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Correlation equalities and some upper bounds for the critical temperature of Ising spin systems†

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Abstract. Starting from correlation identities for Ising systems and using Griffith's and Newman's inequalities, upper bounds for the critical temperature are obtained which improve mean-field results.

Upper bounds $\bar{T}_c$ for the critical temperature T_c for Ising and multi-component spin systems have been obtained by showing (for $T > \bar{T}_c$) the exponential decay of the two-point function (Fisher 1967, Simon 1980, Brydges *et al* 1982). Series expansions in $\tanh \beta J$ and in βJ are analysed by Fisher (1967) and Brydges *et al* (1982) respectively, and spin correlation inequalities and their iteration are used by Brydges *et al* (1982), Lieb (1980) and Simon (1980). The inequality used by Lieb (1980) and its iteration can, in principle, be used to obtain a sequence of temperatures that converge to the critical temperature. However, as pointed out by Simon (1980), computation of successively better approximations to T_c require increasingly lengthier computations.

In this short note, for completeness, we give a simple proof of the mean-field bound for T_c. We then improve this bound for the classical Ising model as follows: starting from a two-point correlation function identity (Callen's identity) (Callen 1963) using Griffith's 1st and 2nd inequalities (Griffith I, II) (see Glimm and Jaffe 1981) and Newman's inequalities (Newman 1975) we establish the inequality

$$\langle S_0 S_l \rangle \leqslant \sum_{|j|=1} a_j \langle S_j S_l \rangle, \qquad 0 \leqslant a_j \leqslant 1, \qquad l \neq 0 \tag{1}$$

for the two-point function $\langle S_0 S_l \rangle$ which when iterated (see Simon 1980) implies exponential decay for $T > \bar{T}_c$. The upper bounds we obtain are lower than those obtained by Simon (1980) and Brydges *et al* (1982).

We first give a simple proof of the mean-field upper bound for T_c. We write the Hamiltonian for a classical lattice spin system as $H = -J \sum_{i,j \in \Lambda} S_i S_j$ where $J > 0$ and the sum is over nearest-neighbour spins on the lattice Λ with the point $0 \in \Lambda$. We define the thermal average $\langle \ldots \rangle$ by

$$\langle \ldots \rangle = Z^{-1} \sum_{\{S_i\}} (\ldots) \, e^{-\beta H}, \qquad Z = \sum_{\{S_i\}} e^{-\beta H}$$

where each S_i is restricted by $|S_i| = 1$. We let ν denote the coordination number of

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the lattice Λ and let $\langle\ldots\rangle_\lambda$, $0\leqslant\lambda<1$ denote $\langle\ldots\rangle$ with H replaced by $H_\lambda=-J\lambda\,\Sigma_{|i|=1}S_0S_i-J\,\Sigma_{i,j\neq 0}S_iS_j$. T_c is defined by

$T_c=[\inf T:\forall T'>T\,\exists m(T')>0$ and $C(T')>0\rightarrow\langle S_0S_l\rangle\leqslant C(T')\exp(-m(T')|l|)]$.

We have

Theorem 1. $T_c\equiv\beta_c^{-1}<J^{-1}\nu^{-1}$.

Proof. Integrating $\mathrm{d}\langle S_0S_l\rangle_\lambda/\mathrm{d}\lambda$ between $\lambda=0$ and $\lambda=1$ we obtain

$$\langle S_0S_l\rangle=\int_0^1\mathrm{d}\lambda\,\beta J\sum_{|j|=1}(\langle S_0^2S_lS_j\rangle_\lambda-\langle S_0S_l\rangle_\lambda\langle S_0S_j\rangle_\lambda)$$

$$\leqslant\beta J\int_0^1\mathrm{d}\lambda\sum_{|j|=1}\langle S_lS_j\rangle_\lambda\leqslant\beta J\sum_{|j|=1}\langle S_lS_j\rangle \qquad (2)$$

where we have used Griffith I (II) in the 1st (2nd) inequality of (2). Iteration of (2) (see Simon 1980) and noticing that $\Sigma_{|j|=1}=\nu$ completes the proof.

Remark. Using Griffith's 3rd inequality, βJ can be replaced by $\tanh\beta J$ in (2) (see Simon 1980 and Brydges *et al* 1982).

We now recall Callen's identity (Callen 1963) and its proof for the two-point function.

Theorem 2. $\langle S_0S_l\rangle=\langle S_l\tanh(\beta J\,\Sigma_{|j|=1}S_j)\rangle$.

Remark. Callen's identity can be generalised to include magnetic fields and more general functions, i.e. can replace S_l by $f(\{S_i\})$ where $S_0\notin\{S_i\}$ and $E_i=-\Sigma_{|j|=1}JS_j$ by $E_i=-\Sigma_{|j|=1}JS_j+h$.

