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The Oguchi Upper Bound on the Magnetization for Ferromagnetic Ising Models

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The Oguchi approximation is shown to give an upper bound on the magnetization for spin-1/2 Ising models with arbitrary ferromagnetic pair couplings. The resulting bound on the critical temperature is shown to better than the mean field bound. For ferromagnetic spin-1/2 models where the three-body approximation predicts a unique magnetization, this too is shown to give a magnetization bound and an even better bound on the critical temperature.

1. INTRODUCTION

Mean field theory gives a good first approximation of the behavior of general ferromagnetic spin models. Griffiths[1] first noticed that for spin-1/2 ferromagnets one could show that the mean field critical temperature was more than an approximation; it gives a rigorous upper bound to the true critical temperature. Using the Dobrushin uniqueness theorem Cassandro *et al.*[2] were able to extend this result to a large class of one-component models. Subsequently Driessler *et al.*[3] and Simon[4] have shown that this bound also holds for multicomponent, Heisenberg-like spin models. Attention was also brought to the mean field magnetization by other researchers. For the spin-1/2 model, Thompson[5] proved that the mean field magnetization was an upper bound to the true magnetization. This result has recently been extended to one-component and multicomponent models by Pearce,[6] Newman,[7] Slawny,[8] and Tasaki and Hara.[9] We note that this automatically implies the related temperature bound.

Extensions of mean field theory, such as the Oguchi[14] and Bethe[15] approximations, are higher-order approximations which one believes give

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better descriptions of the spin models. As mean field theory may be considered a one-body approximation, so the Oguchi method corresponds to a two-body approximation. In this paper we will show that the Oguchi method also gives an upper bound on the magnetization and a bound on the critical temperature of general ferromagnetic spin-1/2 models. For those models where the three-body approximation predicts a unique magnetization, we will show that it too gives a bound on the magnetization and an even better bound on the critical temperature of general ferromagnetic spin-1/2 models.

The proof is a modification of Pearce's proof of the mean field bound. The magnetization bound for the infinite lattice spin system is reduced to an algebraic inequality. This inequality is proven by induction and some facts about spin-1/2 systems. Once one has the magnetization bounds, the results on transition temperatures follow from working with explicit functions.

For spin-1/2 models these are the strongest results to date for general ferromagnetic coupling. For nearest-neighbor models, stronger results exist for the magnetization bound (Krinsky[10]) and the transition temperature bound (Krinsky[10]; Fisher[11]).

2. THE MODELS

Let Λ be a finite lattice with periodic boundary conditions. We assume Λ can be written as a disjoint union of identical smaller lattices X_α, i.e., $\Lambda = \bigcup_\alpha X_\alpha$. At each site i in Λ there is a spin-1/2 Ising variable s taking values in $\Omega = \{-1, 1\}$. The Hamiltonian is defined by

$$\mathscr{H} = -\frac{1}{2} \sum_{i,j \in \Lambda} J_{ij} s_i s_j - h \sum_{i \in \Lambda} s_i$$

where $J_{ij} \geqslant 0$ and $h \geqslant 0$ are ferromagnetic couplings and $J_{ij} = J(|i-j|)$ is translation invariant. We write $J_i(X) = \sum_{j \in \Lambda \setminus X} J_{ij}$ for any fixed $X \varepsilon \{X_\alpha\}$, and use the convention that $J_{ii} = 0$. We assume $J_i(X) < \infty$ for any X. For the Oguchi approximation $J_i(X)$ is independent of i but for the three-body case there usually is i dependence. The spin space for the lattice is $[s] = \otimes_{i \in \Lambda} \Omega_i$; we use normalized counting measures, and expectations are defined as

$$\langle f \rangle_{\Lambda, \mathscr{H}} = \left(\sum_{[s]} f e^{-\beta \mathscr{H}} \right) \Big/ \left(\sum_{[s]} e^{-\beta \mathscr{H}} \right)$$

where $\beta = 1/kT$ is the inverse temperature. Until Section 5 we absorb β into the couplings J_{ij} and h. The magnetization of the model is

$$\langle s_i \rangle = \lim_{|\Lambda| \to \infty} \langle s_i \rangle_\Lambda$$

and the spontaneous magnetization is $\lim_{h\downarrow 0}\langle s_i\rangle$, both of which are independent of $i \in \Lambda$. By general results, in the limit as $|\Lambda| \to \infty$ this magnetization is the same as that obtained by plus-boundary conditions.

