

Coexistence of Phases in Ising Ferromagnets

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Received December 7, 1976

We derive a new inequality for ferromagnetic Ising spin systems and then use it to obtain information about the number of phases which can coexist in such systems. We show in particular that for even interactions only two phases (up and down magnetization) can coexist below the critical temperature at zero magnetic field ($h = 0$) whenever the energy is a continuous function of the temperature. We also prove that the derivatives with respect to h at $h = 0$ of the odd correlation functions (triplet,...) diverge like the susceptibility in the vicinity of the critical temperature (at least for pair interactions). Our results also apply to higher order Ising spins (not just spin $\frac{1}{2}$).

KEY WORDS: Ising ferromagnets; coexistence of phases; new inequalities; critical exponents.

1. INTRODUCTION

The understanding of phase transitions is one of the most interesting and central, perhaps the central, problem of equilibrium statistical mechanics. A system undergoes a first-order phase transition whenever, for some value of the temperature and other relevant thermodynamic parameters, two or more phases can coexist in equilibrium. The different properties of the pure phases manifest themselves also as discontinuities in certain observables as a function of the appropriate thermodynamic variables, e.g., discontinuity of the magnetization as a function of the magnetic field in a ferromagnet. More general phase transitions are said to occur whenever the free energy of the system (and thus also the thermodynamic functions derivable from it) has a nonsmooth, mathematically nonanalytic, behavior as a function of its

Research supported in part by NSF Grant #MPS 75-20638 and USAFOR Grant #73-2430D.

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arguments. Indeed, since statistical mechanics goes beyond thermodynamics to describe also the microscopic correlation in the system, any nonanalytic behavior of the correlation functions (in their dependence on temperature and other suitable variables) may be considered as some sort of phase transition. The relationship between nonanalyticity, coexistence of phases, and the kindred notion of "symmetry breakdown" is one of the interesting questions in this field.⁽¹⁻³⁾

As is well known, it follows from the general formalism of statistical mechanics that such nonanalytic behavior can occur strictly only in infinite systems—the proper mathematical idealization of macroscopic systems that are described thermodynamically by intensive variables.^(1,3) The equilibrium states of such an infinite system are described by Gibbs probability measures on the phase space of the system: the appropriate⁽³⁻⁵⁾ generalization of finite-volume Gibbs ensembles. Equivalently, one may describe the "state" of the infinite system by means of correlation functions. The latter are obtained as infinite-volume limits of the equilibrium correlations in a finite system with specified "boundary conditions." A pure thermodynamic phase then corresponds (loosely speaking) to a set of translation-invariant correlation functions which "cluster" at infinity, i.e., correlations between different local regions of the system decay (however weakly) as the distance between these regions becomes larger and larger. The latter condition is equivalent to the requirement that intensive variables be well defined, i.e., that fluctuations in "all" intensive variables, local functions averaged over the volume of the system, vanish as the volume tends to infinity. The coexistence of several phases then corresponds to the existence, for a given interaction, temperature, and magnetic field, of more than one translation-invariant equilibrium state. This is the same⁽³⁻⁵⁾ as the possibility of obtaining different translation-invariant, infinite-volume limits for the correlation functions from different boundary conditions.

By a very general theory⁽³⁻⁵⁾ it is always possible to decompose any equilibrium state *uniquely* into "extremal" states, the translation-invariant (TI) extremal states corresponding to the pure phases. This means the following: Given any "observable" f , then its expectation value $\langle f \rangle$ in any TI equilibrium state can be written in the form $\langle f \rangle = \sum_{k=1}^m \alpha_k \langle f \rangle_k$, where $\langle f \rangle_k$ is the expectation value of $\langle f \rangle$ in the k th pure phase, $0 < \alpha_k \leq 1$, and $\sum_{k=1}^n \alpha_k = 1$, i.e., α_k measures the fraction of volume occupied by the k th phase. The crucial point here is that the α_k are independent of the observable f : Thus n clearly represents the total number of phases which can coexist (at a given temperature and magnetic field) and the question then is to determine n . (The Gibbs phase rule states that for an m -component fluid, $n \leq m + 2$, but this is far from proven and does not apply to spin systems with general interactions.^(3,6))

