Correlation equalities and upper bounds for the transverse Ising model

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Abstract. Starting from an exact formal identity for the two-state transverse Ising model and using correlation inequalities, approximate upper bounds for the critical temperature and the critical transverse field are obtained, which improve the effective results.

Keywords: rigorous results in statistical mechanics, classical phase transitions (theory), quantum phase transitions (theory)
1. Introduction

The transverse Ising model (TIM) is described by a two-state Ising Hamiltonian with a term representing a field transverse to the spins,

\[ H = - \sum_{ij} J_{ij} S_i^z S_j^z - \Omega \sum_i S_i^x, \]  

where \( J_{ij} > 0 \), \( \Omega \) is the transverse field, \( S_i^z \) and \( S_i^x \) are Pauli spin-\( \frac{1}{2} \) operators and the first sum is over the nearest neighbour spins on the lattice. The model was firstly applied to describe the phase transitions and the properties of hydrogen bonded ferroelectrics [1, 2] and magnetic ordered materials [3]. This model in one dimension has no phase transition at finite temperatures; however, at zero temperature it is ordered up to the critical value of the transverse field. The model has been solved exactly in one dimension [4]–[6]. In high dimensions there are approximations for low-temperature or high-temperature regions [7, 8]. All other calculations are based on mean field type approximations. An effective field theory has been presented which improves the mean field results [9]. Since then many results have been obtained based on the effective field theory. More recently the model has been used to study the phase diagrams of nanowire systems [10] and magnetization of nanoparticles [11]. The objective of this paper is to present approximate upper bounds for the critical couplings. We will apply the results for the \( d = 2 \) square lattice and the \( d = 3 \) cubic lattice.
2. Generalized Callen’s identity for the transverse Ising model

In this section, we describe the methodology used by Sá Barreto et al [9] to derive an identity for the two-spin correlation function of the transverse Ising model. The procedure used in this deduction was presented in reference [9] to obtain an exact relation for the order parameter \( \langle S_i^z \rangle \) which generalizes Callen’s identity [17]. The longitudinal two-spin correlation function \( \langle S_i^z S_i^z \rangle \) can be calculated from

\[
\langle S_i^z S_i^z \rangle = \frac{\text{Tr}(e^{-\beta H} S_i^z S_i^z)}{\text{Tr}(e^{-\beta H})}
\]  

(2)

where \( H \) is given by equation (1). The Hamiltonian can be separated into two parts, \( H = H_i + H' \), where \( H_i \) includes all parts associated with site \( i \) and \( H' \) represents the rest of the Hamiltonian. A direct calculation leads to

\[
\langle S_i^z S_i^z \rangle = \left( S_i^z \frac{\text{Tr}(\langle S_i^z \rangle e^{-\beta H_i})}{\text{Tr}(e^{-\beta H})} \right) - \left( S_i^z \frac{\text{Tr}(\langle S_i^z e^{-\beta H} \rangle - S_i^z) \Delta}{\text{Tr}(e^{-\beta H})} \right)
\]

(3)

where \( \text{Tr}(\langle S_i^z \rangle) \) represents the partial trace with respect to site \( i \) and \( \Delta = 1 - e^{-\beta H} e^{-\beta H'} e^{\beta (H_i + H')} \). Equation (3) is an exact relation. However, it is difficult to use. Therefore, we will make an approximation based on the following decoupling:

\[
\langle S_i^z \left[ \frac{\text{Tr}(\langle S_i^z \rangle e^{-\beta H_i})}{\text{Tr}(e^{-\beta H})} - S_i^z \right] \Delta \rangle \approx \left( S_i^z \frac{\text{Tr}(\langle S_i^z e^{-\beta H} \rangle - S_i^z)}{\text{Tr}(e^{-\beta H})} \right) \langle \Delta \rangle.
\]

(4)

Inserting equation (4) into (3) and using the fact that \( \langle \Delta \rangle \leq 1 \), we obtain

\[
\langle S_i^z S_i^z \rangle \leq \left( S_i^z \frac{\text{Tr}(\langle S_i^z \rangle e^{-\beta H_i})}{\text{Tr}(e^{-\beta H})} \right).
\]

(5)

By expanding \( \Delta \) we see that the approximation is correct to the order of \( \beta^2 \). Moreover, it is consistent with the application of the correlation inequalities that will be used later to obtain the upper bounds for the critical couplings.

