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On Ising models

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Abstract

For various Ising models two approaches are discussed, one is that of simulating lattices, also called gauging on exact equations, the other is that of calculating analytical expressions for the boundary free energy of Ising lattices. The first approach allows to conjecture a solution for some Ising models, that have sofar not been solved, once some exact partial result for the problem is known.
The second approach aims at furnishing such a partial result in the form of a condition for the critical temperature. An example of such a result was recently given for the 2D Ising square lattice with nearest and next-nearest-neighbor interactions. The critical line that separates the ordered (ferromagnetic) phase from the disordered (paramagnetic) phase showed good agreement in the moderate and strong nearest neighbor coupling limit with several results obtained by Monte Carlo, transfer matrix and series expansion results. We extend the discussion of the critical line, finding an excellent fit, now also in other points, like the Padé point, as well as cusp behavior at the Onsager point where the lattice decouples into two 2D square lattices with only nearest-neighbor interaction. Combination of this result with a geometrical argument in the simulation approach leads to a critical exponent $2-\sqrt{2} \approx 0.5858$, comparable to the exponent $4/7 \approx 0.5714$ found from renormalization arguments.

1. Introduction

We would like to refer to the book of Huang [1] for an introduction to Ising problems, although we will not use exactly the same notation. An Ising model consists of spins σ, that can take values -1 of +1. These spins interact according to a lattice structure, which can, in this paper, be the one-dimensional linear chain, Ising's original model without or with next-nearest-neighbor interactions, the two-dimensional square lattice without or with next-nearest-neighbor interactions along diagonals and the three-dimensional cubic lattice. As usual we will assume periodic boundary conditions, so the simplest model is just a cycle. For graph theoretical terminology we refer to Bondy and Murty [2] or any other of the many books on graph theory. The 2D square lattice with diagonals and the cubic lattice are non-planar lattices. It is well-known that in particular non-planar lattices have so far prohibited an exact solution to the corresponding Ising problems. This comes forward very clearly in the approach by Pfaffians, see Green and Hurst [3].

Two spins σ_p and σ_q are assumed to have an interaction energy $-J\sigma_p\sigma_q$, whenever p and q are neighboring vertices on the lattice. For ferromagnetic interaction, $J>0$, the spins σ_p and σ_q will align, as this is the state with the lowest energy. We will distinguish J_x, J_y and J_z for the three possible directions and J_d for the next-nearest-neighbor interaction. k_B and T denote the Boltzmann constant and the absolute temperature and we write H, H_x, H_y, H_z and H_d for respectively J/k_BT, J_x/k_BT, J_y/k_BT, J_z/k_BT and J_d/k_BT. The interaction energy of a spin σ with an external magnetic field M is assumed to be $\mu M\sigma$ and H_μ denotes $\mu M/k_BT$. Including an external magnetic field doubles the number of Ising models we consider.

The Ising problem is to calculate the free energy per element f_N of a lattice of N spins in the limit $N\to\infty$. From $\lim_{N\to\infty} f_N = f$ the relevant thermodynamic quantities can be calculated. The intermediate concept from model to free energy is the partition function, or sum of states,

$$Z_N = \sum_{i=1}^{2^N} e^{-E_i/k_BT} = \sum_{\{\sigma\}} e^{\frac{1}{2}\sum_{p=1}^{N}\sum_{q=1}^{N} H\sigma_p\sigma_q - \sum_{p=1}^{N} H_\mu\sigma_p},$$

where each of the 2^N combinations of spin variables, denoted by {σ} , contributes a term, and σ_p and σ_q only contribute when they are spin variables of neighboring vertices in the lattice.
The free energy per element is given by

$$f_N = -\frac{k_B T}{N}\ln(Z_N) \quad .$$

Van der Waerden [4] introduced, for *M=0*, the "combinatorial" approach in which Z_N is written as the product of $\left(2ch(H_1)...ch(H_p)\right)^N$, where the indices *1* up to *p* correspond to *p* different types of edges on the lattice, and a polynomial $G_N\left(w_1, w_2, ..., w_p\right)$, where $w_i = th(H_i)$, *i=1,2,….,p.* G_N is the generating function for the numbers of multiple cycles on the lattice, so subgraphs of the lattice graph, for which all vertices have even degree. For the simplest lattice, the linear chain, we obtain

$$Z_N = \left(2ch(H)\right)^N\left(1 + w^N\right) \ ,$$

as there are only two subgraphs, the one without edges, all vertices have degree 0, and the cycle of length N, which is the complete cycle lattice itself. So,

$$f_N = -\frac{k_B T}{N}\ln(Z_N) = -\frac{k_B T}{N}\left[N\ln(2ch(H) + \ln\left(1 + w^N\right)\right] = -k_B T\ln\left(2ch(H)\right) - \frac{k_B T}{N}\ln\left(1 + w^N\right)$$

.

Hence

$$f = \lim_{N\to\infty} f_N = -k_B T\ln\left(2ch(H)\right) \quad . \qquad (1)$$

For the 2D square lattice with directions x and y, we have

$$Z_N = \left(2ch(H_x)ch(H_y)\right)^N G_N\left(w_x, w_y\right) \ ,$$

where

$$G_N\left(w_x, w_y\right) = 1 + Nw_x^2 w_y^2 + Nw_x^2 w_y^4 + Nw_x^4 w_y^2 + ... \quad , \qquad (2)$$

as there are N squares, N "horizontal" rectangles of six edges, N "vertical" rectangles of six edges, etc.

