

$$\sum_{\{\sigma_{j,k}\}} \sigma_{0,0} \sigma_{0,N} e^{-\beta E} = (\cosh \beta E_h)^{2L_v(2L_h-1)}(\cosh \beta E_v)^{2L_v(2L_v-1)}2L_h \times$$
Figure 10: Directions in the six-site cluster of the counting lattice.

\[
\times \sum_{\{\sigma_{j,k}\}} \sigma_{0,0} \sigma_{0,N} \prod_{j=-L_v+1}^{L_v} \prod_{k=-L_h+1}^{L_h} (1+\sigma_{j,k} \sigma_{j,k+1} z_h) \prod_{j=-L_v+1}^{L_v} \prod_{k=-L_h+1}^{L_h} (1+\sigma_{j,k} \sigma_{j+1,k} \bar{z}_0). \tag{3.29}
\]

Since \(\sigma_{i,j}^2 = 1\), we can write

\[
\sigma_{0,0} \sigma_{0,N} = (\sigma_{0,0} \sigma_{0,1}) (\sigma_{0,1} \sigma_{0,2}) \ldots (\sigma_{0,N-1} \sigma_{0,N})
\]

and

\[
\sigma_{0,k} \sigma_{0,k+1} (1 + \sigma_{0,k} \sigma_{0,k+1} z_h) = z_h (1 + \sigma_{0,k} \sigma_{0,k+1} \bar{z}_h^{-1}),
\]

so that

\[
\sigma_{0,0} \sigma_{0,N} \prod_{k=0}^{N-1} (1 + \sigma_{0,k} \sigma_{0,k+1} z_h) = z_h^N \prod_{k=0}^{N-1} (1 + \sigma_{0,k} \sigma_{0,k+1} \bar{z}_h^{-1}).
\]

Then the relation (3.29) can be expressed as

\[
\sum_{\{\sigma_{j,k}\}} \sigma_{0,0} \sigma_{0,N} e^{-\beta \mathcal{E}} = (\cosh \beta E_h)^{2L_v(2L_h-1)} (\cosh \beta E_v)^{2L_v(2L_h-1)} z_h^N \prod_{k=0}^{N-1} (1 + \sigma_{0,k} \sigma_{0,k+1} \bar{z}_h^{-1}) \times
\]

\[
\times \prod_{j=-L_v+1}^{L_v} \prod_{k=-L_h+1}^{L_h} \left(1 + \sigma_{j,k} \sigma_{j,k+1} z_h \right) \prod_{j=-L_v+1}^{L_v} \prod_{k=-L_h+1}^{L_h} \left(1 + \sigma_{j,k} \sigma_{j+1,k} \bar{z}_0 \right), \tag{3.30}
\]

where \(\prod_{k=-L_h+1}^{L_h} \) means that the terms with \( j = 0, k = 0, \ldots, N-1 \), are omitted. The last expression is similar to (3.3) and (3.4) except for the factor \(z_h^N\) and for the fact that the weights \(z_h\) of the bonds on the horizontal line connecting \((0,0)\) and \((0,N)\) are now replaced by \(z_h^{-1}\). This is also reflected in the fact that the term \(\prod_{k=0}^{N-1} (1 + \sigma_{0,k} \sigma_{0,k+1} \bar{z}_h^{-1})\) now replaces the corresponding term \(\prod_{k=0}^{N-1} (1 + \sigma_{0,k} \sigma_{0,k+1} z_h)\) in (3.4). One can then argue in the same way as for \(Z_{L_v,L_h}\). Since \(Z_{L_v,L_h}\) is expressible as (3.28), by combining the expressions for the numerator and denominator of (3.1), we obtain that

\[
E \sigma_{0,0} \sigma_{0,N} = \frac{1}{Z_{L_v,L_h}} \sum_{\{\sigma_{j,k}\}} \sigma_{0,0} \sigma_{0,N} e^{-\beta \mathcal{E}} = z_h^N \left(\frac{\det(A')}{\det(A)}\right)^{1/2}, \tag{3.31}
\]

where

\[
A' = A + \delta
\]
or equivalently \( \delta = A' - A \) with

\[
\delta(0, k; 0, k + 1) = -\delta(0, k + 1; 0, k)^T = \begin{pmatrix} R & L & U & D \\ 0 & z_h^{-1} - z_h & 0 & 0 \\ L & 0 & 0 & 0 \\ U & 0 & 0 & 0 \\ D & 0 & 0 & 0 \end{pmatrix}
\] (3.32)

if \( 0 \leq k \leq N - 1 \) and zero otherwise. Observe that the presence of \( \delta \) affects only the “horizontal” edges \((0, k) \rightarrow (0, k + 1)\) and \((0, k + 1) \rightarrow (0, k)\) of the Ising lattice.