A more general result can be represented by equations identical to (3) and (5) but written for \( \langle F(S) \rangle \), where \( F(S) \) is any product function of the spin components, except \( S_i^z \). Relations (3) and (5) are special cases where \( F(S) = S_i^z \). The relation for the longitudinal magnetization \( \langle S_i^z \rangle \) is the special case where \( F(S) = 1 \). Within this description, the decoupling (4) can then be viewed as a 0th order approximation of the exact relation (3) for \( F(S) = 1 \), i.e., equation (5) can be assumed to be obtained from the approximation \( \langle S_i^z - S_i^z \rangle = 0 \), where \( S_i^z = \frac{\text{Tr}(\langle S_i^z \rangle e^{-\beta H_i})}{\text{Tr}(e^{-\beta H_i})} \). For the magnetization, equation (4) has already been used before in other references that use relation (5) and an effective field approach [10]–[16].

Let us write \( H_i = -E_i S_i^z - \Omega S_i^x \), where \( E_i = \sum_j J_{ij} S_j^z \). From equation (5), diagonalizing and taking the partial trace over \( i \), we get for the longitudinal spin correlation function, \( \langle \sigma_i^z \sigma_i^z \rangle \), where \( \sigma_i = 2S_i \),

\[
\langle \sigma_i^z \sigma_i^z \rangle \leq \left( \frac{2 \Omega}{(2\Omega)^2 + \left( \sum_j J_{ij} \sigma_j^z \right)^2} \right)^2 \cdot \tanh \left( \beta \sqrt{(2\Omega)^2 + \left( \sum_j J_{ij} \sigma_j^z \right)^2} \right).
\]

(6)
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Introducing the exponential operator \( e^{(aD)}f(x) = f(x + a) \), \( D = \partial/\partial x \), we obtain

\[
\langle \sigma_i^z \sigma_i^z \rangle \leq \left\langle \sigma_i^z e^{\sum_j (J_{ij}\sigma_j^z)D} \right\rangle f(x)|_{x=0} = \left\langle \sigma_i^z \prod_j e^{(J_{ij}\sigma_j^z)D} \right\rangle f(x)|_{x=0}
\]

(7)

where \( f(x) \) is given by

\[
f(x) = \frac{x}{\sqrt{(2\Omega)^2 + x^2}} \tanh(\beta) \sqrt{(2\Omega)^2 + x^2}.
\]

(8)

Note that \( f(x) = -f(-x) \).

Expanding the exponential in equation (7) and considering that \((\sigma_i^z)^2 = 1\), we obtain

\[
\langle \sigma_i^z \sigma_i^z \rangle \leq \left\langle \sigma_i^z \prod_j \left[ \cosh(J_{ij}D) + \sigma_j^z \sinh(J_{ij}D) \right] \right\rangle f(x)|_{x=0}.
\]

(9)

By a similar procedure the transverse two-spin correlation function \( \langle \sigma_i^x \sigma_i^x \rangle \) is obtained,

\[
\langle \sigma_i^x \sigma_i^x \rangle \leq \left\langle \sigma_i^x \prod_j \left[ \cosh(J_{ij}D) + \sigma_j^z \sinh(J_{ij}D) \right] \right\rangle g(x)|_{x=0},
\]

(10)

where \( g(x) \) is

\[
g(x) = \frac{2\Omega}{\sqrt{(2\Omega)^2 + x^2}} \tanh(\beta) \sqrt{(2\Omega)^2 + x^2} = g(-x).
\]

(11)

The expectation value of \( \sigma_i^x \) is given by

\[
\langle \sigma_i^x \rangle \leq \left\langle \prod_j \left[ \cosh(J_{ij}D) + \sigma_j^z \sinh(J_{ij}D) \right] \right\rangle g(x)|_{x=0}.
\]

(12)

3. Application to the \( d = 2 \) square lattice and the \( d = 3 \) cubic lattice

3.1. The \( d = 2 \) lattice

Considering the four neighbours of \( i \) in equation (9), expanding the product, applying the exponential operators appearing in the powers of \( \cosh(J_{ij}D) \) and \( \sinh(J_{ij}D) \) in \( f(x) \), we obtain

\[
\langle \sigma_i^x \sigma_i^x \rangle \leq A_2 \sum_j \langle \sigma_i^x \sigma_j^x \rangle + B_2 \sum_{j<k<m} \langle \sigma_i^x \sigma_j^x \sigma_k^x \sigma_m^x \rangle
\]