This paper is devoted mainly to the derivation of some results regarding the number of possible phases in an Ising spin system with ferromagnetic interactions. This is the simplest nontrivial system for which such results can be derived in a mathematically rigorous way. The main new result is that for such a system with even spin interactions (pair, quadruple,...) there can coexist, at zero magnetic field, only two phases (up and down magnetization) at all temperatures at which the energy is continuous (in the temperature). In particular, there are no intervals of temperature, below the critical temperature T_c , at which three or more phases can coexist. This extends results previously known only for the two-dimensional Ising spin system with nearest neighbor pair interactions⁽⁷⁾ and for higher dimensional Ising systems only at low temperatures.⁽⁶⁾ It is a simple consequence of our result that the spin-spin correlation $\langle \sigma_i \sigma_j \rangle$ obtained with “zero” or periodic boundary conditions at $h = 0$ approaches, as $|i - j| \rightarrow \infty$, the square of the spontaneous magnetization (below T_c).

The above results are derived in Section 3. They are based on a new inequality for ferromagnetic Ising spin systems, which is derived in Section 2. Section 4 is devoted to proving, on the basis of the new inequality, the equality of the “low-temperature” critical exponents describing the divergence of the derivatives, with respect to the magnetic field, of the odd correlations (triplet,...), i.e., they diverge like the susceptibility. The results are generalized to spin- $\frac{1}{2}n$ ($n > 1$) Ising systems in Section 4.

2. INEQUALITY

Let Λ be a finite set of $|\Lambda|$ sites, which for later application we shall think of as a subset of a regular ν -dimensional lattice, say $\Lambda \subset \mathbb{Z}^\nu$. Let $\sigma_i = \pm 1, i \in \Lambda$, be an Ising spin variable and $\sigma_A = \prod_{i \in A} \sigma_i, A \subset \Lambda$. Let

$$\beta H = - \sum_{K \subset \Lambda} J_K \sigma_K, \quad \beta' H' = - \sum_{K \subset \Lambda} J'_K \sigma_K, \quad \beta = (kT)^{-1} \quad (1)$$

be the energies (times the reciprocal temperatures) of two Ising spin systems in Λ . Define

$$\langle \sigma_A \rangle = Z^{-1} \text{Tr}_{\sigma} \left[\sigma_A \exp \left(\sum J_K \sigma_K \right) \right], \quad \langle \sigma_A \rangle' = (Z')^{-1} \text{Tr}_{\sigma} \left[\sigma_A \exp \left(\sum J'_K \sigma_K \right) \right] \quad (2)$$

to be the equilibrium expectation values of σ_A in the two systems, where

$$Z = \text{Tr}_{\sigma} \left[\exp \left(\sum J_K \sigma_K \right) \right], \quad Z' = \text{Tr}_{\sigma} \left[\exp \left(\sum J'_K \sigma_K \right) \right] \quad (3)$$

are the corresponding partition functions.

We are interested in the difference $\langle \sigma_A \rangle - \langle \sigma_A \rangle'$, which, following Ginibre,⁽⁹⁾ can be written in the form

$$\begin{aligned} \langle \sigma_A \rangle - \langle \sigma_A \rangle' &= (ZZ')^{-1} \text{Tr}_{\sigma', \sigma} \left\{ (\sigma_A - \sigma_A') \exp \left[\sum_K (J_K \sigma_K + J_K' \sigma_K') \right] \right\} \\ &= (ZZ')^{-1} \text{Tr}_{\sigma'} (1 - t_A) \text{Tr}_{\sigma} \left\{ \sigma_A \exp \left[\sum_K (J_K + J_K' t_K) \sigma_K \right] \right\} \end{aligned} \quad (4)$$