Solving the Ising problem for this square lattice was done by Onsager [5] using Lie algebras in the so-called transfer matrix approach, by Kaufman [6] using the theory of spin representations of rotations for the same approach and by Kasteleyn [7] for the combinatorial approach, solving an equivalent problem of counting dimer configurations for the lattice. For an isotropic lattice, $H_x = H_y = H$, they found, see Huang [1],

$$f = -k_B T \ln\left(2ch(2H)\right) - \frac{k_B T}{2\pi}\int_0^{\pi} \ln\left(\frac{1}{2}\left(1+\sqrt{1-\kappa^2 \sin^2\alpha}\right)\right)d\alpha \quad , \tag{3}$$

where

$$\kappa = \frac{e^{2H} - e^{-2H}}{\left(e^{2H} + e^{-2H}\right)^2} \quad .$$

The one-dimensional lattice with external magnetic field is rather simply solved by the transfer matrix method and yields

$$f = -k_B T \ln\left(e^{H} ch(H_\mu) + e^{H}\sqrt{sh^2(H_\mu) + e^{-4H}}\right) . \tag{4}$$

The one-dimensional problem for the lattice with next-nearest-neighbor interactions was solved by Montroll [8] and has the solution

$$f = -J_d - k_B T \ln\left(ch(H) + \sqrt{sh^2(H) + e^{-4H_d}}\right) \quad . \tag{5}$$

For $H_\mu = 0$, respectively $J_d = 0$, both (4) and (5) reduce to (1).

The formulas given are well-known, but are given here for our later discussion. Also for this reason we draw the linear chain with next-nearest neighbors as in Figure 1.

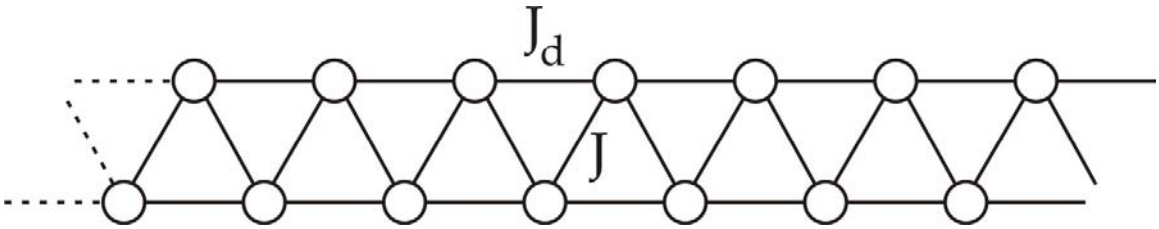

Figure 1
One-dimensional lattice with nearest and next-nearest-neighbor interactions.

We clearly see that this lattice decouples into two linear lattices with interaction strength J_d, in case *J=0*. A similar decoupling into two single square lattices with interaction strength J_d occurs, in case *J=0*, for the isotropic square lattice with next-nearest neighbor interactions. This will be one of our main topics in the coming sections.

2. Simulating lattices. Gauging on equations

The idea of simulating lattices is very simple and can be illustrated by the one-dimensional lattices. The one-dimensional lattice with next-nearest neighbor interaction, with external magnetic field or even with both modifications, can be seen as a simple one-dimensional lattice with an adjusted interaction strength J^*. The solution of such a simulating lattice is just given by (1)

$$f = -k_B T \ln\left(2ch(H^*)\right) \quad , \tag{6}$$

where $H^* = J^* / k_b T$. We only have the problem to find $H^*(H, H_d)$ respectively $H^*(H, H_\mu)$ or even $H^*(H, H_d, H_\mu)$. This idea is somewhat similar to that used in Kadanoff renormalization theory [9], where lattices are turned into smaller lattices by replacing certain subgraph structures by subgraph structures with smaller number of vertices and the problem is to make sure that the coarser lattice has the same properties as the original lattice.
We do ***not*** change the number of vertices, but try to incorporate the presence of next-nearest neighbors or an external magnetic field directly into the interaction strength of the simulating lattice. In the one-dimensional case the simulation by a simple linear chain with modified interaction strength J^* is possible, as we shall see. In the case of the simple square lattice we may expect that simulation, by

that lattice, is possible for the square lattice with next-nearest neighbor interactions, with an external magnetic field, or with both modifications, and even for the simple cubic lattice, that can be seen as a set of linked square lattices.