The matrix \( \delta \), which has dimensions \( 2K \times 2K \) with \( 2K = 4(2L_v)(2L_h) \), is zero everywhere except on its \( 2N \) columns and \( 2N \) rows. Let \( y \) be that \( 2N \times 2N \) submatrix of \( \delta \) where it does not vanish. We have from (3.32) that

\[
y = \begin{pmatrix} y_{RR} & y_{RL} \\ y_{LR} & y_{LL} \end{pmatrix},
\]

where

\[
y_{RR} = \begin{pmatrix} 00 & 01 & \ldots & 0N-1 \\ 00 & R & R & \ldots & R \\ 01 & R & 0 & 0 & \ldots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0N-1 & R & 0 & 0 & \ldots & 0 \end{pmatrix},
\]

\[
y_{LR} = \begin{pmatrix} 01 & 02 & \ldots & 0N \\ 01 & L & 0 & \ldots & 0 \\ 02 & L & -(z_h^{-1} - z_h) & \ldots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0N & L & 0 & 0 & \ldots & -(z_h^{-1} - z_h) \end{pmatrix},
\]

\[
y_{RL} = \begin{pmatrix} 00 & 01 & \ldots & 0N \\ 00 & R & 0 & z_h^{-1} - z_h & \ldots & 0 \\ 01 & R & 0 & z_h^{-1} - z_h & \ldots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0N-1 & R & 0 & 0 & \ldots & z_h^{-1} - z_h \end{pmatrix},
\]

\[
y_{LL} = \begin{pmatrix} 01 & 02 & \ldots & 0N \\ 01 & L & 0 & 0 & \ldots & 0 \\ 02 & L & 0 & 0 & \ldots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0N & L & 0 & 0 & \ldots & 0 \end{pmatrix}.
\]

In the expressions above, following \( \delta \) in (3.32), \( 00, 01, \ldots, 0N-1, 01, \ldots, 0N \) refer to the Ising lattice sites with non-zero weights, and \( R, L \) refer to the site in the cluster of the counting lattice.

Let also \( Q \) be the \( 2N \times 2N \) submatrix of \( A^{-1} \) in this same subspace as \( y \). Then, in view of (3.31),

\[
(\mathbb{E}_{\sigma_0,0}\sigma_{0,N})^2 = z_h^{2N} \frac{\det(A + \delta)}{\det(A)} = z_h^{2N} \det(A^{-1}) \det(A + \delta)
\]
\[ \det(I + A^{-1} \delta) = \det(I + Qy) = \det(y^{-1} + Q) = \det(y^{-1} + Q) \]

so that

\[ (E \sigma_{0,0} \sigma_{0,N})^2 = \det(1 - z_h^2)(y^{-1} + Q). \] (3.35)

### 4 Computation of the inverse

To evaluate \( \det(y^{-1} + Q) \) in (3.35), we need an expression for the inverse \( A^{-1} \) of \( A \) and, more specifically, for the elements of the \( 2N \times 2N \) submatrix \( Q \) of \( A^{-1} \) in the same subspace as \( y \).

Then, we have

\[ Q = \begin{pmatrix} Q_{RR} & Q_{RL} \\ Q_{LR} & Q_{LL} \end{pmatrix}, \] (4.1)

where

\[
Q_{RR} = \begin{pmatrix} 0 & \ldots & A^{-1}(0,0;0,0,N-1)_{RR} \\ A^{-1}(0,1,0;0,0)_{RR} & \ldots & A^{-1}(0,1,0;0,N-1)_{RR} \\ \vdots & \ddots & \vdots \\ A^{-1}(0,N-1;0,0)_{RR} & \ldots & 0 \end{pmatrix},
\]

\[
Q_{LR} = \begin{pmatrix} A^{-1}(0,1,0;0,0)_{LR} & \ldots & A^{-1}(0,1,0;0,N-1)_{LR} \\ A^{-1}(0,2,0;0,0)_{LR} & \ldots & A^{-1}(0,2,0;0,N-1)_{LR} \\ \vdots & \ddots & \vdots \\ A^{-1}(0,N;0,0)_{LR} & \ldots & A^{-1}(0,N;0,0,N-1)_{LR} \end{pmatrix},
\]

\[
Q_{RL} = \begin{pmatrix} A^{-1}(0,0,0;0,0,1)_{RL} & \ldots & A^{-1}(0,0,0;0,N)_{RL} \\ A^{-1}(0,1,0;0,0,1)_{RL} & \ldots & A^{-1}(0,1,0;0,N)_{RL} \\ \vdots & \ddots & \vdots \\ A^{-1}(0,N-1;0,0,1)_{RL} & \ldots & A^{-1}(0,N-1;0,N)_{RL} \end{pmatrix},
\]

\[
Q_{LL} = \begin{pmatrix} 0 & \ldots & A^{-1}(0,1,0;0,N)_{LL} \\ A^{-1}(0,2,0;0,0,1)_{LL} & \ldots & A^{-1}(0,2,0;0,N)_{LL} \\ \vdots & \ddots & \vdots \\ A^{-1}(0,N;0,1)_{LL} & \ldots & 0 \end{pmatrix},
\]

and where zeroes are on the diagonal since \( A^{-1} \) and hence \( Q \) is antisymmetric. The entries \( A^{-1}(\cdot,\cdot,\cdot)_{\cdot,\cdot,\cdot} \) are place holders for the corresponding entries of the matrix \( A^{-1} \) and will need to be evaluated.

