Commun. math. Phys. 6, 121—127 (1967)

Correlations in Ising Ferromagnets. III

A Mean-Field Bound for Binary Correlations*

ROBERT B. GRIFFITHS**

Physics Department, Carnegie Institute of Technology, Pittsburgh, Pennsylvania 15213

Received May 15, 1967

Abstract. An inequality relating binary correlation functions for an Ising model with purely ferromagnetic interactions is derived by elementary arguments and used to show that such a ferromagnet cannot exhibit a spontaneous magnetization at temperatures above the mean-field approximation to the Curie or "critical" point. (As a consequence, the corresponding "lattice gas" cannot undergo a first order phase transition in density (condensation) above this temperature.) The mean-field susceptibility in zero magnetic field at high temperatures is shown to be an upper bound for the exact result.

I. Introduction

Many years ago PEIERLS [1] gave a simple argument for the existence of spontaneous magnetization in an Ising ferromagnet at sufficiently low temperatures. More recently this argument has been turned into a rigorous proof [2, 3], and generalized to include interactions other than the nearest-neighbor ferromagnetic coupling originally considered [4].

The existence of a spontaneous magnetization in the "thermodynamic" sense [5] for an Ising ferromagnet implies a horizontal portion of the pressure-density isotherm in the corresponding "lattice gas" [6]. Thus for this somewhat artificial model, the Peierls argument provides an elementary proof that a first order phase transition, or "condensation", takes place at sufficiently low temperatures.

We shall discuss a complementary problem: a proof of the *absence* of spontaneous magnetization (or first-order phase transition for the analogous lattice gas) at a sufficiently *high* temperature. So far as we know, such a proof has not been given previously for any Ising model with interactions of finite range, apart from linear chains [7]. (It is of interest to note that a proof of the absence of spontaneous magnetization for certain systems with a Heisenberg exchange interaction has recently appeared [8].) It is true that for the Ising ferromagnet on a square lattice,

* Research supported in part by the National Science Foundation.
** ALFRED P. SLOAN research fellow.

YANG [9] has calculated a spontaneous magnetization which vanishes at the temperature where the zero-field free energy has a singularity [10]. However, there is as yet no proof that Yang's value is identical with the thermodynamic result [11], though we may be sure that the former is a lower bound for the latter [5].

By an elementary argument we shall derive an inequality for binary correlation functions in an Ising ferromagnet, and from this deduce an upper bound on the Curie or "critical" temperature, defined as the temperature at which the spontaneous magnetization vanishes. Our bound is essentially the mean-field estimate for the Curie temperature. We also obtain an upper bound for the magnetization μ as a function of magnetic field H, for $H \geqq 0$, above this temperature.

The procedures we employ are analogous to those used in two previous papers on inequalities in Ising ferromagnets [12, 13; hereafter referred to as CIFI and CIFII, respectively]. S. SHERMAN and D. G. KELLY [17] have generalized the arguments in CIFI and CIFII; SHERMAN has also generalized our basic inequality (5) below. M. E. FISHER [16] has independently obtained upper bounds on the Curie temperature by a different technique. He obtains not only mean-field bounds, but also additional upper bounds which lie at even lower temperatures, and are thus more useful in estimating the actual Curie point.

An interesting question as yet unanswered is the following: LEE and YANG [6, 14] have shown that for an Ising ferromagnet and at any temperature, $\mu(H)$ in the thermodynamic limit of an infinite system is analytic for $H > 0$ and $H < 0$ [actually, in the two half-planes Real $(H) > 0$ or < 0]. It is tempting to suppose that μ is also analytic at $H = 0$ when the temperature is sufficiently high. Our argument demonstrates continuity at $H = 0$ for real H at sufficiently high temperatures, but a proof of analyticity (or a counter example) will require more sophisticated techniques.

II. Inequality for Binary Correlation Functions

Let $\mathscr{H}$ be the Hamiltonian for a system of N Ising spins, $\sigma_i = \pm 1$

$$\mathscr{H} = - \sum_{i<j} J_{ij}(\sigma_i \sigma_j - 1) \tag{1}$$

where the interaction is assumed to be ferromagnetic:

$$J_{ij} = J_{ji} \geqq 0; \quad J_{ii} = 0 . \tag{2}$$

Angular brackets denote a thermal average at a temperature $T = (k\beta)^{-1}$:

$$\langle \mathscr{O} \rangle = Z^{-1} \operatorname{Tr}[\mathscr{O} e^{-\beta \mathscr{H}}] , \tag{3}$$

where Z is the partition function:

$$Z = \operatorname{Tr}[e^{-\beta \mathscr{H}}] . \tag{4}$$

Here Tr denotes a trace or a sum over all 2^N configurations [a configuration is an assignment of specific values to each of the σ_i] of the system.

