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Analysis of a Potential Solution to the Simple Cubic Three-dimensional Ising Model

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Abstract

Following a novel approach to solve sofar unsolved Ising problems like the 3D-problem for the simple cubic isotropic lattice, the authors brought forward a potential solution. This potential solution is analyzed to illustrate various aspects of the approach and is replaced by another.

Key words: Ising model, critical exponents, transition equation

AMS Subject Classifications: 82B20

1 Introduction

A novel approach to Ising problems was introduced in [3]. In that paper the idea of gauging on an equation was launched. It enables to simulate models like the 2D+NNN-model, two-dimensional quadratic plus next-nearest neighbours, or the 3D-model, three-dimensional simple cubic, by the 2D-model, two-dimensional quadratic.
In all cases interaction energies are taken equal for nearest neighbour bonds and also for next-nearest neighbour bonds. For the simple cubic lattice that we will consider this means that the interaction energies J_x, J_y and J_z in the x-, y- and z-direction are taken to be equal to J. For the simulating simple quadratic lattice the interaction energies J_x^* and J_y^* in x- and y-direction are taken to be equal to J^*.

With Boltzmann constant k and temperature T the expressions $\frac{J_x}{kT}$, $\frac{J_y}{kT}$,$\frac{J_z}{kT}$,$\frac{J_x^*}{kT}$, $\frac{J_y^*}{kT}$, $\frac{J}{kT}$ and $\frac{J^*}{kT}$ are denoted by H_x, H_y, H_z, H_x^*, H_y^*, H and H^*. $O(H_x^*, H_y^*)$ denotes the solution of the free energy of the anisotropic 2D-problem, while $O(H^*) \equiv O(H^*, H^*)$.

The basic idea of simulation is to express H^* in terms of H and to substitute this expression in $O(H^*)$. Writing

$$H^* = f(H).H$$

we introduced the *simulation strength factor* f(H). In [4] we have shown that for T=0 f(H)=$\frac{3}{2}$, whereas $f(H_{c,2D}) = \frac{H_{c,2D}}{H_{c,3D}}$, where $H_{c,2D}$ and $H_{c,3D}$ are the transition point values for the simulating and the simulated model respectively. $H_{c,2D} = \frac{1}{2}ln(\sqrt{2}+1)$ is known from Onsager's 2D-solution [12] and was conjectured three years earlier by Kramers and Wannier [7]. $H_{c,3D}$ is not known exactly, but Monte Carlo calculations of Blöte *et al.* [1] give $H_{c,3D}$=0.2216544, where the last digit is uncertain. As $H_{c,2D}$=0.4406868... the value of $f(H_{c,2D})$ is 1.9881707... . All calculational results are given with seven digits behind the comma.

For gauging we focus on the transition equations. For the anisotropic lattice we know for the 2D-model that

$$sinh(2H_x)sinh(2H_y) = 1.$$

The transition equation for the 3D-model is unknown, but in [4] we mentioned a possible transition equation. That is the equation we will analyze and that reads

$$\begin{aligned} TE_{3D}(H_x, H_y, H_z) \equiv \\ sinh(2H_x)^2 sinh(2H_y)^2 cosh(2H_z)^2 + sinh(2H_x)^2 cosh(2H_y)^2 sinh(2H_z)^2 + \\ cosh(2H_x)^2 sinh(2H_y)^2 sinh(2H_z)^2 + \\ 6sinh(2H_x)sinh(2H_y)sinh(2H_z)cosh(2H_x)cosh(2H_y)cosh(2H_z) + \\ 8sinh(2H_x)^2 sinh(2H_y)^2 sinh(2H_z)^2 = 1. \end{aligned} \tag{1}$$

For $H_x = H_y = H_z = H$ this equation reads

$$TE_{3D}(H) \equiv 3sinh(2H)^4 cosh(2H)^2 + 6sinh(2H)^3 cosh(2H)^3 + 8sinh(2H)^6 = 1,$$

that gives $H_{c,3D}$=0.2216379..., differing 165.10^{-7} from the Monte Carlo value.
The gauging equation reads, see [4],

$$TE_{2D}(H^*) = TE_{3D}(H).$$

As for H_z=0 the 2D-transition equation should be recovered we see from Equation (1) that $TE_{2D}(H^*) = sinh(2H^*)^4$ so that

$$sinh(2H^*)^4 = 3sinh(2H)^4 cosh(2H)^2 + 6sinh(2H)^3 cosh(2H)^3 + 8sinh(2H)^6 \tag{2}$$

is the gauging equation that expresses H^* in terms of H and gives the potential 3D-solution $O(H^*)$. In line with the reasoning in [3] we will now try to find "truth certificates" for Equation (1).