(13)

where

\[
A_2 = \frac{1}{8}[f(4J) + 2f(2J)] > 0, \quad B_2 = \frac{1}{8}[f(4J) - 2f(2J)] < 0
\]

(14)

and \( j, k \) and \( m \) are neighbours of \( i \) and \( f(\cdots) \) is given by equation (8).

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3.2. The $d = 3$ lattice

After a similar calculation we obtain for the cubic lattice

$$
\langle \sigma_l^z \sigma_i^z \rangle \leq A_3 \sum_j \langle \sigma_l^z \sigma_j^z \rangle + B_3 \sum_{j < k < m} \langle \sigma_l^z \sigma_j^z \sigma_k^z \sigma_m^z \rangle + C_3 \sum_{j < k < m < n < p} \langle \sigma_l^z \sigma_j^z \sigma_k^z \sigma_m^z \sigma_n^z \sigma_p^z \rangle \quad (15)
$$

where

$$
A_3 = \frac{1}{5}[f(6J) + 4f(4J) + 5f(2J)] > 0, \quad B_3 = \frac{1}{5}[f(6J) - 3f(2J)] < 0,
$$

and

$$
C_3 = \frac{1}{5}[f(6J) - 4f(4J) + 5f(2J)] > 0 \quad (16)
$$

and $j, k, m, n$ and $p$ are neighbours of $i$ and $f(\cdots)$ is given by equation (8).

4. Exponential decay of the two-point functions and the upper bounds

Upper bounds for the critical temperature $T_c$ for Ising and multi-component spin systems have been obtained by showing (for $T > T_c$) the exponential decay of the two-point function [18]–[20]. The procedure to obtain these upper bounds for the critical couplings of the transverse Ising model is as follows. We start from the two-point correlation functions (13) and (15) and we make use of Griffiths inequalities (Griffiths I, II) [21, 23, 24] and Newman and Lebowitz inequalities [22, 24]. A proof of Griffiths inequalities has been given for the XY model with no external field [21]. Extensions of Griffiths–Kelly–Sherman inequalities to quantal systems, under external fields, both longitudinal and transverse, have been proved [23, 24]. The physical reason why the Griffiths and similar inequalities are valid for the quantal XY-type Hamiltonian is that the off-diagonal interaction, namely $H_1(x) = \sum_A J_{A}^x \sigma_A^x$, ($J_{A}^x \geq 0$), produces a decrease of the ferromagnetic correlation among the $\sigma_j^x$-spins, but it is not sufficiently large to create a cooperative effect to induce an antiferromagnetic correlation. In other words, one can say that $H_1(x)$ is a dynamical random force acting on $z-z$ correlations [23]. We establish the inequality for the two-point function

$$
\langle \sigma_l^z \sigma_i^z \rangle \leq \sum_j a_j \langle \sigma_l^z \sigma_j^z \rangle, \quad 0 \leq a_j \leq 1, \quad (17)
$$

which when iterated [19] implies exponential decay for $T > T_c$. Due to the use of the approximation (4), the upper bounds thus obtained are not exact. Nevertheless, all the steps that follow the substitution of equation (4) in (3) in order to obtain the two-spin correlation function relation given by equation (17) are based on rigorous correlation function inequalities.

4.1. Upper bounds for $d = 2$

From equation (13), using Griffiths II ($\langle \sigma_l^z \sigma_j^z \sigma_k^z \sigma_m^z \rangle \geq \langle \sigma_l^z \sigma_j^z \rangle \langle \sigma_k^z \sigma_m^z \rangle$) in the second term and considering $B_2 < 0$, we get

$$
\langle \sigma_l^z \sigma_i^z \rangle \leq \sum_j a_j \langle \sigma_l^z \sigma_j^z \rangle \quad (18)
$$

where $j \neq k$ are neighbours of $i$, and

$$
a_j = A_2 - |B_2| \langle \sigma_l^z \sigma_k^z \rangle_{1d} \quad (19)
$$

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Table 1. Estimates for $\Omega_c/\Omega_c^{\text{MFA}}$ for $d = 2$ and 3.