Proof. Carrying out the sum over S_0 in the numerator of $\langle S_0S_l\rangle$ we obtain

$$\langle S_0S_l\rangle=Z^{-1}\sum_{\{S_i\},i\neq 0}S_l\,2\sinh\Big(\beta J\sum_{|j|=1}S_j\Big)\exp\Big(\beta J\sum_{\substack{|m-n|=1\\ m,n\neq 0}}S_mS_n\Big)$$

$$=Z^{-1}\sum_{\{S_i\},i\neq 0}S_l2\sinh\Big(\beta J\sum_{|j|=1}S_j\Big)$$

$$\times\Big[\sum_{S_0}\exp\Big(\beta J\sum_{|a|=1}S_0S_a\Big)\Big/\sum_{S_0}\exp\Big(\beta J\sum_{|a|=1}S_0S_a\Big)\Big]\exp\Big(\beta J\sum_{m,n\neq 0}S_mS_n\Big)$$

$$=Z^{-1}\sum_{\{S_i\}}S_l\tanh\Big(\beta J\sum_{|j|=1}S_j\Big)\exp\Big(\beta J\sum_{m,n}S_mS_n\Big) \qquad (3)$$

where we have noted that

$$\Big[\sum_{S_0}\exp\Big(\beta J\sum_{|a|=1}S_0S_a\Big)\Big]=\Big[2\cosh\Big(\beta J\sum_{|a|=1}S_a\Big)\Big]$$

and that $S_l\,2\sinh(\beta J\,\Sigma_{|j|=1}S_j)$ is independent of S_0.

Specialising Callen's theorem to the case of a dimension $d=2, 3$ cubic lattice we obtain correlation function identities as

Theorem 3. (a) For $d=2$

$$\langle S_0 S_l\rangle = A \sum_i \langle S_i S_l\rangle + B \sum_{i<j<k} \langle S_i S_i S_j S_k\rangle \tag{4}$$

where

$$A = \tfrac{1}{8}[\tanh(4\beta J) + 2\tanh(2\beta J)]$$

$$B = \tfrac{1}{8}[\tanh(4\beta J) - 2\tanh(2\beta J)].$$

(b) For $d=3$

$$\langle S_0 S_l\rangle = A \sum_i \langle S_i S_l\rangle + B \sum_{i<j<k} \langle S_i S_j S_k S_l\rangle + C \sum_{i<j<k<m<n} \langle S_i S_j S_k S_m S_n S_l\rangle \tag{5}$$

where

$$A = (1/2^5)[\tanh(6\beta J) + 4\tanh(4\beta J) + 5\tanh(2\beta J)]$$

$$B = (1/2^5)[\tanh(6\beta J) - 3\tanh(2\beta J)]$$

$$C = (1/2^5)[\tanh(6\beta J) - 4\tanh(4\beta J) + 5\tanh(2\beta J)].$$

The sums over i, j, k, m, n are over the nearest neighbours of 0 to which we have given a numerical ordering.

Proof. Letting $E_0 = -\Sigma_{|j|=1} JS_j$, Callen's identity can be written as

$$\langle S_0 S_l\rangle = \langle S_l \exp(\beta E_0 \mathrm{D}) \tanh x|_{x=0}\rangle$$

where D is the differentiation operator d/dx or as

$$\langle S_0 S_l\rangle = \left\langle S_l \prod_{|j|=1} [\exp(\beta J S_j \mathrm{D})]\right\rangle \tanh x|_{x=0}.$$

Using $S_i^2 = 1$ we have

$$\langle S_0 S_l\rangle = \left\langle S_l \prod_{|j|=1} [\cosh(\beta J \mathrm{D}) + S_j \sinh(\beta J \mathrm{D})]\right\rangle \tanh x|_{x=0}.$$

Carrying out the indicated differentiation and after some elementary algebra we arrive at the equalities (4) and (5).

Remark 1. Equations (4) and (5) can also be obtained from (3) directly using the definition of the random variable $\tanh(\beta J \Sigma_{|j|=1} S_j)$ and inserting projections over configurations, i.e. if all $S_j = 1$ then insert $\Pi_{|j|=1} \frac{1}{2}(1+S_j)$, etc.

Remark 2. Of course, equalities of this type hold in any dimension, for $J \leq 0$ or complex J and for discrete spin systems.

From equations (4) and (5) we now obtain an inequality of the form

$$\langle S_0 S_l\rangle \leq \sum_{|j|=1} a_j \langle S_l S_j\rangle$$

where a_j is a sum of products of two-point functions.