2 Analysis

We will investigate various properties of the potential solution.

2.1 Choice of the transition equation

One of the first properties that TE_{3D} should have is symmetry in the variables H_x, H_y and H_z. Another obvious property required is that for H_x=0, H_y=0 or H_z=0 the transition equation for the 2D-model is recovered. Both are properties of the TE_{3D} in Equation (1).

A third requirement comes from results known for the strongly anisotropic lattice, in which both $H_x \ll H_z$ and $H_y \ll H_z$. It is known, see [2] and [5], that asymptotically Equation (3) holds.

$$sinh(2H_z)sinh(2H_x + 2H_y) = 1. \tag{3}$$

The left hand side reads

$$sinh(2H_z)sinh(2H_x)cosh(2H_y) + sinh(2H_z)cosh(2H_x)sinh(2H_y).$$

Apart from the exponents 2 we recognize the second and third term in equation (1). In fact we first considered TE_{3D}'s in which these exponents 2 did not occur. What changed our mind was what is discussed in [4] concerning the transition equation for the 2D-triangular lattice. The solution for the anisotropic triangular lattice was given by Houtappel [6] and the transition equation reads

$$TE_{TR,1} = sinh(2H_1)sinh(2H_2) + sinh(2H_1)sinh(2H_3) + sinh(2H_2)sinh(2H_3) = 1, \tag{4}$$

where H_1, H_2 and H_3 correspond to the interactions in the three directions. For $H_1 = H_2 = H_3 = H$ one finds $H_{c,TR} = \frac{1}{4}ln(3)$. In [4] we pointed out that Equation (4) is a correct transition equation, but that there are other transition equations that give the same value. Lin [9] has given the solutions for the magnetization of various models. For the triangular model he gives

$$M_{TR} = [1 - \frac{1}{TE_{TR,2}}]^{\frac{1}{8}},$$

where, in the isotropic case,

$$TE_{TR,2} \equiv 3sinh(2H)^4 + 2sinh(2H)^3cosh(2H)^3 + 2sinh(2H)^6. \tag{5}$$

This expression is clearly different from $TE_{TR,1} = 3sinh(2H)^2$, but also $TE_{TR,2} = 1$ is a transition equation giving $H_{TR} = \frac{1}{4}ln(3)$. In [4] we therefore distinguished *correct* transition equations, giving the transition point, and *right* transition equations, giving not only the transition point but also the right formula for the magnetization. The example of

the triangular lattice, like the 3D-model having vertices of degree 6, often called coordination number in the literature, gave us the suggestion that the right transition equation for the 3D-model might look like $TE_{TR,2}$ in Equation (5). We therefore chose expressions in sinh(2H) and cosh(2H) that were all of degree 6. Next to $sinh(2H)^4cosh(2H)^2$ we chose $sinh(2H)^3cosh(2H)^3$ and $sinh(2H)^6$ as terms that we wanted to have integer coefficients. The integers 3, 6 and 8 were chosen to get the transition point right. We now pose some more stringent demands on the transition equation.