3. THE APPROXIMATIONS

One obstacle to solving the lattice model exactly is that the configuration sum with the Boltzmann factor is hard. Since each spin has one degree of freedom, in the thermodynamic limit, the sum has an infinite number of degrees of freedom. Mean field theory avoids this problem by making a self-consistent approximation. All spins save one are replaced by an effective average magnetization. The magnetization of this last spin is then calculated exactly in this effective field. Consistency is obtained by demanding that the calculated magnetization be equal to the assumed magnetization of the other spins. The number of degrees of freedom has been reduced to one and this new model is tractable. This is the basis for calling mean field theory a one-body approximation. Thus, the mean field approximation consists of using the region $X = \{s\}$ and the Hamiltonian

$$\mathscr{H}_1 = [-mJ_i(X) - h]s$$

to find the largest root m of the equation

$$m = \langle s \rangle_{X, \mathscr{H}_1}$$

For spin-1/2, this reduces to the familiar

$$m = \tanh\left(\sum_{j\in\Lambda} J_{ij} m\right) \tag{1}$$

The extensions to mean field theory considered here use the same basic self-consistency approach. However, now one has a privileged region X as opposed to a privileged spin, exterior to which all spins are replaced by their assumed effective average magnetization. The spins in the interior of X take values in Ω, their proper spin space. In general we call a method an n-body approximation if the number of spins in X is n. The Hamiltonian in use is then

$$\mathscr{H}_n = -\frac{1}{2}\sum_{i,j\in X} J_{ij} s_i s_j - \sum_{i\in X} [h + mJ_i(X)]\, s_i$$

and one imposes the consistency condition

$$m = \langle s \rangle_{X, \mathscr{H}_n}$$

The largest such m for a given set of J_{ij} and h is taken to be the magnetization of the simplified model.

For the Oguchi approximation, the region X is taken to be any set of two spins, although in practice one uses two nearest neighbors. One point to notice is that the magnetization predicted may *a priori* depend on which site in X one uses for this self-consistent procedure. Since the coupling $J_{ij} = J_{ji}$, it is easy to see that the expected magnetization of both spins in the region X will be the same, and so the Oguchi magnetization is unambiguous. If for some model the sites or couplings are chosen so that the predicted magnetization is site dependent, the proof of the Oguchi bound may be modified so that the Oguchi bound corresponds to the larger of the two predicted magnetizations. The Oguchi region is $X = \{s, t\}$, the coupling between spins s and t is J, and the Hamiltonian is

$$\mathscr{H}_2 = -Jst - [h + J_i(X)m](s + t) \tag{2}$$

For the three-body approximation, if the three sites are equivalent, say by symmetry, there is an unambiguous magnetization and this is an upper bound. If the three sites separately predict different magnetizations, the present proof breaks down and one does not have a bound. For the symmetric case, the three-body Hamiltonian in a region $X = \{s, t, u\}$ is

$$\mathscr{H}_{3,\text{sym}} = -J(st + tu + su) - [h + mJ_i(X)](s + t + u) \tag{3}$$

where J is again the pair coupling in the region X.