Recall that the matrix \( A \) is made up of blocks \( A(j,k;j',k') \) given by (3.26) if \( j' = j, k' = k \), and otherwise, by (3.20) and (3.21) with the rows and columns labeled 1 and 2 removed. For practical purpose, it is convenient to replace \( A \) by the following matrix \( \bar{A} \) which, as indicated below, has a cyclic structure,

\[
\bar{A} = I_{2L_v} \otimes I_{2L_h} \otimes \begin{pmatrix} 0 & 1 & -1 & -1 \\ -1 & 0 & 1 & -1 \\ 1 & -1 & 0 & 1 \\ 1 & 1 & -1 & 0 \end{pmatrix}
\]
\[ +I_{2L_v} \otimes \tilde{H}_{2L_h} \otimes \begin{pmatrix} 0 & z_h & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} + I_{2L_v} \otimes \tilde{H}_{2L_h}^T \otimes \begin{pmatrix} 0 & 0 & 0 & 0 \\ -z_h & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \]

\[ +\tilde{H}_{2L_v} \otimes I_{2L_h} \otimes \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & z_v \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} + \tilde{H}_{2L_v}^T \otimes I_{2L_h} \otimes \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -z_v \\ 0 & 0 & 0 & 0 \end{pmatrix} \], \quad (4.2)

where \( \otimes \) indicates the Kronecker product and where

\[
\tilde{H}_n = \begin{pmatrix} 0 & 1 & 0 & \ldots & 0 \\ 0 & 0 & 1 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \ldots & 1 \\ -1 & 0 & 0 & \ldots & 0 \end{pmatrix}
\]

is an \( n \times n \) matrix with a near-cyclic structure and corresponding eigenvalues \( e^{i\theta} \), \( \theta = \pi(2\ell - 1)/n \), \( \ell = 1, \ldots, n \) (McCoy and Wu (1973), p. 84). The matrix \( \tilde{A} \) differs from \( A \) only at the rows and columns corresponding to the boundary positions \((j, k)\), that is, when \( j = -L_h + 1, L_h \) or \( k = -L_v + 1, L_v \). Indeed, a row and a column of \( A \) associated with a position \((j, k)\) away from the boundary contain 5 non-zero blocks \( A(j; k, j, k), A(j, k; j, k), A(j, k; j, k + 1), A(j, k + 1; j, k) \) and \( A(j + 1, k; j, k) \). These blocks are captured by the respective 5 terms in the sum (4.2).

We will consider below the so-called thermodynamic limit of \( L_h, L_v \to \infty \). Since the difference between \( A \) and \( \tilde{A} \) is only at the columns and rows corresponding to the \((j, k)\) which are at boundary positions, in the thermodynamic limit, the elements of \( A^{-1} \) away from these columns and rows will be those of \( \tilde{A}^{-1} \). Since the elements in (4.1) are away from the boundary, we will thus suppose without loss of generality that \( A \) is actually given by (4.2).

The advantage of working with \( A \) given by (4.2) is that it now has a cyclic structure which makes it easier to compute its inverse. One can show (McCoy and Wu (1973), pp. 183, 148-150) that the entries of its inverse are

\[
A^{-1}(j, k; j', k') = \frac{1}{2L_h} \sum_{\theta} e^{i\theta(k-k')} (B^{-1}(\theta))_{j,j'}, \quad (4.3)
\]

where the sum is over \( \theta = \pi(2\ell - 1)/2L_h, \ell = 1, \ldots, 2L_h \), and where the \( 4(2L_v) \times 4(2L_v) \) matrix \( B(\theta) \) is given by

\[
B_{j,j}(\theta) = \begin{pmatrix} R & L & U & D \\ 0 & -1 + z_h e^{i\theta} & 1 & -1 \\ -1 - z_h e^{-i\theta} & 0 & 1 & -1 \\ 1 & 0 & -1 & -1 \end{pmatrix}, \quad (4.4)
\]

for \(-L_v + 1 \leq j \leq L_v\),

\[
B_{j,j+1}(\theta) = -B_{j+1,j}(\theta)^T = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & z_v & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad (4.5)
\]
for \(-L_v + 1 \leq j \leq L_v\), and all other matrix elements are zero. A matrix \((B^{-1}(\theta))_{j,j'}\) in (4.3) has dimension \(4 \times 4\). Labeling its rows and columns by \(R, L, U\) and \(D\) as in (4.4), denote its elements as \((B^{-1}(\theta))_{j,j''}\) with the labels \(l, l' = R, L, D, U\). One can further show (McCoy and Wu (1973), p. 185, formulas (2.26)) that, as \(L_v \rightarrow \infty\) (thermodynamic limit),

\[
(B^{-1}(\theta))_{jR,j'R} = -(B^{-1}(\theta))_{jL,j'L} = \begin{cases} -\alpha^{-j'\prime-j}(1-z_h^2)^{-1}, & \text{if } j \neq j' \prime, \\ 0, & \text{if } j = j' \prime, \end{cases}
\]  

(4.6)

and that

\[
(B^{-1}(\theta))_{jR,j'\prime L} = -(B^{-1}(\theta))_{jL,j'\prime R} = \frac{z_h(1-z^2_h)}{1+z_v} \frac{1}{1+z_v} e^{i\theta} \left( \frac{1-\alpha_1 e^{i\theta}}{1-\alpha_1 e^{-i\theta}} \right)^{1/2},
\]

(4.7)

where * stands for the Hermitian transpose, \(\delta_{j,j'}\) is here the Kronecker delta (1 if \(j = j'\), 0 if \(j \neq j'\)),

\[
\alpha_1 = \frac{z_h(1-z_v)}{1+z_v}, \quad \alpha_2 = \frac{z^2_h(1-z_v)}{1+z_v},
\]

(4.8)

(See formula (3.16) on p. 121, and formula (3.3) on p. 87 in McCoy and Wu (1973) for a definition of \(\alpha\).) The square root in (4.7) is such that it is positive at \(\theta = \pi\).