The problem of finding H^* is based on the idea of gauging on an, preferably exact, equation for the variables of the simulated lattice. By this we mean that if for some problem an equation between the variables is known, valid in some region of values of the variables, the unknown function H^* may be adapted to that equation, so as to assure that the simulating Ising model has the same behavior, for values in that region, as the simulated Ising model.
We will illustrate this idea by means of the one-dimensional models for which we already have the exact solutions. The point is, of course, not to solve these models again, but to illustrate the simulation process.
In the one-dimensional case there are obvious exact equations on which one can gauge. These are the exact solutions themselves. From equating the right hand sides of (1) and (4) we get

$$2ch\left(H^*\right)= e^{H}\left[ch(H_\mu) + \sqrt{sh^2(H_\mu) + e^{-4H}}\right], \qquad (7)$$

as *gauging equation*. From (7) $H^*(H, H_\mu)$ can be solved. Likewise equating the right hand sides of (1) and (5) we get

$$-k_B T \ln\left(2ch(H^*)\right)= -J_d - k_B T \ln\left(ch(H) + \sqrt{sh^2(H) + e^{-4H_d}}\right),$$

as gauging equation for $H^*(H, H_d)$, which can be rewritten as

$$2ch(H^*) = e^{Hd}\left[ch(H) + \sqrt{sh^2(H) + e^{-4Hd}}\right] \quad . \qquad (8)$$

It is remarkable that (7) and (8) have precisely the same structure.
In the two-dimensional case the simple square lattice has Onsager's solution (3) that we will shortly write as *O(H)*. If diagonal edges are added to the lattice we want to simulate the addition of the next-nearest-neighbor interactions by replacing H by H^*, thus getting $O(H^*)$.
Now we do not have the exact solution at all. However, we do have an equation on which we can gauge.

By a calculation of the boundary free energy Zandvliet [10] found;

$$e^{-2J_x/k_BT_c}+e^{-2J_y/k_BT_c}+e^{-2(J_x+J_y)/k_BT_c}\left(2-e^{-4J_d/k_BT_c}\right)=e^{4J_d/k_BT_c}, \tag{9}$$

for the critical point. Similar approaches have been adopted by Müller-Hartmann and Zittartz [11], Burkhardt [12] and Southern [13]. In Figure 2 the phase diagram of the isotropic square lattice Ising model with nearest-neighbor and next-nearest-neighbor interaction is presented. The critical line between the layered antiferromagnetic phase and the paramagnetic phase can be found by the transformation $J_y \to -J_x$ and $J_d \to -J_d$ in Equation (9).

The Onsager equation for the order-disorder transition temperature for the simple square lattice is recovered from (9) by putting $J_d = 0$, which gives,

$$sh\left(\frac{2J_x}{k_BT_c}\right)sh\left(\frac{2J_y}{k_BT_c}\right)=1 \quad .$$

For $J_x = J_y = J$ and $J/k_BT_c = H_c$ this gives

$$sh(2H_c)=1 \quad . \tag{10}$$

When we want to simulate by a simple square Ising lattice we should have

$$sh(2H_c^*)=1\,. \tag{11}$$

For gauging, equation (9) can now be used. For the isotropic lattice we have, from (9),

$$2e^{-2H_c}+e^{-4H_c}\left(2-e^{-4H_{d,c}}\right)=e^{4H_{d,c}},$$

or,

$$2e^{-2H_c-4H_{d,c}}+e^{-4H_c}\left(2e^{-4H_{d,c}}-e^{-8H_{d,c}}\right)=1 \tag{12}$$