4. PROOF OF THE MAGNETIZATION BOUNDS

Theorem 1. If there is an m, m only a function of β, such that

$$\sum_{[s]} \left[e^{-\beta \mathscr{H}_n} \left(\prod_{s_i \in X} (m - s_i)^{p_i} \right) \right] \geqslant 0 \tag{4}$$

for all p_i integral and non-negative, then

$$\langle m - s \rangle_{\Lambda, \mathscr{H}} \geqslant 0$$

Proof. Following Pearce[6] we write

$$\mathscr{H} = \sum_{X_\alpha \in \Lambda} \mathscr{H}_n(X_\alpha) - \frac{1}{2} \sum{}' \, [J_{ij}(m - s_i)(m - s_j) - J_{ij} m^2]$$

In the second sum, $\sum'$, we sum over all pairs i and j where i and j lie in different X_α's. We have

$$\langle m - s \rangle_{\Lambda, \mathscr{H}} = Z^{-1} \left\langle (m - s) \exp \left[\sum{}' \frac{1}{2} J_{ij}(m - s_i)(m - s_j) \right] \right\rangle_{\Lambda, \Sigma_\alpha \mathscr{H}_n(X_\alpha)}$$

where

$$Z = \left\langle \exp\left[\sum{}' \frac{1}{2} J_{ij}(m - s_i)(m - s_j)\right]\right\rangle_{\Lambda, \sum_\alpha \mathscr{H}_n(X_\alpha)}$$

By expanding the exponential in a Taylor series, $\langle m - s\rangle_{\Lambda,\mathscr{H}}$ factors over regions X_α and by hypothesis each resulting expectation is non-negative. Therefore

$$m \geqslant \langle s\rangle_{\Lambda,\mathscr{H}} \tag{5}$$

For any given Λ, the best bound m is the minimum m such that Eq. (4) still holds; however, any greater value of m will still be a bound. Writing this Λ dependence out explicitly as m_Λ, we find that an examination of the specific form of m_Λ, say, e.g., Eq. (9) for the Oguchi approximation, shows that m_Λ is an increasing function of $|\Lambda|$. Since $m_\Lambda \leqslant 1$ for all Λ, $\lim_{|\Lambda| \to \infty} m_\Lambda = m$ exists. Then we know from Eq. (5) that $m \geqslant \langle s\rangle$ for the thermodynamic limit. This infinite volume m will be the desired upper bound.

We will show that the hypothesis (4) is true for spin-1/2 models by using the following lemma.

Lemma 1. If

$$\sum_{[s]} \mathrm{Ker}(m - s)^p\, s^a \sim (-)^a \qquad \text{and} \qquad 0 \leqslant m \leqslant 1$$

then

$$\sum_{[s]} \mathrm{Ker}(m - s)^{p+1}\, s^a \sim (-)^a$$

Here s is taken to be any s_i. Since s is spin 1/2, $a = 1$ or 0 exhausts all the possibilities. "$\sim$" is a shorthand for "has the sign of" and $(-)^a$ will mean nonnegative [also written $(+)$] or nonpositive, as $a = 0$ or 1, respectively. We are only interested in the sign of this sum since we only wish to show that the left-hand side of Eq. (4) $\sim (+)$. p will be any positive integer and Ker (short for Kernel) will be any function. Later we will take [k is nonnegative and typically equal to $h + mJ_i(X)$]

$$\mathrm{Ker} = \exp[Jst + k(s + t)]$$

and

$$\mathrm{Ker} = \{\exp[Jst + k(s + t)]\}(m - t)^q\, t^b$$

for the Oguchi model.

The idea behind the proof is to introduce a dummy sum. By coupling this dummy sum to the assumption, and letting the coupling go to infinity, one makes the $p \to p+1$ transition. We get information about the sign of the sum by examining the coupled system at arbitrary finite coupling. Since this sign will not depend on the magnitude of the coupling, we get the result for the infinite coupling limit. We note this idea is suggested by Griffiths.[12]

Proof. Let u be a dummy variable. For spin 1/2

$$\lim_{K \to \infty} \frac{e^{Ksu}}{(\sum_{x,y=\pm 1} 2e^{Kxy})} = \delta_{su}$$

so

$$\sum_{[s]} \text{Ker}(m-s)^{p+1} s^a = \lim_{K \to \infty} \frac{1}{(\sum_{x,y} 2e^{Kxy})} \sum_{[s],u} e^{Ksu} \,\text{Ker}(m-s)^p s^a (m-u) \quad (6)$$