When \(j = j' = 0\), these formulas (4.6) and (4.7) simplify to

\[
(B^{-1}(\theta))_{0R,0R} = -(B^{-1}(\theta))_{0L,0L} = -(1-z^2_h)^{-1}
\]

(4.9)

and

\[
(B^{-1}(\theta))_{0R,0L} = -(B^{-1}(\theta))_{0L,0R} = \frac{1}{1-z^2_h} \left( \frac{z_h e^{i\theta} - e^{i\theta} \left( \frac{1-\alpha_1 e^{i\theta}}{1-\alpha_1 e^{-i\theta}} \right)^{1/2}}{(1-\alpha_1 e^{i\theta})(1-\alpha_2 e^{i\theta})} \right).
\]

(4.10)

Letting \(L_v \rightarrow \infty\), \(L_h \rightarrow \infty\) (thermodynamic limit) in (4.3), we get the \(4 \times 4\) matrices

\[
\lim_{L_h \rightarrow \infty} \lim_{L_v \rightarrow \infty} A^{-1}(0,k;0,k') = \frac{1}{2\pi} \int_0^{2\pi} e^{i\theta(k-k')} (B^{-1}(\theta))_{0,0} d\theta.
\]

(4.11)

For example, each matrix has \(R, L\) entries

\[
\lim_{L_h \rightarrow \infty} \lim_{L_v \rightarrow \infty} A^{-1}(0,k;0,k')_{RL} = \frac{1}{2\pi} \int_0^{2\pi} e^{i\theta(k-k')} (B^{-1}(\theta))_{0R,0L} d\theta.
\]

Substituting (4.9)–(4.10) into (4.11), we obtain for the entries of the \(2N \times 2N\) matrix \(Q\) in (4.1) that

\[
\lim_{L_h \rightarrow \infty} \lim_{L_v \rightarrow \infty} A^{-1}(0,k;0,k')_{RR} = \lim_{L_h \rightarrow \infty} \lim_{L_v \rightarrow \infty} A^{-1}(0,k;0,k')_{LL} = 0
\]

(4.12)

and

\[
\lim_{L_h \rightarrow \infty} \lim_{L_v \rightarrow \infty} A^{-1}(0,k;0,k')_{RL} = z_h (1-z^2_h)^{-1} \delta_{k-k'+1,0} \frac{1}{2\pi} \int_0^{2\pi} e^{i(k-k'+1)\theta} \left( \frac{1-\alpha_1 e^{i\theta}}{1-\alpha_1 e^{-i\theta}} \right)^{1/2} d\theta.
\]
and using \( N \) we now want to substitute (4.12), (4.13) and (4.16) into the expression (3.35). Observe from \( \lim_{\theta \to \infty} \int_{L} e^{i \theta (k - k') + 2} d\theta = 2\pi \delta_{k - k', 0} = 2\pi \delta_{k' - k, 0} \). One gets similarly

\[
\lim_{L_h \to \infty} \lim_{L_v \to \infty} A^{-1}(0, k; 0, k')_{LR} = -z_h (1 - z_h^{-2})^{-1} \delta_{k - k', 0}
\]

\[
(1 - z_h^{-2})^{-1} (2\pi)^{-1} \int_{0}^{2\pi} e^{i (k - k') \theta} \left( \frac{(1 - \alpha_1 e^{-i \theta})(1 - \alpha_2 e^{i \theta})}{(1 - \alpha_1 e^{i \theta})(1 - \alpha_2 e^{-i \theta})} \right)^{1/2} d\theta
\]

\[
= \frac{1}{1 - z_h^{-2}} (-z_h \delta_{k - k', 0} + a_{k' - k}).
\]

We now want to substitute (4.12), (4.13) and (4.16) into the expression (3.35). Observe from (4.1) and (4.12)–(4.16) that the \( 2N \times 2N \) matrix \( Q \) becomes, in the thermodynamic limit,

\[
\lim_{L_h \to \infty} \lim_{L_v \to \infty} Q = \begin{pmatrix}
0 & 0 & \ldots & 0 & \frac{z_h - a_0}{1 - z_h} & \frac{-a_1}{1 - z_h^2} & \ldots & \frac{-a_{N - 1}}{1 - z_h^2} \\
0 & 0 & \ldots & 0 & \frac{-a_1}{1 - z_h^2} & \frac{a_1}{1 - z_h} & \ldots & \frac{-a_{N - 2}}{1 - z_h} \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
\frac{-a_0}{1 - z_h} & \frac{a_0}{1 - z_h^2} & \ldots & \frac{a_{N - 1}}{1 - z_h} & 0 & 0 & \ldots & 0 \\
\frac{-a_0}{1 - z_h^2} & \frac{a_0}{1 - z_h} & \ldots & \frac{a_{N - 2}}{1 - z_h} & 0 & 0 & \ldots & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
\frac{-a_{N - 1}}{1 - z_h} & \frac{-a_{N - 2}}{1 - z_h^2} & \ldots & \frac{-a_0}{1 - z_h^2} & 0 & 0 & \ldots & 0
\end{pmatrix}
\]