2.2 3D-1D and 3D-2D crossover behavior

We have mentioned the 3D-1D crossover behaviour in Equation (3). We take H_x=H_y=H and Equation (1) reads

$$\begin{aligned} 2sinh(2H)^2cosh(2H)^2sinh(2H_z)^2 + sinh(2H)^4cosh(2H_z)^2 + \\ 6sinh(2H)^2cosh(2H)^2sinh(2H_z)cosh(2H_z) + \\ 8sinh(2H)^4sinh(2Hz)^2 = 1. \end{aligned} \tag{6}$$

For $H \ll H_z$ the second and fourth term, containing $sinh(2H)^4$, are majorized and $sinh(2H_z) \approx cosh(2H_z)$, leading to

$$sinh(2H_z)^2[2sinh(2H)^2cosh(2H)^2 + 6sinh(2H)^2cosh(2H)^2] \approx 1.$$

Comparison with Equation (3), that now reads

$$sinh(2H_z)sinh(4H) = 1$$

or

$$sinh(2H_z)^2sinh(4H)^2 = 1$$

leads to the conclusion that for obtaining a truth certificate with respect to the 3D-1D crossover behaviour, the coefficient 6 had rather be 2. This is a second deviation, next to the slightly wrong transition point. As the 3D-1D crossover behaviour is well-established, this means that now also the coefficient 8 has to be adapted. Assuming the demands posed sofar the coefficient should be replaced by 63.3760522..., a somewhat unlikely non-integer value.

Before adapting the transition equation we investigate the interesting 3D-2D crossover behaviour for our candidate transition equation. Again we consider Equation (6), but now investigate the transition curve in the neighbourhood of H_z=0, i.e. for $H_z \ll H$. A most remarkable outcome is obtained.
Differentiating Equation (6) to H only the derivative of the second and the third term give contributions that do not contain a factor $sinh(H_z)$ and therefore remain for H_z=0. These contributions lead to

$$\frac{dH_z}{dH} = -\frac{3}{2}\sqrt{2}$$

in the 2D-Onsager point, where H_z=0.

This outcome is unsatisfactory in the light of the fact that it has been argued in [10] and [11] that the transition curve should have a vertical cusp in the 2D-Onsager point, so slope infinity. However, here a simple result from calculus can be used to enforce a cusp. We consider the functions $y = x^\epsilon$ for x going to 0. For ϵ=0 the limit is 1, for positive ϵ the limit is 0 and for negative ϵ the value goes to infinity.
We can now multiply the fourth term in Equation(1) with $sinh(2H_x)^\epsilon sinh(2H_y)^\epsilon sinh(2H_z)^\epsilon$. This leads to a horizontal cusp for negative ϵ. The effect on the left hand side of the transition equation vanishes in the limit of ϵ going to 0. A positive ϵ leads to an infinite slope for the transition curve, so to a vertical cusp.
So a very small change in the transition equation has a dramatic effect on the behaviour of the transition curve at the 2D-Onsager point. We will come back to this point in our summary.

The behaviour at the 2D-Onsager point is investigated in the literature, see e.g. Lee [8] by considering $H_z = \lambda H$ and asking for the behaviour, as function of λ of

$$A(\lambda) = \frac{T_c(\lambda) - T_c(0)}{T_c(0)} = \frac{\frac{kT_c(\lambda)}{J} - \frac{kT_c(0)}{J}}{\frac{kT_c(0)}{J}} = \frac{\frac{1}{H_c(\lambda)} - \frac{1}{H_c(0)}}{\frac{1}{H_c(0)}} = \frac{H_c(0)}{H_c(\lambda)} - 1.$$

It is conjectured [11] that $A(\lambda)$ behaves as $\lambda^{\frac{1}{\Phi}}$, where Φ is the susceptibility exponent $\frac{7}{4}$ for the 2D-model. The derivative of $A(\lambda)$ then would behave as $\frac{4}{7}\lambda^{-\frac{3}{7}}$, so tends to infinity as λ tends to zero.
In order to compare with this conjecture we remark that at λ=0

$$\frac{dA(\lambda)}{d\lambda} = -\frac{H_c(0)}{H_c(\lambda)^2}.\frac{dH_c(\lambda)}{d\lambda} = -\frac{\frac{dH_c(\lambda)}{d\lambda}}{H_c(0)} = +\frac{3}{2}\sqrt{2}.$$

Again no truth certificate is obtained as far as this conjecture is concerned. Note that

$$T_c(\lambda) - T_c(0) = A(\lambda).T_c(0)$$

and derivation to λ yields at λ=0

$$\frac{dT_c(\lambda)}{d\lambda} = \frac{3}{2}\sqrt{2}.T_c(0).$$

Unlike for $A(\lambda)$, the derivative depends on the interaction strength J, as $T_c(0) = \frac{J}{kH_c(0)}$.So the slope with which $T_c(\lambda)$ departs from $T_c(0)$ increases with J. The stronger the interaction, the steeper the slope.