For any fixed K, using the identity

$$e^{Ksu} = \cosh K + su \sinh K$$

the right-hand side (RHS) of Eq. (6) is

$$\text{RHS} \sim (\cosh K) \left[\sum_{[s]} \text{Ker}(m-s)^p s^a\right]\left[\sum_u (m-u)\right]$$
$$+ (\sinh K) \left[\sum_{[s]} \text{Ker}(m-s)^p s^{a+1}\right]\left[\sum_u (m-u)u\right]$$

We calculate two of the sums explicitly:

$$\sum_u (m-u) = m - \sum_u u = m \sim (+)$$

$$\sum_u (m-u)u = m \sum_u u - 1 = -1 \sim (-)$$

Therefore, using the induction hypothesis, we can write

$$\text{RHS of Eq. (5)} \sim (+)(-)^a(+) + (+)(-)^{a+1}(-)$$
$$\sim (-)^a$$

Since this holds for any K positive, it also holds in the limit and we have

$$\sum_{[s]} \text{Ker}(m-s)^{p+1} s^a \sim (-)^a \quad \blacksquare$$

With these two results we are set to show the following.

Theorem 2. Equation (4) holds for the Oguchi Hamiltonian.

Proof. By the lemma, if

$$\sum e^{-\beta\mathscr{H}_2}(m-s)^p\, s^a \sim (-)^a \qquad \text{for} \quad p=1 \tag{7}$$

and

$$\sum e^{-\beta\mathscr{H}_2}(m-s)^p\, s^a (m-t)^q\, t^b \sim (-)^{a+b} \qquad \text{for} \quad p=q=1 \tag{8}$$

we know the above equations are true for all p, q positive. Equation (4) is just the case $a=b=0$ and we will have the needed non-negativity.

Up till now we have not specified the value of m; let us now define $m=m_{\text{Oguchi}}$ where m_{Oguchi} is the largest m such that the left-hand side of Eq. (7) is identically zero for $p=1$, $a=0$. Explicitly,

$$m=\left(\sum_{[s]} se^{-\beta\mathscr{H}_2}\right)\Big/\left(\sum_{[s]} e^{-\beta\mathscr{H}_2}\right) \tag{9}$$

That takes care of the case $a=0$ for Eq. (7). For $a=1$, we notice $s(m-s)\leqslant 0$ for both $s=\pm 1$ and so the sum must be nonpositive, which is what was needed.

Now Eq. (8) may be written, using Eq. (2) for the Hamiltonian,

$$\begin{aligned}\sum e^{-\beta\mathscr{H}_2}&(m-s)\, s^a(m-t)\, t^b \\ &=(\cosh J)\left[\sum_s e^{ks}(m-s)\, s^a\right]\left[\sum_t e^{kt}(m-t)\, t^b\right] \\ &\quad+(\sinh J)\left[\sum_s e^{ks}(m-s)\, s^{a+1}\right]\left[\sum_t e^{kt}(m-t)\, t^{b+1}\right]\end{aligned}$$

By the correlation inequality GKS II[16] we see that m defined by $\mathscr{H}_2=-Jst-k(s+t)$ is greater than m defined by $\mathscr{H}=-ks$, which tells us that $\sum e^{ks}(m-s)\geqslant 0$. The signs of the above terms are then

$$\begin{aligned}\sum e^{-\beta\mathscr{H}_2}(m-s)\, s^a(m-t)\, t^b &\sim (+)(-)^a(-)^b+(+)(-)^{a+1}(-)^{b+1} \\ &\sim (-)^{a+b}\end{aligned}$$

as needed. ∎

Theorem 3 (three-body case). If $X=\{s,t,u\}$ and there is a Hamiltonian $\mathscr{H}_3$ on X such that $\langle s\rangle=\langle t\rangle=\langle u\rangle=m$, then Eq. (4) holds.

