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LETTER TO THE EDITOR

Accurate determination of the critical line of the square Ising antiferromagnet in a field

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Abstract. Several points on the critical line of the simple quadratic antiferromagnetic Ising model in a field are located with high precision. This is accomplished by means of finite-size scaling of the magnetic correlation length of $n\times\infty$ strips. The latter quantities were determined by means of the transfer matrix method for strip widths up to $n=20$. An expression, possibly with the exact form, is constructed which reproduces the critical line with an accuracy to the order of 10^{-10}.

Until recently, the location of the critical line of two-dimensional Ising antiferromagnets in a field has mostly been restricted to numerical methods [1-4]. An exception is the 'super-exchange model' solved by Fisher [5]; in that rather special case the field acts only on part of the spins and can be transformed away with the decoration transformation. A related example was recently given by Giacomini [6]. An interesting conjecture was devised by Müller-Hartmann and Zittartz [7] for the critical line of the model on the square lattice; however, it was later shown not to be exact [3].

A new development is based on the analytic approach. The principle works as follows. The antiferromagnetic Ising model, with only nearest-neighbour interactions and a field, is generalised to a vertex model. By introducing a gauge variable into the weak-graph expansion by Wegner [8], Wu [9] has shown that the partition function of the vertex model is invariant under continuous O(2) transformations acting on the vertex weights. Therefore, it is required that also the critical manifold of the vertex model is invariant under that transformation. This requirement imposes restrictions on the shape of the critical surface. These restrictions can be augmented by the assumption that the critical surface corresponds with the zeros of a homogenous polynomial in the vertex weights [9-12]. When supplemented with additional knowledge, e.g. the exactly known zero-field critical point and numerical results for non-zero fields in the Ising subspace, the location of the critical surface can be further restricted. Finally, the assumption that the critical surface has the simplest form allowed by the gauge invariance and the additional data may be used to determine the Ising critical line uniquely (i.e. if we neglect the inaccuracy of the numerical results). This was recently achieved for the Ising model on the honeycomb lattice [13]. In that case, the availability of highly accurate numerical data [14] was crucial: in the first instance, an analytic expression for the critical line was constructed that fitted the numerical

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results up to deviations of the order of 10^{-6}. Since the numerical inaccuracy was smaller, it could nevertheless be concluded that the expression was not the exact one: the deviations were significant in spite of the fact that they were very small. The next-simplest expression allowed by the gauge invariance of the critical manifold was found fully consistent with the numerical precision of the order of 10^{-9} in the critical points.

This technique was also applied to the Ising model on the square lattice by Wu and Wu [15], leading to an expression for the critical line that might have the exact form. This expression contains constants with a finite numerical accuracy, reflecting the numerical inaccuracies of a few times 10^{-6} in the critical points derived in [4].

One of the goals of the present work is to reduce the numerical inaccuracy of the critical line (or a number of points on the critical line) of the square Ising antiferromagnet to a level comparable to that of the honeycomb model. This may not only lead to a more accurate determination of the aforementioned constants, but also enable a more stringent test of the form of the expression for the critical line proposed in [15]. This task was accomplished by means of transfer-matrix calculations and finite-size scaling (for reviews see [16]) of the correlation length.

To this purpose we consider the Ising model on an $n\times\infty$ strip on the square lattice with periodic boundaries in the finite direction, and with a reduced Hamiltonian

$$\mathcal{H}/kT=-K\sum_{\langle i,j\rangle}s_is_j-H\sum_k s_k. \tag{1}$$

The first sum is over all nearest-neighbour pairs. The associated coupling (interaction divided by kT) K is negative. Also the reduced magnetic field H contains a factor $1/kT$. The magnetic correlation length ξ_n in the length direction of the strip follows from the two largest (in absolute value) eigenvalues λ_1 and λ_2 of the transfer matrix:

$$\xi_n^{-1}(K,H)=\log|\lambda_1/\lambda_2|. \tag{2}$$

At the critical point, the magnetic correlation length is expected to have the following finite-size dependence

$$n\xi_n^{-1}(K,H)\simeq\pi/4 \tag{3}$$

for asymptotically large n, in accordance with Ising universality [17]. Thus, the critical coupling $K_c(H)$ can be estimated by solving numerically for K in (3). These solutions, which are denoted $K_{1,n}$, can be subjected to a number of iterated fits described, e.g. in [14], yielding $K_{i,n}$, $i=2,3,\ldots$. This procedure greatly accelerates the convergence to $K_c(H)$ with increasing n.