Note from (3.33) that

\[
y^{-1} = \begin{pmatrix}
0 & 0 & \ldots & 0 & \frac{-z_h}{1 - z_h} & 0 & \ldots & 0 \\
0 & 0 & \ldots & 0 & \frac{-z_h}{1 - z_h^2} & 0 & \ldots & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & \ldots & 0 & 0 & 0 & \ldots & \frac{-z_h}{1 - z_h^2} \\
\frac{z_h}{1 - z_h} & 0 & \ldots & 0 & 0 & 0 & \ldots & 0 \\
\frac{z_h}{1 - z_h^2} & 0 & \ldots & 0 & 0 & 0 & \ldots & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & \ldots & \frac{z_h}{1 - z_h^2} & 0 & 0 & \ldots & 0
\end{pmatrix}
\]
Then,

\[(1 - z_h^2)(y^{-1} + Q) = \begin{pmatrix}
0 & 0 & \ldots & 0 & -a_0 & -a_1 & \ldots & -a_{N-1} \\
0 & 0 & \ldots & 0 & -a_1 & -a_0 & \ldots & -a_{N-2} \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & \ldots & 0 & -a_N & -a_{N-1} & \ldots & -a_0 \\
a_0 & a_1 & \ldots & a_N & 0 & 0 & \ldots & 0 \\
a_1 & a_0 & \ldots & a_N & 0 & 0 & \ldots & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
a_{N-1} & a_{N-2} & \ldots & a_1 & 0 & 0 & \ldots & 0
\end{pmatrix},
\]

or

\[(1 - z_h^2)(y^{-1} + Q) = \begin{pmatrix}
0 & -B^T \\
B & 0
\end{pmatrix},
\]

where \(B = (a_{j-k})_{1 \leq j,k \leq N}\) and 0 is a \(N \times N\) zero matrix. By using the formula \(\det((A B; C D)) = \det(AD - CB)\) if \(AB = BA\) for \(N \times N\) blocks \(A, B, C\) and \(D\), we deduce that

\[\det((1 - z_h^2)(y^{-1} + Q)) = (\det(B))^2.\]

Using the expression (3.35) for \((E\sigma_{00}\sigma_{0N})^2\), this leads to the following expression which now involves the determinant of an \(N \times N\) matrix:

\[S_N := \lim_{L_h \to \infty} \lim_{L_v \to \infty} E\sigma_{00}\sigma_{0N} = \det \begin{pmatrix}
a_0 & a_1 & a_2 & \ldots & a_{N+1} \\
a_1 & a_0 & a_1 & \ldots & a_{N+2} \\
a_2 & a_1 & a_0 & \ldots & a_{N+3} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
a_{N+1} & a_{N+2} & a_{N+3} & \ldots & a_1
\end{pmatrix}. \tag{4.17}\]

One can similarly show (McCoy and Wu (1973), p. 199, formula (3.31)) that

\[\bar{S}_N := \lim_{L_h \to \infty} \lim_{L_v \to \infty} E\sigma_{00}\sigma_{N0} = \det \begin{pmatrix}
\tilde{a}_0 & \tilde{a}_1 & \tilde{a}_2 & \ldots & \tilde{a}_{N+1} \\
\tilde{a}_1 & \tilde{a}_0 & \tilde{a}_1 & \ldots & \tilde{a}_{N+2} \\
\tilde{a}_2 & \tilde{a}_1 & \tilde{a}_0 & \ldots & \tilde{a}_{N+3} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
\tilde{a}_{N+1} & \tilde{a}_{N+2} & \tilde{a}_{N+3} & \ldots & \tilde{a}_0
\end{pmatrix}, \tag{4.18}\]

where \(\tilde{a}_n\) is defined as \(a_n\) in (4.14) but using \(\tilde{\varphi}\) instead of \(\varphi\), defined by

\[\tilde{\varphi}(\theta) = \left(\frac{\sinh 2\beta E_h \sinh 2\beta E_v - e^{-i\theta}}{\sinh 2\beta E_h \sinh 2\beta E_v - e^{i\theta}}\right)^{1/2}. \tag{4.19}\]

5 The strong Szegö limit theorem

We are now interested in the behavior of the determinants \(S_N\) and \(\bar{S}_N\) in (4.17) and (4.18), resp., as \(N \to \infty\) at the critical temperature \(T = T_c\), which is such that

\[1 = \sinh 2\beta E_h \sinh 2\beta E_v, \quad \beta = 1/T_c. \tag{5.1}\]