Proof. The three cases to consider are

$$\text{(i)}\quad \sum_{[s]} e^{-\beta\mathscr{H}_3}(m-s_i)\, s_i^a \sim (-)^a \qquad \forall i\in X$$

$$\text{(ii)}\quad \sum_{[s]} e^{-\beta\mathscr{H}_3}(m-s_i)\, s_i^a(m-s_j)\, s_j^b \sim (-)^{a+b} \qquad \forall i,j\in X,\ i\neq j$$

$$\text{(iii)}\quad \sum_{[s]} e^{-\beta\mathscr{H}_3}(m-s)\, s^a(m-t)\, t^b(m-u)\, u^c \sim (-)^{a+b+c}$$

where again Lemma 1 brings us to Eq. (4). As before, define $m = m_{3\text{-body}}$ where $m_{3\text{-body}}$ is the largest m such that the left-hand side of (i) is identically zero for $a = 0$, and then (i) is satisfied. Case (iii) can be shown by rewriting the coupling terms in the Boltzmann factor as cosh and sinh as done in Theorem 2. We demonstrate Case (ii) by using GKS II, which says

$$\langle s\rangle\langle t\rangle - \langle st\rangle \leqslant 0$$

Let y be a dummy variable. The left-hand side (LHS) of Case (ii) is

$$\text{LHS}(a=0, b=0 \text{ or } 1) = \lim_{K\to\infty} \sum_{[s],y} \frac{e^{Kty}}{(\sum 2e^{Kxz})} e^{-\beta\mathscr{H}_3}(m-s)\, t(m-y)\, y^b$$

Fix K. The RHS may be written as

$$\begin{aligned}\text{RHS} &\sim (\cosh K)\left[\sum_{[s]} e^{-\beta\mathscr{H}_3}(m-s)t\right]\left[\sum_{y}(m-y)\, y^b\right] \\ &\quad + (\sinh K)\left[\sum_{[s]} e^{-\beta\mathscr{H}_3}(m-s)\right]\left[\sum_{y}(m-y)\, y^{b+1}\right] \\ &\sim (+)(-)(-)^b + (+)(+)(-)^{b+1} \\ &\sim (-)^{b+1}\end{aligned}$$

as needed. The case $(a=1,\ b=0)$ may similarly be shown. Since $s(m-s)\leqslant 0$, $s(m-s)\, t(m-t)\geqslant 0$, which takes care of the case $a=b=1$. This exhausts the possibilities and Case (ii) is shown. ■

5. PROOF OF THE CRITICAL TEMPERATURE BOUNDS

The magnetizations predicted by the Oguchi and three-body Hamiltonians have been shown to be upper bounds on the magnetization of the true Hamiltonian. We expect these magnetization bounds to be a decreasing series as the number of spins in X is increased. To get a quantitative feel for these bounds, we now examine the critical temperatures predicted by these two methods. In this section we will explicitly show the β-dependence.

Theorem 4. Given a Hamiltonian $\mathscr{H}$ we have

$$T_c(\text{true}) \leqslant T_c(\text{symmetric three-body}) \leqslant T_c(\text{Oguchi}) \leqslant T_c(\text{mean field})$$

We recall that the critical temperatures of the approximation schemes are obtained as the solution to

$$\left.\frac{\partial \langle s \rangle_{\Lambda, \mathscr{H}}}{\partial m}\right|_{m=0} = 1$$

Using the explicit equation obeyed by the magnetization for the mean field approximation, Eq. (1), the mean field critical temperature is determined by

$$\beta_{\text{MF}} \sum_j J_{ij} = 1 \tag{10}$$

The corresponding equation for the Oguchi case is ($\beta_0 \equiv \beta_{\text{Oguchi}}$)

$$\beta_0 \left(\sum_j J_{ij} - J \right) (1 + \tanh J\beta_0) = 1 \tag{11}$$

and the symmetric three-body case gives

$$\beta_3 \left(\sum_j J_{ij} - 2J \right) \left[1 + 2 \left(\frac{\tanh J\beta_3 + \tanh^2 J\beta_3}{\tanh^3 J\beta_3 + 1} \right) \right] = 1$$

We remark that examination of the proofs below show that equality is obtained only for the pair coupling $J = 0$ and that otherwise one has strictly better bounds.