Theorem 6[1]. If σ_p and σ_q are two distinct spins (i.e., $p \neq q$) in the system described by (1) and (2), the following inequality holds:

$$\langle \sigma_p \sigma_q \rangle \leqq \sum_{m(\neq p)} \langle \sigma_m \sigma_q \rangle \tanh \beta J_{pm} \tag{5}$$

or

$$\langle \sigma_p \sigma_q \rangle \leqq \tanh \beta J_{pq} + \sum_{m(\neq p,q)} \langle \sigma_m \, \sigma_q \rangle \tanh \beta J_{pm} \,. \tag{6}$$

One obtains (6) from (5) by removing the term $m = q$ from the summation and noting that $\langle \sigma_q^2 \rangle = \sigma_q^2 = 1$.

Proof of Theorem 6. Our diagrammatic and notational conventions coincide with CIFI and CIFII. A diagram representing the Hamiltonian (1) or associated partition function consists of small circles, representing spins, and lines or bonds connecting pairs of spins k and l if J_{kl} in (1) is not zero. A factor

$$X_{kl} = \exp(-2\beta J_{kl}) \tag{7}$$

associated with this bond always lies between 0 and 1, by condition (2).

Setting X_{kl} equal to zero (equivalent to $J_{kl} \to \infty$) serves to "combine" spins k and l. That is, if a single spin k' replaces k and l in a new diagram, the "reduced diagram", and one lets

$$X_{k'm} = X_{km} X_{lm} \tag{8}$$

for all m, the new partition function (a polynomial in the X_{ij}) and correlation functions (Z^{-1} times a polynomial in the X_{ij}) are precisely those obtained by setting $X_{kl} = 0$ in their respective predecessors. Further, if all bonds in the original diagram are ferromagnetic [(2) is satisfied], the same is true for the reduced diagram.

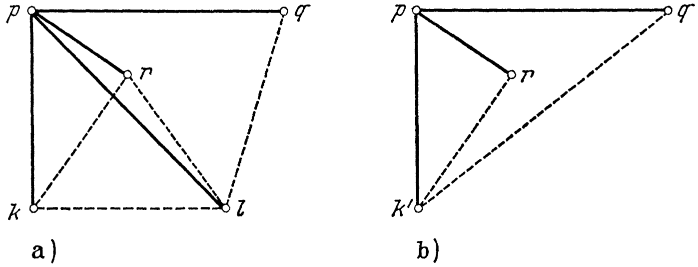

Fig. 1. a The solid lines denote primary bonds and the dotted lines some of the possible secondary bonds. b The reduced diagram obtained from (a) by setting $X_{kl} = 0$.

[1] The numbering is consecutive with that in CIFI, CIFII.

In connection with (5) it is useful to distinguish the bonds which connect p to some other spin, which we term "primary bonds", from all the remaining "secondary bonds" (Fig. 1). Consider the special case where there are no secondary bonds (i.e., the corresponding J_{kl} are zero). An elementary computation yields:

$$\langle \sigma_p \sigma_q \rangle = \tanh \beta J_{pq} \tag{9}$$

and, since the remaining terms on the right side of (6) are non-negative [every $\langle \sigma_k \sigma_l \rangle$ is non-negative in an Ising ferromagnet by theorem 1 of CIFI], the inequality (6) is clearly satisfied.

The proof of (5) is equivalent to showing that

$$W = \sum_{m(\neq p)} [Z \langle \sigma_m \sigma_q \rangle] \tanh \beta J_{pm} - [Z \langle \sigma_p \sigma_q \rangle] \tag{10}$$

is non-negative. Now $Z\langle \sigma_m \sigma_q \rangle$ is a polynomial in the X_{ij} and a linear function of any particular X_{kl}. Hence W is a linear function of the factor associated with any *secondary* bond [due to the appearance of $\tanh \beta J_{pm}$ it is *not* a linear function of a primary-bond factor].