3 Adjusting the transition equation

We mentioned three fallacies of our potential transition equation.

1. The transition point 0.2216379 differs, though only slightly, from the best known value 0.2216544.

2.The known 3D-1D crossover behaviour suggests that the integer coefficient 6 in the last but one term should be 2.

3. The 3D-2D crossover behaviour with respect to conjectures in the literature, for example that $\frac{dH_c(\lambda)}{d\lambda}$ should be infinite at the 2D-Onsager point, implying a cusp (with respect to the vertical in the phase diagram there).

As we have seen we easily achieve a cusp as meant in 3, either a horizontal or a vertical one by changing the exponents 1 in the forelast term to $1+\epsilon$, ϵ chosen negative respectively positive. The candidate transition equation is extremely sensitive to this choice.

The interplay of 1. and 2. allows "tuning" in the following way. The integer coefficients 6 and 8 can be changed to 2 and C. This does not have an effect on the behaviour of the 3D-2D crossover. Now either the integer C is tuned to achieve a transition point close to 0.2216544, or this value is assumed to be correct and C is solved from the equation resulting from substitution of this value. As we already remarked the latter results in that C should be 63.3760522... . We would prefer an integer coefficient for all terms of the transition equation.

As we have mentioned $A(\lambda)$ behaves like $\lambda^{\frac{4}{7}}$ by conjecture, but Monte Carlo calculations of Lee [8] indicate $\Phi \approx 1.49$, so practically $\frac{3}{2}$ and behaviour like $\lambda^{\frac{2}{3}}$. For this reason no truth certificate can be given sofar. However, it is possible to replace the term with $sinh(2H)^6$ by a term with $sinh(2H)^{30/7}$, in case $\Phi = \frac{7}{4}$ is considered to be a correct conjecture. Each factor has then an exponent $\frac{10}{7}$, in particular one factor is $sinh(2H_z)^{\frac{10}{7}}$. Note that this does not influence the 3D-1D crossover behaviour as then this factor is majorized by $sinh(2H_z)^2$ and so is the term.

Differentiation of the term to H yields a term with factors $sinh(2H_z)^{\frac{3}{7}}$ and $\frac{dH_z}{dH}$. On the other hand the derivative of $A(\lambda)$ behaves like $\lambda^{-\frac{3}{7}}$, i.e., for small λ, as $sinh(2H_z)^{-\frac{3}{7}}$, but then so does $\frac{dH_z}{dH}$. The choice of the exponent $\frac{10}{7}$ leads to compensating behaviour of the two mentioned factors arising from differentiation.

With the exponent $\frac{30}{7} = 4\frac{2}{7}$ we can determine the required coefficient that turns out to be about 16.3. A similar calculation can be made if we believe the Monte Carlo result of Lee to be right, that pleads for a behaviour of $A(\lambda)$ like $\lambda^{\frac{2}{3}}$. The exponent must then be 4 and the coefficient is about 13.2.
Both results are unsatisfactory. We therefore chose the coefficient to be precisely 15 and calculated the required exponent E of the last term of the transition equation. It turned out to be E=4.1547580... . The natural question is now the one about the 3D-2D crossover

behaviour. We choose for this the compensation principle that compensates for the divergent behaviour of the derivative of $A(\lambda)$, like we discussed before. On one hand there will occur a factor $sinh(2H_z)^{\frac{E}{3}-1}$, on the other hand the derivative behaves as $sinh(H_z)^{\frac{1}{\Phi}-1}$. Compensation occurs when

$$\frac{E}{3} - 1 = -(\frac{1}{\Phi} - 1),$$

or

$$\Phi = \frac{3}{6-E}.$$

Now a small miracle occurs. With the exponent E determined by demanding all truth certificates, considered sofar, to hold, we obtain $\Phi = 1.6258030...$, which differs only 0.0008 from 1.625=$\frac{13}{8}$. Note that $\frac{7}{4} = \frac{14}{8}$ whereas $\frac{3}{2} = \frac{12}{8}$. When we assume Φ to be $\frac{13}{8}$ precisely, then $E = \frac{54}{13}$. With this value for E we find a coefficient 14.9893219... for the assumed truth certificates, in particular the assumed transition value. As candidate transition equation we have now found

$$TE_{3D} \equiv 3sinh(2H)^4cosh(2H)^2 + 2sinh(2H)^3cosh(2H)^3 + 15sinh(2H)^{\frac{54}{13}} = 1. \quad (7)$$