Proof. Clearly all the critical temperatures are upper bounds to the true transition temperature. We show that

$$\sum_j (\beta_{C,\text{MF}} - \beta_{C,\text{Oguchi}}) J_{ij} \leqslant 0$$

which implies that $T_{C,\text{Oguchi}} \leqslant T_{C,\text{MF}}$. As we are now working only with critical temperatures, henceforth we drop the subscript c. By Eqs. (10) and (11), we have

$$\sum_j J_{ij}(\beta_{\text{MF}} - \beta_0) = 1 - \left(\frac{1}{1 + \tanh \beta_0 J} + \beta_0 J \right)$$

Examine the RHS. Let $x = \beta_0 J$ and note that x is non-negative. When $x = 0$, the RHS $= 0$. Now

$$\frac{\partial}{\partial x}(\text{RHS}) = \frac{1}{(1+\tanh x)^2} \cdot \frac{1}{\cosh^2 x} - 1$$

Since this is negative for all positive x, we see that the RHS is nonpositive, as needed.

To show $\beta_3 \geqslant \beta_0$, we note that if

$$g(x) = \left(\sum_j J_{ij} x - 2Jx\right)\left[1 + 2\,\frac{(\tanh Jx + \tanh^2 Jx)}{\tanh^3 Jx + 1}\right]$$

then $g(x)$ is an increasing function of positive x. We will show that $g(\beta_0) \leqslant 1$. Since $g(\beta_3) = 1$, this implies that $\beta_3 \geqslant \beta_0$. If $y = \beta_0 J$ and $T = \tanh y$, clearly

$$y \geqslant \frac{T}{1+T} \geqslant \frac{T}{(1+T)}\,\frac{(1+T-T^2)}{(1+T+T^2)}$$

Then

$$\frac{1}{1+T} - y \leqslant \frac{1}{1 + 2\left[\dfrac{T(T+1)}{T^3+1}\right]}$$

But

$$\frac{1}{1+T} = \sum_j J_{ij}\beta_0 - 2J\beta_0$$

by Eq. (11) so we have shown $g(\beta_0) \leqslant 1$. ■

We present some sample calculational results obtained with these methods. The values for $T_{C,\text{MF}}$ and $T_{C,0}$ are obtained from Eqs. (10) and (11). We remark that while each of the three spins in the three-body model is predicting zero magnetization, this is a bound on the magnetization. Thus we can obtain an upper bound on T_C, call it $T_{C,3}$, corresponding to $\max_{s \in X} T_{C,3}(s)$. This is what is listed under T_C 3-body. For nearest-neighbor models better magnetization and T_C bounds than our bounds may be obtained by different methods. For instance, the T_C bound for the three-dimensional nearest-neighbor model obtained by Fisher's self-avoiding walk method[11] is much better than our best bound, the $T_{C,3}$ bound (see model A). However, we emphasize that our method is not restricted to

Table I. Critical Temperature Bounds

Model[a]	Mean field	Oguchi	Three-body	Best known
A	6	5.847	5.825	4.796[b]
B	3.290	3.021	2.897	—[c]

[a] The models are: A = three-dimensional (3-D) nearest-neighbor cubic lattice; B = 1-D $J_{ij} = |i-j|^{-2}$ model.
[b] Fisher.[11] Best guess is $T_C \approx 4.684$, Domb.[17]
[c] Best guess is $T_C \approx 1.58$, Bhattacharjee *et al.*[13]

nearest-neighbor models. For these non-nearest-neighbor models our method gives new and better magnetization and T_C bounds. As an example, we calculate the T_C bounds for the one-dimensional $1/r^2$ model (see model B).

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