Suppose the factor X_{kl} for a particular secondary bond is set equal to zero. Let W_0 represent the value of W in (10) when X_{kl} is everywhere replaced by zero, and let W_1 represent (10) for the corresponding reduced diagram in which the spins k and l are combined to form a single spin k' (Fig. 1), with $X_{k'm}$ defined by (8).

When X_{kl} is zero, the correlations $\langle \sigma_k \sigma_q \rangle$ and $\langle \sigma_{l,e} \sigma_q \rangle$ are equal to $\langle \sigma_{k'} \sigma_q \rangle$; however, W_0 differs from W_1 in that the sum over m for the former includes one more term than the latter. The difference is

$$W_0 - W_1 = Z \langle \sigma_{k'} \sigma_q \rangle [\tanh \beta J_{pk} + \tanh \beta J_{pl} - \tanh \beta (J_{pk} + J_{pl})]. \tag{11}$$

For J's satisfying (2), the quantity in square brackets is never negative. Also, by CIFI, $\langle \sigma_{k'} \sigma_q \rangle \geqq 0$. Thus W will be non-negative in the limit $X_{kl} = 0$ provided W for the corresponding reduced diagram (which contains one less spin) is non-negative.

We shall now prove theorem 6 by induction. Suppose it is true for any system of $N - 1$ spins and for any system having N spins and at most n secondary bonds. We shall show that it holds for N spins and $n + 1$ secondary bonds. Assume the $n + 1$st bond joins spins k and l. As W is linear in X_{kl}, we can prove it is non-negative by showing this is the case for $X_{kl} = 0$ and $X_{kl} = 1$. In the latter instance, the bond kl is erased and we have n secondary bonds for which W is non-negative by hypothesis. In the former instance W is non-negative because (see preceding paragraph) this is true by our hypothesis for the corresponding reduced diagram containing $N - 1$ spins. As we have previously established (5) for $n = 0$ and N arbitrary (note that for $N = 2$, the only possibility is $n = 0$), the proof of theorem 6 is complete.

III. Upper bound for the Curie Temperature

The Hamiltonian

$$\mathscr{H} = -\sum_{1 \leqq i < j}\sum J_{ij}\sigma_i\sigma_j - H\sum_i \sigma_i \tag{12}$$

for an Ising system of N spins in a magnetic field $H \geqq 0$ may be written in the form[2]

$$\mathscr{H} = -\sum_{0 \leqq i < j}\sum J_{ij}\sigma_i\sigma_j \tag{13}$$

provided one defines

$$J_{oj} = J_{jo} = H \geqq 0 \tag{14}$$

for all $j \geqq 1$, and requires in addition that σ_0, the "ghost spin", always have the value $+1$. Let $\langle\ \rangle_0$ denote an average with the restriction $\sigma_0 = +1$ [only configurations satisfying these restrictions are used in (3) and (4)], whereas $\langle\ \rangle$ denotes the unrestricted average in which σ_0 may be $+1$ or -1.

The equality

$$\langle\sigma_k\rangle_0 = \langle\sigma_k\sigma_0\rangle \tag{15}$$

is easily verified by writing out the right hand side in terms of sums over configurations for which $\sigma_0 = +1$ and $\sigma_0 = -1$, and noting that (13) is unchanged if every σ_i is replaced by $-\sigma_i$.

The average magnetization per spin, μ_N, is equal to

$$\mu_N(H, T) = N^{-1}\sum_k{}' \langle\sigma_k\rangle_0 = N^{-1}\sum_k{}' \langle\sigma_k\sigma_0\rangle \tag{16}$$

where a prime on the summation indicates the omission of $k = 0$. The bulk magnetization $\mu(H, T)$ is the limit of $\mu_N(H, T)$ in the "thermodynamic" or $N \to \infty$ limit; one must, of course, place some restrictions on the sequence of systems by which the limit is achieved (for example, a series of cubes) and on the form of the exchange interaction J_{ij} [15]. When speaking of "$N \to \infty$" we shall assume these restrictions are satisfied. A theorem of Lee and Yang [6] states that if (2) is satisfied (all interactions ferromagnetic), μ is an analytic function of H at fixed T for $H > 0$. At $H = 0$ μ (which is an odd function of H) may be continuous, or it may possess a jump discontinuity or "spontaneous magnetization" which we define [5] as

$$\mu_o(T) = \lim_{H \to 0+} \mu(H, T)\,. \tag{17}$$

The "Curie temperature" T_c is the temperature where $\mu_0(T)$ goes to zero [μ_0 is monotone non-increasing in T if (2) is satisfied — see CIFII]; more precisely, the least upper bound of all the temperatures for which μ_0 is greater than zero.