The determinants \(S_N\) and \(\bar{S}_N\) are defined in terms of functions \(\varphi(\theta)\) and \(\tilde{\varphi}(\theta)\) in (4.15) and (4.19). We will need expressions of these functions at the critical temperature.
Lemma 5.1  At the critical temperature $T_c$, $\phi(\theta)$ in (4.15) becomes

$$\phi(\theta) = \left( \frac{1 - \alpha_1 e^{i\theta}}{1 - \alpha_1 e^{-i\theta}} \right)^{1/2} e^{i(-1/2)(\theta - \pi)},$$

and $\tilde{\phi}(\theta)$ in (4.19) becomes

$$\tilde{\phi}(\theta) = e^{i(-1/2)(\theta - \pi)}.$$

Proof: Consider first $\tilde{\phi}(\theta)$ in (4.19), which becomes by (5.1),

$$\tilde{\phi}(\theta) = \left( \frac{1 - e^{-i\theta}}{1 - e^{i\theta}} \right)^{1/2} = \left( -e^{-i\theta} \right)^{1/2} = ie^{-i\theta/2} = e^{i(-1/2)(\theta - \pi)}.$$

Turning to the function $\phi(\theta)$ in (4.15), recall that the parameters $\alpha_1$ and $\alpha_2$ were defined in (4.8), and $z_h$ and $z_v$ in (3.5). We first show that if (5.1) holds, then $\alpha_2 = 1$. To do so, use the relations $\cosh^2 x - \sinh^2 x = 1$ and $2(\sinh x)(\cosh x) = \sinh 2x$. Then, by using $(1 - z_h^2)/(2z_h) = (\sinh 2\beta_E h)^{-1}$ for $k = h, v$, the relation (5.1) can be expressed as $(1 - z_h^2)(1 - z_v^2) = 4z_hz_v$. This is the same as $(1 - z_hz_v)^2 = (z_h + z_v)^2$ or $1 - z_hz_v = z_h + z_v$. The latter yields $1 = z_h^{-1}(1 - z_v)/(1 + z_v) = \alpha_2$. This now implies that

$$\alpha_1 = z_h^2 \alpha_2 = z_h^2 < 1.$$

Hence, by (5.4), $\phi(\theta)$ in (4.15) becomes (5.2). $\Box$

To obtain the asymptotic behavior of the determinants $S_N$ and $\tilde{S}_N$ as $N \to \infty$, we will apply the so-called “strong Szegő limit theorem”. This theorem concerns the limiting behavior, as $N \to \infty$, of the $N \times N$ Toeplitz determinant

$$D_N = \det \begin{pmatrix}
    c_0 & c_{-1} & \cdots & c_{-N+1} \\
    c_1 & c_0 & \cdots & c_{-N+2} \\
    \vdots & \vdots & \ddots & \vdots \\
    c_{N-1} & c_{N-2} & \cdots & c_0
\end{pmatrix},$$

where the entries $c_n$ are the Fourier coefficients of a function $C$ on the unit circle, that is,

$$c_n = \frac{1}{2\pi} \int_0^{2\pi} d\theta \ e^{-in\theta} C(e^{i\theta}).$$

Thus, $C(e^{i\theta}) = \sum_{n=\infty}^{\infty} c_n e^{-in\theta}$ is the discrete Fourier transform of the sequence $\{c_n\}$. In the case of interest here, $C(e^{i\theta})$ is chosen to be either $\phi(\theta)$ or $\tilde{\phi}(\theta)$.

The classical strong Szegő limit theorem supposes that $C(e^{i\theta})$ is “smooth” and allows one to conclude that

$$D_N \sim E(C)\mu^N,$$

as $N \to \infty$, where $\mu$ and $E(C)$ are two constants given by

$$\mu = \frac{1}{2\pi} \int_0^{2\pi} d\theta \ \ln C(e^{i\theta}), \quad E(C) = \exp \left\{ \sum_{n=1}^{\infty} n(\ln C)^n(\ln C)_{-n} \right\},$$

and $(\ln C)^n$ denotes the $n$th Fourier coefficient of the function $\ln C(e^{i\theta})$. See Szegő (1952). A typical assumption for (5.7) to hold is that $C(\xi)$ be continuous on the unit circle $|\xi| = 1$. Note that this is not the case with the functions $\tilde{\phi}(\theta)$ and $\phi(\theta)$ in (5.3) and (5.2). For example, note
that \( \tilde{\phi}(0) = ie^{-i\theta} = i \) and \( \tilde{\phi}(2\pi) = ie^{-i\pi} = -i \). In the case when \( C(\xi) \) is not continuous, the function \( C(e^{i\theta}) \) and the determinant \( D_N \) are said to have a singularity.

Though conjectured in the past by Fisher and Hartwig (1968), the asymptotic behavior of determinants with singularities has been established only recently in Bootcher and Silbermann (1985), Ehrhardt and Silbermann (1997), Deift et al. (2009). We state next a corollary of Theorem 2.5 in Ehrhardt and Silbermann (1997) which will be sufficient for our purposes. Suppose the function \( C(e^{i\theta}) \) can be expressed as

\[
C(e^{i\theta}) = b(e^{i\theta})t_{\beta}(e^{i\theta}),
\]

where

\[
t_{\beta}(e^{i\theta}) = e^{i(\beta(\theta-\pi))}, \quad \beta \in \mathbb{R}.
\]

Note that the function \( t_{\beta}(e^{i\theta}) \) satisfies \( t_{\beta}(e^{i0}) = e^{-i\beta\pi} \), \( t_{\beta}(e^{i2\pi}) = e^{i\beta\pi} \), and hence is a discontinuous function on the unit circle (unless \( \beta \) is an integer). The function \( b(e^{i\theta}) \) will be assumed to be continuous on the unit circle. We will also need the Wiener-Hopf factorization of \( b \), namely,

\[
b(e^{i\theta}) = b_+(e^{i\theta})g(b)b_-(e^{i\theta}),
\]

where the factors are defined as

\[
b_{\pm}(e^{i\theta}) = \exp \left\{ \sum_{n=1}^{\infty} e^{\pm i\theta n}(\ln b)_{\pm n} \right\}, \quad g(b) = \exp((\ln b)_0)
\]

and where \( (\ln b)_n \) denotes the \( n \)th Fourier coefficient of the function \( \ln b \).