It is obvious how the equation reads in the anisotropic case. This equation has all the right properties, truth certificates that we considered, as well as integer coefficients 3, 2 and 15, but for a deviation in the critical point for which we now have $H_c = 0.2216328....$ The deviation is 0.0000216... .

We have been able to weave the 3D-2D crossover behaviour into the transition equation, but there remains the question which value of Φ is the right one. $\frac{7}{4}$ is the theoretically conjectured value. $\frac{3}{2}$ is a value based on Monte Carlo results. $\frac{13}{8}$ is the best fitting value in our simulation approach.

4 Discussion and summary

By constructing TE_{3D} in Equation(7) we have adapted the transition equation so that it obtained all the truth certificates we could sofar consider. We should indicate at which points uncertainties are present.
The symmetry in the variables H_x, H_y and H_z is assured, as is the reduction to the proper 2D-transition equation if any of these variables has value zero. The 3D-1D crossover, that is well-known, was used to adapt the equation originally considered.
The uncertainty of the 3D-2D crossover behaviour has two aspects. First, there is the aspect of the exponent $\frac{1}{\Phi}$ of λ in $A(\lambda)$. We have indicated how the choice of Φ affects the exponent of the third term in Equation (7). For $\frac{7}{4}$, $\frac{13}{8}$ respectively $\frac{3}{2}$ the exponent has the values $4\frac{2}{7}$, $4\frac{2}{13}$ respectively 4. We defended our choice by demanding integer coefficients

for the terms. Second, there is the fact that the equation does not show a cusp behaviour at the 2D-Onsager point. However, introducing an exponent $1+\epsilon$ for the factors sinh(..) in the terms of the anisotropic version corresponding to the second and third term of Equation(7), we can create a cusp, horizontal for negative ϵ or vertical for positive ϵ. After introducing these exponents and gauging we obtain $H^*(H,\epsilon)$ for the simulating 2D-lattice, leading to $O(H,\epsilon)$ and, finally, to

$$O_{3D}(H) = \lim_{\epsilon \downarrow 0} O(H,\epsilon), \tag{8}$$

as a candidate solution for the free energy of the isotropic 3D simple cubic Ising model.

As was discussed in [4], the magnetization can then be given as

$$M_{3D} = \lim_{\epsilon \downarrow 0} [1 - \frac{1}{TE_{3D(H,\epsilon)}}]^{\frac{3}{8}} \tag{9}$$

and the simulation strength factor on the interval [0,1] for $1 - \frac{T}{T_{c,3D}}$ reads

$$f(H) = \lim_{\epsilon \downarrow 0} \frac{H^*(H,\epsilon)}{H}. \tag{10}$$

These three equations summarize our results.

Some final remarks should be made about the fact that we allow a deviation from the Monte Carlo value for the transition point. Seeing Monte Carlo results as a kind of measurement an important aspect is the certainty of such results. For the critical exponent β_{3D} we have seen [4] that there is considerable disagreement in the literature and that calculations on larger lattices showed that the outcome of a value $\frac{5}{16}$ shifted to an outcome closer to $\frac{3}{8}$. The value $H_c = 0.2216544$ was used as one of our truth certificate criteria. It is remarkable that this value comes out when $1 + \epsilon$, as we introduced for creating the vertical cusp, is 1.0006961... . Now any bulk calculation might show ϵ as function of H and N, the number of spins contained in the finite lattice considered, with the property that ϵ goes to zero with N going to infinity, thus creating the cusp in a natural way. But that means that Monte Carlo calculations on larger lattices may show that H_c is to be adjusted to a slightly lower value.

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