Setting $q = 0$ in (6) and using the definitions (14) and (16), one obtains

$$\mu_N \leqq \tanh \beta H + N^{-1} \sum_{p \neq m}' \sum' \langle \sigma_m \sigma_0 \rangle \tanh \beta J_{pm} \leqq \tag{18}$$
$$\leqq \tanh \beta H + G(\beta)\, \mu_N$$

where

$$G(\beta) = \max_m \Big(\sum_{p(\neq m)}' \tanh \beta J_{pm} \Big) . \tag{19}$$

Consider the particular case where J_{ij} is equal to J if spins i and j are nearest neighbors on a regular lattice, and 0 otherwise. If each spin has z nearest neighbors, G is equal to

$$G(\beta) = z \tanh \beta J . \tag{20}$$

Provided the temperature T exceeds T_m defined by

$$z \tanh (J/k T_m) = 1 , \tag{21}$$

G is less than 1, and (18) may be rewritten as

$$\mu_N (H, T) \leqq \frac{\tanh (H/kT)}{1 - z \tanh (J/kT)} \tag{22}$$

with, of course, $H \geqq 0$. The right side of (22), since it is independent of N, is also an upper bound for the bulk magnetization. Thus for $T > T_m$, $\mu_0(T)$ vanishes[3] and we conclude that

$$T_c \leqq T_m . \tag{23}$$

The usual "mean-field" Curie temperature T_M defined by

$$zJ/k T_M = 1 \tag{24}$$

is slightly larger than T_m, though the difference is only 2% for $z = 4$ and decreases as z increases.

Note that (22) also provides a bound on the zero field susceptibility

$$\chi_0 = (\partial \mu_N / \partial H)_{T, H=0} \leqq [kT(1 - \tanh J/kT)]^{-1} \tag{25}$$

provided T is greater than T_m. This bound also holds in the $N \to \infty$ limit provided the limiting function μ actually possesses a derivative at $H = 0$.

References

1. PEIERLS, R.: Proc. Cambridge Phil. Soc. **32**, 477 (1936).
2. GRIFFITHS, R. B.: Phys. Rev. **136**, A437 (1964).
3. DOBRUSHIN, R. L.: Teoriya Veroyatnostei i ee Primeneniya **10**, 209 (1965). [English translation: Theory of Probability and its Applications **10**, 193 (1965)].

[2] Equation (13) differs from (1) by an additive constant which does not, of course, affect the correlation functions and the validity of theorem 6.

[3] For $H \geqq 0$, $\mu_N(H, T)$ is non-negative since the binary correlations in (16) are all non-negative [CIFI], and thus $\mu(H, T)$ is also non-negative. The non-negativity also follows from the convexity of the free energy, [15].

4. Ginibre, J., A. Grossman, and D. Ruelle: Commun. Math. Phys. **3**, 187 (1966).
5. Griffiths, R. B.: Phys. Rev. **152**, 240 (1966).
6. Lee, T. D., and C. N. Yang: Phys. Rev. **87**, 410 (1952).
7. Baur, M. E., and L. H. Nosanow: J. Chem. Phys. **37**, 153 (1962).
8. Mermin, N. D., and H. Wagner: Phys. Rev. Letters **17**, 1133, 1307 (1966).
9. Yang, C. N.: Phys. Rev. **85**, 808 (1952).
10. Onsager, L.: Phys. Rev. **65**, 117 (1944).
11. Schultz, T. D., D. C. Mattis, and E. H. Lieb: Rev. Mod. Phys. **36**, 856 (1964).
12. Griffiths, R. B.: J. Math. Phys. 8, 478 (1967).
13. — J. Math. Phys. 8, 484 (1967).
14. Yang, C. N., and T. D. Lee: Phys. Rev. **87**, 404 (1952).
15. Griffiths, R. B.: Math. Phys. **5**, 1215 (1964).
16. Fisher, M. E.: Phys. Rev. (to be published).
17. Kelly, D. G., and S. Sherman (to be published).