|        | $d = 2, z = 4$ | $d = 3, z = 6$ |
|--------|----------------|----------------|
| MFA    | 1              | 1              |
| EFT    | 0.688          | 0.784          |
| HTE    | 0.770          | 0.860          |
| Present work | 0.643         | 0.813          |

4.2. Upper bounds for $d = 3$

From equation (15), using Griffiths II on the second term $B_3 < 0$, Newman’s inequality $\langle \sigma_i^z F \rangle \leq \sum_j \langle \sigma_i^z \sigma_j^z \rangle \langle dF/d\sigma_j^z \rangle$, $F$ are polynomials with positive coefficients) combined with Griffiths I ($\langle \sigma_3^z \rangle \leq 1$) on the third term $C_3 > 0$, we get

$$\langle \sigma_i^z \sigma_i^z \rangle \leq \sum_j a_j \langle \sigma_i^z \sigma_j^z \rangle$$

(20)

where $j \neq k$ are neighbours of $i$, and

$$a_j = A_3 - |B_3| \langle \sigma_j^z \sigma_k^z \rangle_{1d} + 5C_3.$$  

(21)

4.3. Numerical results

The two-spin correlation function appearing in equations (19) and (21), $\langle \sigma_j^z \sigma_k^z \rangle_{1d}$, is the one-dimensional model two-spin correlation function separated by a distance of two lattice sites. For the one-dimensional transverse Ising model the exact value of this function at the critical value $\Omega_c = J$ is [4]

$$\langle \sigma_j^z \sigma_k^z \rangle_{1d} = \frac{1}{4} \left( \frac{2}{\pi} \right)^2 \frac{H^4(2)}{H(4)}$$

(22)

where $H(n) = 1^{n-1}2^{n-2}\ldots(n-1)$. For the one-dimensional Ising model the exact value of the spin correlation function separated by a distance of two lattice sites is

$$\langle \sigma_j^z \sigma_k^z \rangle_{1d} = \tanh^2 \beta J.$$  

(23)

In the following, we will use result (22) in equations (19) and (21) to calculate the upper bound for $\Omega_c$ at $T_c = 0$ and result (23) in equations (19) and (21) to calculate the upper bound for $T_c$ at $\Omega = 0$. Evaluating numerically the value of $T$ such that $\sum_j a_j \leq 1$, $a_j > 0$, we obtain, by a sufficient condition (see equation (17)), the upper bounds for $T_c$ as a function of $\Omega_c$, shown in figure 1, together with the curve for the mean field results. We use equation (23) for the one-dimensional two-spin correlation function in obtaining figure 1. This curve represents the upper bounds for $(T_c, \Omega_c)$. In particular, the mean field values are $\Omega_c^{\text{MFA}} = zJ/2$ and $T_c^{\text{MFA}}(0) = zJ/k_B$. The values for $\Omega_c$ and $T_c(0)$, which are the upper bounds for $d = 2, z = 4$ and $d = 3, z = 6$, obtained in the present calculation are (a) $d = 2, z = 4$; $k_BT_c/J = 3.014$ and $\Omega_c = 1.3755/J$, (b) $d = 3, z = 6$; $k_BT_c/J = 5.423$ and $\Omega_c = 2.4466/J$.

In table 1, we compare the results obtained by the effective field calculation (EFT) [9], the high temperature expansion (HTE) [7, 8] and the present results for $\Omega_c$.

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Figure 1. Phase diagram of the TIM model for $z = 4$ and 6. The solid line is the mean field approximation result. The results for our approach evaluated by using the spin correlation function separated by two sites, equation (23), are given by the dotted ($z = 4$) and dashed ($z = 6$) lines.

5. Concluding remarks

In this paper we have obtained approximate upper bounds for the critical couplings of the transverse Ising model. The procedure was based on an approximation for an exact identity for the two-spin correlation functions and on rigorous inequalities for the spin correlation functions. The approximate relation for the two-spin correlation function, equation (5), used in this procedure is consistent with the rigorous inequalities, equation (17), since both act in the same direction of the inequalities. The upper bounds were applied for two- and three-dimensional models.

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