For the determination of the correlation lengths, two different transfer matrices were used: (i) with the transfer direction (i.e. the length direction of the strip) parallel to a set of lattice edges, and (ii) with the transfer direction rotated by an angle of $\pi/4$. Technical details of the transfer matrix calculations can be found in [14], which describes the construction of transfer matrices for two different directions on the honeycomb lattice. Firstly, the square lattice can be obtained by adding extra bonds into the brick representation of the honeycomb lattice. Thus, the first transfer matrix for the square lattice is constructed by adding a set of horizontal couplings into the first transfer matrix of [14]. Thereby the periodicity in the transfer direction reduces to one. Secondly, the square lattice can be obtained by contracting all bonds having a specified direction on the honeycomb lattice. Thus, the second transfer matrix for the square lattice is obtained from the second transfer matrix constructed in [14] by making the vertical bonds ferromagnetic and infinitely strong (and dividing out the infinite constant in the appropriate Boltzmann weights). The transfer matrix thus obtained is symmetric, so that the spin inversion redefinition described in [14] is unnecessary.

Using the first transfer matrix construction, a computer program was written for the calculation of the magnetic correlation length (2). We have used finite size parameters $n=2, 4, \ldots, 20$. Odd system sizes were ignored because the associated frustration occurring in antiferromagnetic systems leads to a scaling behaviour that is different from that expressed by (3). Solutions of (3) as described in [14] were thus obtained for several values of H. Iterated fits up to $K_{4,n}(H)$ were obtained from these solutions. They show a rapid apparent convergence. Best estimates of the critical points are based on $K_{3,n}(H)$ and $K_{4,n}(H)$, and are shown in table 1. Results were also obtained in the limit $K \to -\infty$, by solving (3) for $\mu = -2H - 8K$, which remains finite. This quantity is the chemical potential of a hard-square lattice gas [3]. The final result is included in table 1.

Table 1. Best estimates of critical points t_c of the square antiferromagnetic Ising model in a field H. The temperature-like parameter t stands for the nearest-neighbour coupling K or for the chemical potential μ of a hard-square lattice gas. The columns under $t_{c,1}$ and $t_{c,2}$ were obtained from the first- and the second-transfer matrix mentioned in the text respectively. Estimated numerical inaccuracies in the last decimal places are shown between parentheses.

H	t	$t_{c,1}$	$t_{c,2}$
0	K	−0.440 686 795 (2)	−0.440 686 7935 (2)
0.25	K	−0.446 044 361 (3)	−0.446 044 3601 (2)
0.5	K	−0.461 733 921 (3)	−0.461 733 9203 (2)
0.75	K	−0.486 729 978 (3)	−0.486 729 9778 (2)
1.0	K	−0.519 652 443 (3)	−0.519 652 4427 (2)
1.25	K	−0.559 055 720 (3)	−0.559 055 7206 (2)
1.5	K	−0.603 617 782 (3)	−0.603 617 7818 (2)
1.75	K	−0.652 221 358 (3)	−0.652 221 3579 (2)
2.0	K	−0.703 964 205 (3)	−0.703 964 2060 (2)
2.5	K	−0.814 184 087 (3)	−0.814 184 0877 (2)
3.0	K	−0.930 301 817 (3)	−0.930 301 8177 (2)
4.0	K	−1.171 715 306 (5)	−1.171 715 3059 (2)
∞	μ	1.334 015 10 (5)	1.334 015 1004 (8)

Using the second transfer matrix, (3) was similarly solved for finite sizes $2, 3, \ldots, 19$. No odd-even alternation occurs in this case. Best estimates of the critical couplings were based on $K_{4,n}$; they are also shown in table 1.

During the fitting procedures, we observed that the differences $K_{4,n}(H) - K_{4,m}(H)$, for $m > n$, were usually at most of the same order of magnitude as the differences $K_{4,n}(H) - K_{4,n-1}(H)$. Thus, the latter difference, taken for the largest available value of n, served as the basis of our estimation of the numerical uncertainties in the data shown in table 1. Although the largest system size for the first transfer matrix is larger, this effect is outweighed by the larger number of system sizes in the case of the second transfer matrix. We observe that the data in table 1 are consistent with each other, and with existing results [1-4], and with the exact value $K_c(0) = \frac{1}{2}\log(1+\sqrt{2}) = 0.440\,686\,793\,509\,771\,513\ldots$.