**Theorem 5.1** (Strong Szegő limit theorem for determinants with singularity). Suppose that the function \( C(e^{i\theta}) \) can be expressed as (5.8) where \( b(e^{i\theta}) \) is infinitely differentiable on the unit circle. Then, the determinant \( D_N \) in (5.6) satisfies, as \( N \to \infty \),

\[
D_N \sim E g(b)^N N^{-\beta^2},
\]

where \( g(b) \) is defined in (5.9), and

\[
E = E(b)b_+(1)^{\beta}b_-(1)^{-\beta}G(1+\beta)G(1-\beta).
\]

In (5.11), \( b_+(1) \), \( b_-(1) \) are defined in (5.9),

\[
E(b) = \exp \left( \sum_{n=1}^{\infty} n(\ln b)_n(\ln b)_{-n} \right)
\]

and

\[
G(1+z) = (2\pi)^{z/2}e^{-(z+1)z/2-\gamma z^2/2} \prod_{n=1}^{\infty} \left\{ \left( 1 + \frac{z}{n} \right)^n e^{-z^2/2n} \right\}
\]

stands for the so-called Barnes \( G \)-function (\( \gamma \) is the Euler’s constant).

\[
^9\text{The result we use follows the statement of Theorem 2.5 in Ehrhardt and Silbermann (1997).}
\]
6 Long-range dependence at critical temperature

Applying Theorem 5.1 to the determinants \( S_n \) and \( \tilde{S}_N \) in (4.17) and (4.18) with the respective functions \( \phi(\theta) \) and \( \tilde{\phi}(\theta) \) in (4.15) and (4.19) at the critical temperature yields the following result which concludes the proof of Theorem 2.1.

**Theorem 6.1** Let \( S_n \) and \( \tilde{S}_N \) be the determinants in (4.17) and (4.18). At the critical temperature (5.1), as \( N \to \infty \),

\[
S_N = \lim_{L_h \to \infty} \lim_{L_v \to \infty} \mathbb{E} \sigma_{0,0} \sigma_{0,N} \sim \left( \frac{1 + \alpha_1}{1 - \alpha_1} \right)^{1/4} AN^{-1/4},
\]

(6.1)

\[
\tilde{S}_N = \lim_{L_h \to \infty} \lim_{L_v \to \infty} \mathbb{E} \sigma_{0,0} \sigma_{N,N} \sim AN^{-1/4},
\]

(6.2)

where \( \alpha_1 \) is defined in (4.8),

\[ A = G(1/2)G(3/2) = 0.6450024 \ldots \]

and \( G \) is the Barnes \( G \)-function in (5.12).

**Proof:** Consider first the determinant \( S_N \) with the function \( \phi(\theta) \) in (5.2). We will apply Theorem 5.1. Note that \( \phi(\theta) \) can be written as in (5.8),

\[
\phi(\theta) = b(e^{i\theta})t_{\beta}(e^{i\theta}),
\]

where

\[
b(e^{i\theta}) = \left( \frac{1 - \alpha_1 e^{i\theta}}{1 - \alpha_1 e^{-i\theta}} \right)^{1/2}, \quad t_{\beta}(e^{i\theta}) = e^{i\beta(\theta - \pi)}, \quad \beta = -1/2.
\]

(6.3)

The factors (5.9) of \( b \) in its Wiener-Hopf factorization are

\[
b_+(e^{i\theta}) = (1 - \alpha_1 e^{i\theta})^{1/2}, \quad b_-(e^{i\theta}) = \frac{1}{(1 - \alpha_1 e^{-i\theta})^{1/2}}, \quad g(b) = 1.
\]

(6.4)

In particular,

\[
b_+(1) = (1 - \alpha_1)^{1/2}, \quad b_-(1) = 1/(1 - \alpha_1)^{1/2}
\]

and hence \( b_+(1)^{-1/2}b_-(1)^{-1/2} = (1 - \alpha_1)^{-1/2} \). For \( b(e^{i\theta}) \) in (6.3), we have

\[
\ln b(e^{i\theta}) = \frac{1}{2} \ln(1 - \alpha_1 e^{i\theta}) - \frac{1}{2} \ln(1 - \alpha_1 e^{-i\theta}) = -\frac{1}{2} \sum_{k=1}^{\infty} \frac{\alpha_k^1 e^{ik\theta}}{k} + \frac{1}{2} \sum_{k=1}^{\infty} \frac{\alpha_k^1 e^{-ik\theta}}{k}
\]

and hence the Fourier coefficients of the function \( \ln b \) are given by

\[
(ln b)_n = \frac{1}{2\pi} \int_{0}^{2\pi} d\theta e^{-in\theta} \ln b(e^{i\theta}) = \begin{cases} \frac{-\alpha_n^1}{2n}, & \text{if } n > 0, \\ 0, & \text{if } n = 0, \\ \alpha_n^{1|n|}, & \text{if } n < 0, \end{cases}
\]