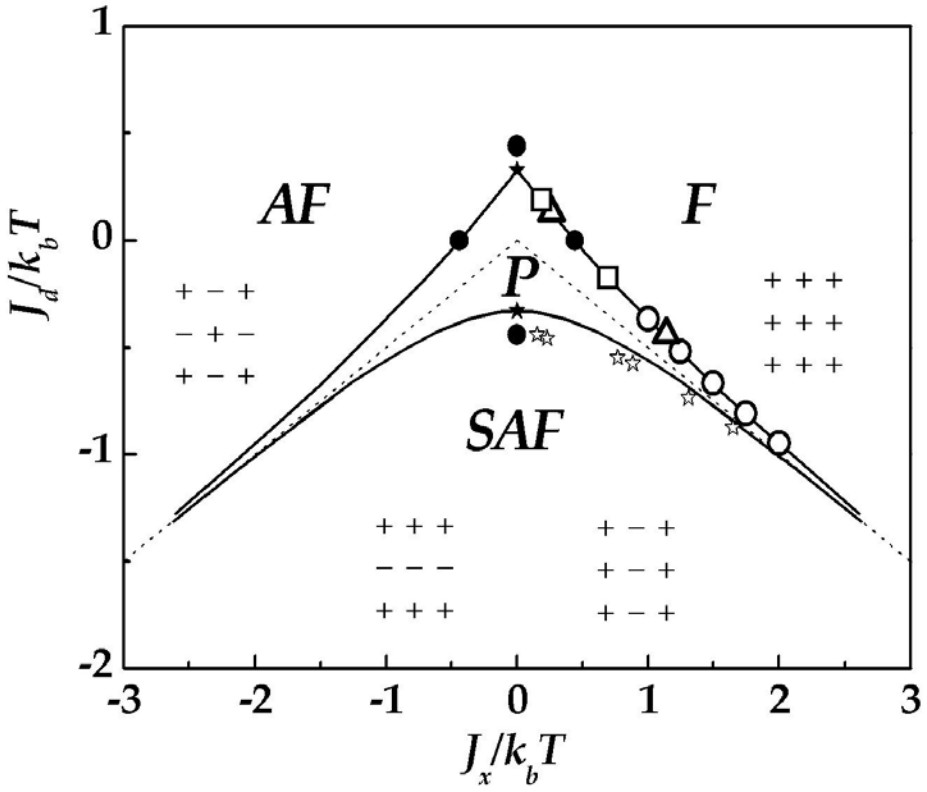

Figure 2

The phase diagram of the isotropic square lattice Ising model with nearest- and next-nearest-neighbor interactions. The solid lines refer to the phase boundaries between the ferromagnetic (*F*), antiferromagnetic (*AF*), superantiferromagnetic (*SAF*) and paramagnetic (*P*) phases as derived in [10]. The data points are series expansions results (triangles, Oitmaa [14]), finite scaling of transfer matrix results (squares, Nightingale [15]), Onsager's exact result (filled circles, Onsager [5]), Monte Carlo simulations (open circles, Blöte, Campagner and Hoogland [16] and open stars, Landau [17]) and free-fermion approximation (closed stars, Fan and Wu [18]). The dotted line gives the asymptotic strong-coupling slope ($J_d = -\frac{1}{2}|J_x|$).

As gauging equation we now find

$$2e^{-2H_c^*}+e^{-4H_c^*}=2e^{-2H_c-4H_{d,c}}+e^{-4H_c}\left(2e^{-4H_{d,c}}-e^{-8H_{d,c}}\right), \tag{13}$$

from which $H_c^*(H_c,H_{d,c})$ can be solved. The left hand-side of Equation (13) is an expression that has the same form as the right hand-side for $H_{d,c}=0$ and, equated to 1, gives an equation that can be transformed into Equation (11).

Equation (9) is in good agreement with results obtained by simulations, especially in the neighborhood of the Onsager point $(H_c,0)$. We may therefore expect that $O(H^*)$, where we replace T_c by T, gives a good approximation to the exact solution of the 2D square lattice with next-nearest-neighbor interactions. From (12) we first check that for $H_{d,c}=0$ we find

$$2e^{-2H_c}+e^{-4H_c}=1\ ,$$

or

$$2+e^{-2H_c}=e^{2H_c}\ ,$$

which is Equation (10). Then we consider the critical line as given by (13) deleting the indices c, to express H_d in terms of H and find, putting $e^{-2H}=a$ and $e^{-4H_d}=b$,

$$2ab+a^2\left(2b-b^2\right)=1\ ,$$

or

$$a^2b^2-2(a+a^2)b+1=0\ .$$

Solving for b we find

$$b = \frac{2(a^2+a)+\sqrt{4(a^2+a)^2-4a^2}}{2a^2},$$

or

$$H_d = -\frac{1}{4}\ln\left[1+e^{2H}+\sqrt{\left(1+2e^{2H}\right)}\right] . \qquad (14)$$

For $\frac{dH_d}{dH}$ we find in the Onsager point $(H_c,0)$ the value $-\frac{1}{2}\sqrt{2}$ for the direction coefficient of the critical line as described by (14). For small H_d the strength of the simulating lattice is given by the particularly simple result $H^* = H + \sqrt{2}H_d$. The curve described by (12) has the strong coupling asymptote $H_d = -\frac{1}{2}H$, see [10]. Both results, i.e. the slope of $-\frac{1}{2}\sqrt{2}$ near the Onsager point $(H_c,0)$ and the slope $-\frac{1}{2}$ for $H \to \infty$, are properties of the exact solution as has already been pointed out by Burkhardt [19].

3. Fitting the critical line

The result (12) did not give satisfactory results for values of *H* close to 0 and did not show a cusp near the Onsager point $(0,H_c)$, where H=0 and the lattice decouples into two simple square lattices. We therefore demanded the following:

1. The curve should go through both Onsager points $(H_c,0)$ and $(0,H_c)$.
2. The slope of the curve in $(H_c,0)$ should be $-\frac{1}{2}\sqrt{2}$.
3. The slope should tend to $-\frac{1}{2}$ for $H \to \infty$.

We found the following formula for a critical line satisfying these demands:

$$H_d = H_c - \frac{1}{2} H \left(1 + \left(\frac{H}{H_c} \right)^{\sqrt{2}-2} \right) \quad . \tag{15}$$

For $H=0$ we find $H_d = H_c$. For $H = H_c$ we find $H_d = 0$. The slope $\left(\frac{dH_d}{dH} \right)_{H=H_c}$ in the Onsager point $(H_c,0)$ is $-\frac{1}{2}\sqrt{2}$. In the strong coupling limit the slope becomes $-\frac{1}{2}$. We have compared this fit with known results [5,14,16,20] and found, to our great surprise, a very good agreement. The results are summarized in Table I.

	Fit results for $H_{d,c}$	Transfer matrix results [16,20], series expansion result [14] and exact results [5]
$H=0$	$\frac{1}{2}\ln\left(\sqrt{2}+1\right)$	$\frac{1}{2}\ln\left(\sqrt{2}+1\right)$ [5]
$H = H_d$	0.1901	0.19019269 [16,20]
$H = 2H_d$	0.1314	0.131404 [14]
$H = \frac{1}{2}\ln\left(\sqrt{2}+1\right)$	0	0 [5]
$H = -4H_d$	-0.1743	-0.174305 [16,20]

Table I
Comparison of critical line formula (15) with known exact and numerical results.