In order to obtain a closed-form expression describing the whole critical line of the square Ising antiferromagnet, we have repeated the analysis of [15] on the basis of the new numerical results. Thus we have fitted the unknowns in the invariant polynomial of degree 4 (f_{4+} as defined in [15]), using the data in the last column of table 1. Unfortunately, we found that the polynomial of degree 4 is unable to reproduce the critical points with an accuracy better than about 10^{-7}. Thus the polynomial of degree 4 cannot be the exact expression for the critical line.

The next-simplest candidate is the polynomial of degree 6. Using the notation and definitions of [15], it is given by

$$f_{6+} = c_1 I_1^6 + c_2 I_2^3 + c_3 I_3^3 + c_4 I_1^4 I_2 + c_5 I_1^2 I_2^2 + c_6 I_1^4 I_3 + c_7 I_1^2 I_3^2 + c_8 I_2^2 I_3 + c_9 I_2 I_3^2 + c_{10} I_1^2 I_2 I_3 \qquad (4)$$

where the I_i are known fundamental invariant polynomials given in [15]; they depend only on K and H. The c_i are the unknowns that remain to be determined (in fact there are only nine unknowns, because only the ratios of the c_i matter). The fundamental invariants I_4 and I_5 do not appear in (4); they were eliminated using the relations $I_4 = -\frac{1}{2}I_1^3 + \frac{1}{2}I_1 I_2 + I_1 I_3$ and $64 I_5^2 = I_2 I_3^2 - I_4^2$.

In addition to the data presented in table 1, also the curvature of the critical line at zero field is known with a high precision. In the limit $H \to 0$, its behaviour is

$$K_c(H) \simeq -\tfrac{1}{2}\log(1+\sqrt{2}) - 2uH^2/\log(1+\sqrt{2}). \qquad (5)$$

The constant u can be determined by substituting the highly accurate number $B = 0.193\,595\,186\,268\,2647\ldots$, which was defined and determined by Kong *et al* [18, 19], for D in equation (24) of a paper by Kaufman [20]. This yields $u = 0.038\,012\,325\,934\,4205\ldots$.

Each of the $K_c(H)$ data points including the exact value at $H = 0$, as well as the constant u, leads to a linear equation ($f_{6+} = 0$) that may serve to solve for the c_i. In order to suppress loss of accuracy during the solution of a resulting set of linear equations, we have used quadruple precision in this part of the calculation. Since the number of data points exceeds the number of unknowns, the remaining data points could be used to check the accuracy of the resulting expression for the critical line after solving for the c_i. The solutions thus obtained are still dependent on the choice

Table 2. Results for the coefficients c_i as solved from the set of linear equations given by $f_{6+} = 0$ using the data described in the text. This set of coefficients describes the critical line $K_c(H)$ with an accuracy of the order of 10^{-10}.

i	c_i
1	1
2	$-6.237\,774\,177\,232\,442 \times 10^{-5}$
3	$-4.388\,465\,499\,901\,184 \times 10^{-3}$
4	$-4.719\,220\,855\,085\,813 \times 10^{-1}$
5	$1.241\,878\,555\,056\,222 \times 10^{-2}$
6	$-9.463\,046\,463\,634\,868 \times 10^{-1}$
7	$5.644\,026\,087\,337\,113 \times 10^{-1}$
8	$4.221\,148\,633\,657\,529 \times 10^{-4}$
9	$2.681\,027\,308\,907\,968 \times 10^{-4}$
10	$-9.331\,064\,823\,834\,851 \times 10^{-2}$

of the data points used to solve the linear equations. The constants c_i as obtained from one of the resulting fits are shown in table 2. Once the c_i are known, one can use the equation $f_{6+}=0$ to solve for $K_c(H)$. For details see [15]. This solution reproduces the zero-field critical point and the constant u with a precision of the order of 10^{-14} (i.e. consistent with the machine precision), and the remaining data points within a margin of 10^{-10}, well within the estimated errors quoted in table 1. Thus, the description of the critical line by the invariant polynomial f_{6+} is consistent with all available data, and therefore $f_{6+}=0$ may be considered a candidate for the exact formula for the critical line Ising antiferromagnet on the square lattice.

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