(6.5)

so that

\[
E(b) = \exp \left( \sum_{n=1}^{\infty} n(ln b)_n(ln b)_{-n} \right) = \exp \left( -\frac{1}{4} \sum_{n=1}^{\infty} \frac{(\alpha_n^1)^n}{n} \right)
\]
\[ \exp \left( \frac{1}{4} \ln(1 - \alpha_1^2) \right) = (1 - \alpha_1^2)^{1/4}. \] (6.6)

In view of (6.6), (5.11) and (6.4), we deduce (6.1). The result (6.2) for the determinant \( \tilde{S}_N \) can be obtained similarly.\( \square \)

**Remark.** The asymptotic behavior (6.2) of \( \tilde{S}_N \) was obtained in McCoy and Wu (1973) directly without using the strong Szegö limit theorem as follows. In view of (5.3), the elements \( \tilde{a}_n \) of \( \tilde{S}_n \) can be evaluated as
\[ \tilde{a}_n = \frac{1}{2\pi} \int_0^{2\pi} d\theta e^{-in\theta} e^{-i\theta/2} = \frac{2}{\pi(2n+1)}. \]

Hence, by (4.18),
\[ \tilde{S}_N = (2\pi^{-1})^N \det \left( \frac{1}{2m-2n+1} \right)_{0 \leq m,n \leq N-1}. \] (6.7)

The latter determinant is the special case of the so-called Cauchy determinant,
\[ \tilde{D}_N = \det \left( \frac{1}{\mu_m + \nu_n} \right)_{0 \leq m,n \leq N-1}, \] (6.8)

where \( \mu_m = 2m+1 \) and \( \nu_n = -2n \). It is known (for example, McCoy and Wu (1973), p. 261) that
\[ \tilde{D}_N = \frac{\prod_{0 \leq m<n \leq N-1} (\mu_m - \mu_n)(\nu_m - \nu_n)}{\prod_{m=0}^{N-1} \prod_{n=0}^{N-1} (\mu_m + \nu_n)}. \] (6.9)

Applying (6.9) to (6.7) allows one to evaluate the determinant \( \tilde{S}_N \) directly, and to deduce the asymptotic behavior (6.2). See McCoy and Wu (1973), pp. 261-264. In particular, one can show that the constant \( A = G(1/2)G(3/2) \) in Theorem 6.1 can also be written as
\[ A = e^{-\gamma/4 + \bar{A} - 1/4} \]
where
\[ \gamma = \lim_{N \to \infty} \left( \sum_{l=1}^{N} l^{-1} - \ln N \right) = 0.5772157 \ldots \]
is the Euler’s constant, and
\[ \bar{A} = \sum_{l=1}^{\infty} l \left( \ln \left( 1 - \frac{1}{4l^2} \right) + \frac{1}{4l^2} \right). \]

The constant \( A \) is numerically about \( A = 0.6450024 \ldots \) as stated in Theorem 6.1.

**Proof of Corollary 2.1:** Suppose \( E_h = E_v = E \) and set \( c = \cosh \beta E, s = \sinh \beta E, c_2 = \cosh 2\beta E \) and \( s_2 = \sinh 2\beta E \). We have
\[ \frac{1 + \alpha_1}{1 - \alpha_1} = \frac{c^2 - s^2 + 2sc}{c^2 + s^2} = \frac{1 + s_2}{\sqrt{1 + s_2^2}}, \]

where the last equality follows from the relations \( c^2 - s^2 = 1, 2cs = s_2 \) and \( c^2 + s^2 = c_2 = \sqrt{1 + s_2^2} \).

But (2.10) yields \( s_2 = 1 \), and therefore
\[ \frac{1 + \alpha_1}{1 - \alpha_1} = \sqrt{2}. \] \( \square \)
7 Conclusion

Benoît Mandelbrot was interested in any phenomenon exhibiting power laws, be it in Mathematics, Physics, Finance, Geology or Hydrology. He passed this interest to his student Murad Taqqu – the second author of this paper, – who in turn passed it to his own student, Vladas Pipiras – the first author.

Power laws often occur at critical junctures, where there is a “phase transition”. This is a typical situation in Physics. We have focused here on the Ising model in two dimensions and shown that at critical temperature, the correlations between the spin at the origin and one at “distance” $N$ decreases like $N^{-1/4}$. New research on the Ising model – as well as on other lattice and growth models – has recently explored their behavior when the edges of the lattice become infinitely small. These scaling limits are generally characterized by conformal invariance, and involve the Schramm-Loewner Evolution (SLE), the Conformal Loop Ensemble (CLE) and related probabilistic objects (see Schramm (2000), Werner (2004), Lawler (2005)). For example, the interface between the +1 and −1 spins in the Ising model at critical temperature has long been conjectured to converge to the SLE model with parameter $\kappa = 16/3$. This is studied rigorously in a series of recent papers by Smirnov (2009, 2010). SLE techniques were used by Lawler et al. (2001) to show that the Hausdorff dimension of the frontier of planar Brownian motion is equal to 4/3. This celebrated result has been conjectured by Mandelbrot (1982).

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References


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