Equation (15) can be transformed into

$$\frac{sh(2H+4H_d)}{sh\left(2H_c\left(2-\left(\frac{H}{H_c}\right)^{\sqrt{2}-1}\right)\right)}=1.$$

The critical line formula is in excellent agreement with the known points of the critical line in the region $0 \le H \le H_c$, where formula (12) still gives deviations. The deviations occur from the fifth digit on. Moreover, the critical line has a cusp at $(0, H_c)$ with exponent $\sqrt{2}-1 \approx 0.4142$. This should be compared with the exponent 4/7≈0.5714 resulting from renormalization theory, see van Leeuwen [21]. We will discuss the exponent further in another section. Formula (15) should be compared with that result from renormalization theory. We therefore consider the formula

$$H_d = H_c - H_c\left(\frac{H}{H_c}\right)^{4/7} \quad , \tag{16}$$

describing a curve with exponent 4/7 that goes through $(H_c, 0)$ as well. In order to compare Equation (16) with Equation (15), we put $y = {H_d}/{H_c}$ and $x = {H}/{H_c}$. We find

$$y = 1 - x^{4/7} \tag{17}$$

and

$$y = 1 - \frac{1}{2}x(1 + x^{\sqrt{2}-2}) \quad . \tag{18}$$

With this substitution the Onsager points are (1,0) and (0,1), respectively.
We want to know where the influence of the decoupling and its corresponding formation of the cusp is starting to be felt strongly. For this we intersect both curves (17) and (18) to find x=0.024, so very c lose to x=0.

The picture that comes forward is that for the critical line in the phase diagram three regions should be distinguished: (i) $H \geq H_c$, (ii) $H_c \geq H \geq 0.024 H_c$ and (iii) $0.024 H_c \geq H \geq 0$.
In region (i) the result (12) describes the critical line very well, and so does (15) in region (ii). In region (iii) the cusp formation, due to the decoupling, becomes dominant.

4. Some other domain wall calculations

In the neighborhood of the Onsager point $(H_c, 0)$ we will illustrate the domain wall calculation, that led to Equation (12) in [10], for a skew domain wall, making an angle of 45^0 with the x-direction, see Figure 3.

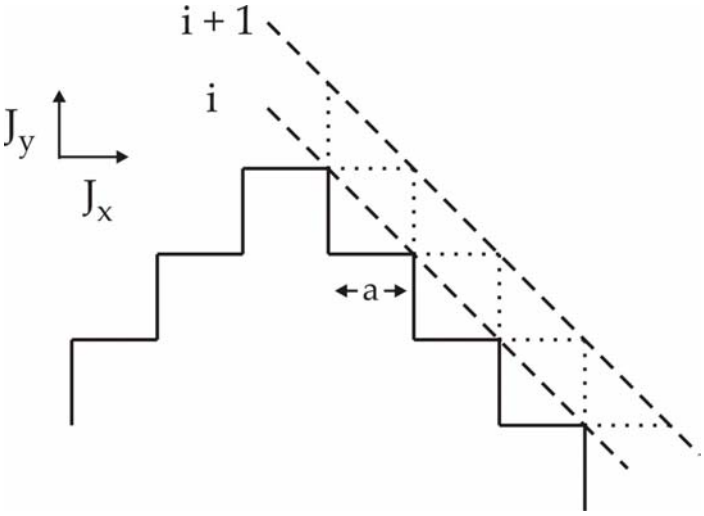

Figure 3
Domain wall calculation for skew wall.

We first consider the simple square lattice. For the skew wall, indicated by the dotted lines in Figure 3, we calculate the free energy needed to form kinks in the wall, analogous to the procedure in [10]. The dotted line *i* separates + spins from – spins. At zero temperature the formation energy of such a boundary per length $\frac{1}{2}\sqrt{2}a$, is given by

$$E_{(11)} = 2J_x + 2J_y \quad ,$$

the energy required to flip the spins near the boundary, so those on the dotted line *(i+1).* The kinks considered in the calculation are assumed not to include overhangs and are kinks perpendicular to the skew wall. Calculating first the energy needed for the formation of kinks reaching to increasing distance from the line *i*, we can calculate the partition function of the skew, i.e. (11), boundary and find

$$Z_{(11)} = \left(e^{-2J_x / k_B T} + e^{-2J_y / k_B T} \right) \sum_{n=0}^{\infty} e^{-2n(J_x + J_y)/k_B T} = \frac{e^{-2J_x / k_B T} + e^{-2Jy / k_B T}}{1 - e^{-2(J_x + J_y)/k_B T}}.$$

Per unit length a, we find for the boundary free energy

$$F_{(11)} = -\sqrt{2} k_B T \ln\left(Z_{(11)}\right).$$

This expression for the skew domain wall free energy is exactly the same as the expression derived by Onsager [5].
To determine the transition temperature, at which $F_{(11)} = 0$, we put $Z_{(11)} = 1$, to find

$$e^{-2J_x / k_B T_c} + e^{-2J_y / k_B T_c} = 1 - e^{-2(J_x + J_y)/k_B T_c} \quad ,$$

or

$$sh\left(\frac{2J_x}{k_B T_c}\right) sh\left(\frac{2J_y}{k_B T_c}\right) = 1 \quad ,$$

the Onsager formula for the transition temperature again . Taking into account isotropic next-nearest-neighbor interactions as well, a similar calculation yields,

$$Z_{(11)} = \left(\frac{e^{-(2J_x + 4J_d)/k_B T} + e^{-(2J_y + 2J_d)/k_B T}}{1 - e^{-2(J_x + J_y + 2J_d)/k_B T}} \right) \cdot \left(\frac{e^{-(2J_y + 4J_d)/k_B T} + e^{-(2J_x + 2J_d)/k_B T}}{1 - e^{-2(J_x + J_y + 2J_d)/k_B T}} \right)$$

.