Using Griffiths II on the second term of (4), i.e., $\langle S_lS_iS_jS_k\rangle \geq \langle S_lS_i\rangle\langle S_jS_k\rangle$, and noticing that B is negative, we get for $d=2$

$$\langle S_0S_l\rangle \leq A \sum_{|i|=1} \langle S_lS_i\rangle - |B|(\langle S_lS_1\rangle\langle S_2S_3\rangle + \langle S_lS_1\rangle\langle S_2S_4\rangle + \langle S_lS_1\rangle\langle S_3S_4\rangle + \langle S_lS_2\rangle\langle S_3S_4\rangle).$$

Using Griffiths II on the second term of (5) ($B<0$) and Newman's inequality ($\langle S_iF\rangle \leq \Sigma_j \langle S_iS_j\rangle\langle \partial F/\partial S_j\rangle$, F are polynomials with positive coefficients) on the third term of (5), we get

$$\langle S_iS_jS_kS_mS_nS_l\rangle$$
$$\leq \langle S_lS_i\rangle\langle S_jS_kS_mS_n\rangle + \langle S_lS_j\rangle\langle S_iS_kS_mS_n\rangle + \langle S_lS_j\rangle\langle S_iS_jS_mS_n\rangle$$
$$+ \langle S_lS_m\rangle\langle S_iS_jS_kS_n\rangle + \langle S_lS_n\rangle\langle S_iS_jS_kS_m\rangle$$

and by Griffiths I ($\langle S_A\rangle \leq 1$),

$$\langle S_iS_jS_kS_mS_n\rangle \leq \langle S_lS_i\rangle + \langle S_lS_j\rangle + \langle S_lS_k\rangle + \langle S_lS_m\rangle + \langle S_lS_n\rangle.$$

Therefore we get for (5)

$$\langle S_0S_l\rangle \leq A \sum_{|i|=1} \langle S_iS_l\rangle - |B|(10\langle S_lS_6\rangle\langle S_jS_k\rangle + 6\langle S_lS_5\rangle\langle S_jS_k\rangle$$
$$+ 3\langle S_lS_4\rangle\langle S_jS_k\rangle + \langle S_lS_3\rangle\langle S_jS_k\rangle) + C5 \sum_{|i|=1} S_lS_i.$$

By bounding the resulting two-point function occurring in the previous results from below with the two-point function of a one-dimensional infinite chain (which follows from Griffiths II), we arrive at

$$\langle S_0S_l\rangle \leq \sum_{|j|\neq 1} \bar{a}_j\langle S_lS_j\rangle$$

where,

$$\text{for } d=2: \quad \bar{a}_j = A - |B|\langle S_jS_k\rangle_{1D}$$
$$\text{for } d=3: \quad \bar{a}_j = A - |B|\langle S_jS_k\rangle_{1D} + 5C$$

where $\langle S_jS_k\rangle_{1D} = \tanh^2\beta J$ is the lower bound with $|j|=|k|=1$, $j\neq k$. Evaluating numerically the value of T such that $\Sigma_{|j|=1}\bar{a}_j \leq 1$, $\bar{a}_j>0$, we obtain, by the sufficient condition (1), the following upper bounds for T_c.

Theorem 4. (a) $d=2$; $kT_c/J \leq 3.013\,99$, $d=3$; $kT_c/J \leq 5.423\,15$.

We make some concluding remarks.

(i) The identities (4)–(5) are lattice analogues of the formal equations of motion satisfied by the two-point Euclidean vacuum expectation of a limiting (Ising limit) φ^4 quantum field theory, i.e.

$$(\Delta_x^{\mathrm{E}} + m^2)(\Omega, \varphi(l)\varphi(x)\Omega) = (\Omega, \varphi(l)(\mathrm{d}\varphi^4/\mathrm{d}\varphi)(x)\Omega).$$

For $d=2$ the scaling limit exists and defines a Wightman field theory (Schor and O'Carroll 1982); it would be interesting to investigate the scaling limit of (4). The scaling limit equality is not to be confused with the non-linear partial differential equation obeyed by the scaling limit two-point function as obtained by Jimbo *et al* (1980). For $d>4$ possibly these equalities can be useful in making triviality statements about field theories and/or mean-field statements about critical exponents (see Aizenman 1981 and Frohlich 1982).

(ii) In ordinary quantum mechanics, the imaginary time equation of motion is well defined, for example in one dimension we have

$$m(\mathrm{d}^2/\mathrm{d}s^2)(\psi_0, x \exp(-H_s)x\psi_0) = (\psi_0, V'(x) \exp(-H_s)x\psi_0)$$

where $H = p^2/2m + V(x) - E_0$ is the Hamiltonian and ψ_0 is its ground state eigenfunction with eigenvalue E_0. Such relations could possibly be exploited to analyse the spectrum of H.

(iii) Equalities for '+boundary' conditions which involve the magnetisation are obtained from (4) and (5) taking $S_l = 1$. Note that the coefficients on the right-hand side are the same. The temperature where the magnetisation vanishes as determined from those inequalities is the same as given by theorem 4.

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