The introduction of a next-nearest-neighbor interaction breaks the symmetry and therefore we have to consider two elementary steps of the skew domain wall.

We find

$$\left(e^{-(2J_x+4J_d)/k_BT_c}+e^{-(2J_y+2J_d)/k_BT_c}\right)\left(e^{-(2J_y+4J_d)/k_BT_c}+e^{-(2J_x+2J_d)/k_BT_c}\right)=$$
$$\left(1-e^{-2(J_x+J_y+2J_d)/k_BT_c}\right)^2$$

, (19)

which should be compared with (9). For small J_d the wall calculations for both choices of the wall, the straight (10) and the skew (11), yield essentially the same result. Although there are small differences this shows that the boundary free energy calculations, as carried out, result in good approximating equations for the critical line.

A second interesting case is the square 2D antiferromagnetic Ising model with nearest-neighbor interaction and an external magnetic field. For the sake of simplicity we consider here only the case of an isotropic nearest neighbor coupling.
For this model there is an interesting result of Müller-Hartmann and Zittartz [11] derived by the transfer matrix method.
They found, for $H_x = H_y = H$,

$$ch(H_\mu) = sh^2(2H) \tag{20}$$

for the transition point. In the absence of an external magnetic field, $H_\mu = 0$, this equation leads to the well-known Onsager result.

The gauging on this equation takes the particularly simple form

$$sh(2H^*) = \frac{sh(2H)}{\sqrt{ch(H_\mu)}}. \tag{21}$$

From this gauging equation we can find $H^*(H,H_\mu)$ and therewith $O(H^*)$ as potential solution to this particular Ising problem. Like for the solution $O(H^*(H,H_d))$, for the square lattice with diagonal edges, for this solution $O(H^*(H,H_\mu))$ should be tested on its validity by comparison with the known data like series expansions and, of course, on whether spontaneous magnetization, as calculated by Yang [22] for the ferromagnetic case, can be recovered from $O(H^*(H,H_\mu))$. The technique used can also be applied if we include diagonal interactions next to an external magnetic field.

5. Yet another approach and discussion of the cusp.

In this last section we would like to point out that the decoupling process can be studied also by the high temperature developments of van der Waerden.
We start with considering the linear lattice with next-nearest-neighbors, see Figure 1. If H=0, we have two simple linear chains. The partition function for the two decoupled chains of length *N/2* is

$$Z_N = \left(2ch(H_d)\right)^N \left(1 + 2{w_d}^{N/2} + {w_d}^N\right), \tag{22}$$

as there are only four graphs to consider. As soon as H is taken to be unequal to zero, the two linear lattices couple. For the partition function this means that

$$Z_N = \left(2ch(H_d)ch(H)\right)^N G_N(w,w_d) \quad . \tag{23}$$

The change for G_N is enormous. Instead of four contributions, now many contributions with low exponents occur. We focus on the low exponents for *w*. The lowest exponent is 2, when part of one chain is combined with part of the other chain, via two edges connecting the two chains;

$$G_N(w,w_d) = 1 + N{w_d}^2 w^2 + terms + 2{w_d}^{N/2} + {w_d}^N \quad . \tag{24}$$

For the free energy per element we find

$$f_N = -\frac{k_B T}{N}\ln\left(Z_N\right) = -k_B T \ln\left(2ch(H_d)ch(H)\right) - k_B T \ln\left({G_N}^{1/N}(w,w_d)\right). \tag{25}$$

Developing $G_N{}^{1/N}(w,w_d)$ to lowest order in w we find $1+g(w,w_d)=1+w_d^2w^2+$ other terms involving w^2. Then

$$f=-k_BT\ln\left(2ch(H_d)ch(H)(1+g(w,w_d))\right)\ , \tag{26}$$

is an equation on which we can gauge again. As $f=-k_BT\ln\left(2ch(H^*)\right)$ is the outcome for the simulating lattice we have

$$2ch(H^*)=2ch(H_d)ch(H)\left[1+g(w,w_d)\right]\ . \tag{27}$$

For w=0 we have $2ch(H^*)=2ch(H_d),$ so $H^*=H_d$, as should be. The terms involving w^2 are easily surveyed as they stem from N graphs with 1,2,3 etc. edges in one linear chain , in combination with 1 or 2, 2 or 3, 3 or 4, etc., edges in the other linear chain of N/2 vertices. The cofactors of w^2 are ${w_d}^2$, ${w_d}^3$, ${w_d}^4$, etc., watching out for double counting. These sum up to ${w_d}^2\left(\frac{1}{1-w_d}\right)$, so $g(w,w_d)={w_d}^2w^2\left(\frac{1}{1-w_d}\right)$, a minor correction on ${w_d}^2w^2$. Developing the exact solution (5) as a series in w, shows that the solution we found this way for the one-dimensional lattice with next-nearest-neighbors hardly differs from the exact solution.

We therefore now look at the coupling process in the two-dimensional case, our main topic. Why is the behavior in the Onsager points $(H_c,0)$ and $(0,H_c)$ so different? Let us first consider the point $(H_c,0)$. The 'dominating' lattice is a simple square lattice with,

$$Z_N=\left(2ch^2(H)\right)^N\left(1+Nw^4+2Nw^6+...\right). \tag{28}$$

The addition of diagonal edges has the effect that now

$$Z_N=\left(2ch^2(H)ch^2(H_d)\right)^N G_N(w,w_d)\,, \tag{29}$$

and in $G_N(w, w_d)$, in lowest order in w_d, terms occur like $w^2 w_d$ and $w^2 {w_d}^2$ for a square of the original lattice. In Figure 4(a) we have shown the addition of diagonal edges to a square.

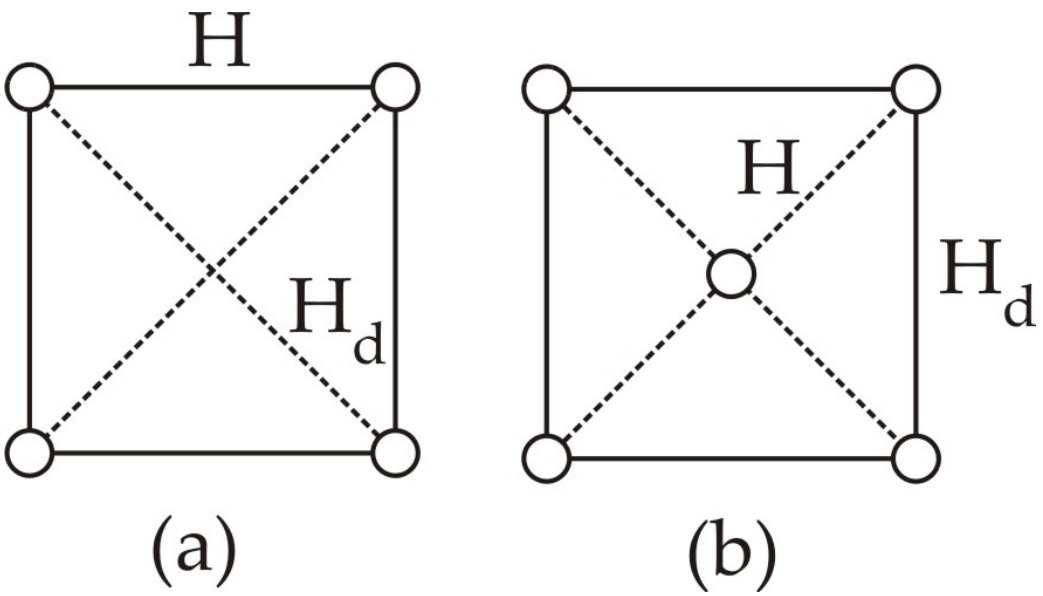

Figure 4
Extra contributions to $G_N(w, w_d)$.

There are two triangles contributing $2w^2 w_d$ to G_N and two cycles of length four contributing $2w^2 {w_d}^2$, next to w^4. In the neighborhood of the other Onsager point $(0, H_c)$, the addition of edges coupling the two lattices gives per square extra contributions, $4w_d w^2 + 4{w_d}^2 w^2 + 4{w_d}^3 w^2$, see Figure 4(b).
One is inclined to think that this is what makes the difference. Gauging on the lowest order terms by

$$ {w_d}^{*4} = {w_d}^4 + 4w^2 \left(w_d + {w_d}^2 + {w_d}^3 \right) \ , \qquad (30) $$

however, does not yield anything essentially different. The point that we should notice is that the contributions from the combination of edges stemming from both lattices via connecting coupling edges are the important ones.

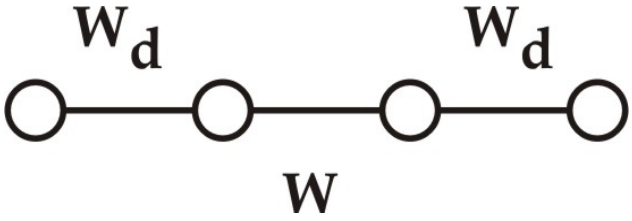

Figure 5
The essential coupling of the two sublattices.

We will make a very simple calculation. Consider, in the coupled lattice, the three consecutive edges depicted in Figure 5, where the edges with label w_d stem from different lattices. In a simulation by a simple square lattice instead of w_d as contribution from an edge now $w_d + w_d\sqrt{w}$ should be taken, as next to the ability to form multiple cycles, closed polygons, on one of the original lattices, two edges connected by an edge with interaction strength *J*, are able to form closed polygons, then contributing a factor ${w_d}^2 w$ to a term. Hence we gauge by

$$w^* = w_d + w_d\sqrt{w} \ . \tag{31}$$

For the critical point of the simulating lattice we have $w_c^* = \frac{1}{2}\sqrt{2}$, hence

$$w_{d,c} + w_{d,c}\sqrt{w_c} = \frac{1}{2}\sqrt{2} \ , \tag{32}$$

for very small, but non-zero, w_c. Deleting the index c for ease, we have

$$w_d = \frac{1}{2}\sqrt{2}.\frac{1}{(1+\sqrt{w})} \tag{33}$$

for the critical line. Therefore

$$\frac{dw_d}{dw} = \frac{1}{4}\sqrt{2}.\frac{1}{(1+\sqrt{w})^2} w^{-1/2} \ . \tag{34}$$

But this extremely simple argumentation then gives that there must be a cusp and, moreover, that the exponent must be in the neighborhood of ½. The fact that we considered hyperbolic tangents does not play a role. So next to the equations (17) and (18) we also have

$$y = 1 - x^{1/2} \quad , \tag{35}$$

as outcome for the shape of the cusp, with an exponent even closer to 4/7 than $\sqrt{2}-1$ was.

There is one final remark we would like to make about the exponent. Two edges from the two different square lattices couple by an edge that makes an angle of 45^0 with them. In the simulation the effect of this connecting edge on the strength of the simulating interaction energy is therefore not as strong as in the 1D case. This weakening involves a factor √2. As a weaker effect of H on H_d means that, because H is very small, the exponent of the cusp must be higher, we should multiply a given exponent, in which this geometrical aspect has not yet been taken into account, by √2. Applying this argumentation to our fitting curve, with exponent √2-1, then leads to an exponent √2(√2-1)=2-√2=0.586… , very close to 4/7=0.571… .

We consider this argumentation somewhat speculative. It should only be seen as giving support to the exponent 4/7 found in renormalization theory. Yet, the agreement of 2-√2 with 4/7 seems to indicate that the geometric aspect does play an important role in understanding the critical line near the Onsager point $(0, H_c)$.

Conclusions

We have proposed a method, which we have called gauging on exact equations, that allows one to map an Ising model that incorporates nearest neighbor and next-nearest-neighbor interactions or an external magnetic field, or both, on an Ising model that involves only nearest neighbor interactions. In this work we have illustrated the gauging method by using transition equations obtained from vanishing of the domain wall free energy.

Moreover, we present a fit for the critical line of the 2D Ising square lattice with nearest-neighbor and ferromagnetic next-nearest neighbor interactions. Finally, we discuss the cusp in the phase diagram that occurs for a vanishing nearest-neighbor interaction.

Note

For the 3D Ising model we have also tried to derive an expression for the 2D domain wall free energy. However, up to now our attempts are still unsuccessful. During the course of our work we found the following equation;

$$sh(2H_x)sh(2H_y)e^{2H_z} + sh(2H_x)sh(2H_z)e^{2H_y} + sh(2H_y)sh(2H_z)e^{2H_x} = 1,$$

which gives very satisfactory results. First, the well-known result of Onsager is recovered for $H_x = 0$, $H_y = 0$ or $H_z = 0$. Second, in the isotropic case we find H_c = 0.2233800, which should be compared to 0.2216546, from Monte Carlo simulations [23].
For the isotropic model we have

$$3e^{2H} sh^2(2H) = 1,$$

which leads to the gauging equation

$$sh^2(2H^*) = 3e^{2H} sh^2(2H) ,$$

from which we can solve H^* to obtain $O(H^*)$ as potential solution for the 3D case, assuming that indeed the 3D model can be simulated by a 2D model. The incorporation of an external field leads to an equation analogous to the conjecture of Müller-Hartmann and Zittartz, see Equation (20). The gauging equation for the 3D case plus an external magnetic field can be written as

$$sh(2H^*) = \sqrt{\frac{3}{ch(H_\mu)}} e^{H} sh(2H) .$$

As a final remark we would like to point out that it seems as if the gauging equations for different models can be partitioned into different *gauging classes*. We have the impression that this phenomenon can be tied up with the theory of universality classes, another point that deserves further research. The various results both exact and conjectured are summarized in Table II. The case 2D with next-nearest-neighbors is special as the gauging is problematic, since different

gauging equations are required in the interval $0 \le H \le H_c$. For this reason this case has not been included in Table II. It will be considered in a future publication.

Model	Solution *f* or gauging equation
1D	$-k_B T \ln\left(2ch(H)\right)$
1D + field	$-k_B T \ln\left(e^H ch(H_\mu) + e^H \sqrt{sh^2(H_\mu) + e^{-4H}} \right)$
1D + NNN	$-J_d - k_B T \ln\left(ch(H) + \sqrt{sh^2(H) + e^{-4H_d}} \right)$
2D	$-k_B T \ln\left(2ch(2H)\right) - \frac{k_B T}{2\pi} \int_0^\pi \ln\left(\frac{1}{2}\left(1 + \sqrt{1 - \kappa^2 \sin^2 \alpha} \right) \right) d\alpha$ where $\kappa = \frac{e^{2H} - e^{-2H}}{\left(e^{2H} + e^{-2H}\right)^2}$, $(sh(2H^*) = sh(2H))$
2D + field	$sh(2H^*) = \frac{sh(2H)}{\sqrt{ch(H_\mu)}}$
3D	$sh(2H^*) = \sqrt{3} e^H sh(2H)$
3D + field	$sh(2H^*) = \sqrt{\frac{3}{ch(H_\mu)}} e^H sh(2H)$

Table II
Solutions and gauging equations for different Ising models.

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