where we have introduced the Ising variables $\sigma_i' = \pm 1$ and $t_i = \sigma_i' \sigma_i = \pm 1$. It follows now from the Griffith, Kelley, and Sherman (GKS) inequalities^(1,10) that when

$$J_K \geq |J_K'|, \quad \text{for all } K \subset \Lambda \quad (5)$$

then the trace over σ on the right side of (4) is nonnegative. Let $A = B \Delta C = B \cup C \setminus B \cap C$ be the symmetric difference between the sets B and C ; then $t_A = t_B t_C = \pm 1$ and

$$1 - t_B t_C \geq \pm (t_B - t_C) \quad (6)$$

Substituting (6) on the right side of (4) and going back to the σ' variables, we obtain our basic inequality for $\sigma_A = \sigma_B \sigma_C$,

$$\langle \sigma_B \sigma_C \rangle - \langle \sigma_B \sigma_C \rangle' \geq |\langle \sigma_B \rangle \langle \sigma_C \rangle' - \langle \sigma_B \rangle' \langle \sigma_C \rangle| \quad (7a)$$

Noting that $\sigma_C = \sigma_A \sigma_B$, we can rewrite (7a) in the form

$$\langle \sigma_A \rangle - \langle \sigma_A \rangle' \geq |\langle \sigma_B \rangle \langle \sigma_A \sigma_B \rangle' - \langle \sigma_B \rangle' \langle \sigma_A \sigma_B \rangle| \quad (7b)$$

The inequalities (7a) and (7b) are valid whenever (5) holds. From (7b) in particular we have the following result:

Lemma 1. Let (5) hold. Then $\langle \sigma_A \rangle = \langle \sigma_A \rangle'$ and $\langle \sigma_B \rangle = \langle \sigma_B \rangle' \neq 0$ imply $\langle \sigma_A \sigma_B \rangle = \langle \sigma_A \sigma_B \rangle'$ for all $A, B \subset \Lambda$.

Corollary. Let (5) hold. Then (i) $\langle \sigma_i \rangle = \langle \sigma_i \rangle' \neq 0$ for all the one-site sets $i \in A$ implies $\langle \sigma_A \rangle = \langle \sigma_A \rangle'$ for all $A \subset \Lambda$; and (ii) $\langle \sigma_i \sigma_j \rangle = \langle \sigma_i \sigma_j \rangle' \neq 0$ for all $i, j \in \Lambda$ implies $\langle \sigma_E \rangle = \langle \sigma_E \rangle'$ for all sets E containing an even number of sites, $|E|$ even.

Proof. By Lemma 1, $\langle \sigma_i \rangle = \langle \sigma_i \rangle' \neq 0$ and $\langle \sigma_j \rangle = \langle \sigma_j \rangle' \neq 0$ imply $\langle \sigma_i \sigma_j \rangle = \langle \sigma_i \sigma_j \rangle'$. Furthermore, since $J_K \geq 0$ it follows from the GKS inequalities that $\langle \sigma_A \sigma_B \rangle \geq \langle \sigma_A \rangle \langle \sigma_B \rangle \geq 0$. Hence $\langle \sigma_i \sigma_j \rangle \geq \langle \sigma_i \rangle \langle \sigma_j \rangle > 0$. The rest follows by induction. The proof of (ii) is similar since $\langle \sigma_B \rangle = \langle \sigma_B \sigma_k \sigma_l \sigma_k \sigma_l \rangle$ for all $B \subset \Lambda$.

We can also rewrite (7a) in the form

$$\langle \sigma_B \sigma_C \rangle - \langle \sigma_B \sigma_C \rangle' \geq |\langle \sigma_B \rangle [\langle \sigma_C \rangle - \langle \sigma_C \rangle'] - \langle \sigma_C \rangle [\langle \sigma_B \rangle - \langle \sigma_B \rangle']| \quad (7c)$$

and consider the case where $J_A' \geq 0$, $\delta_A \geq 0$, $J_A = J_A' + \delta_A$. We then find the following result:

Lemma 2. With the above definition let $J_K \geq 0$; then

$$\partial \langle \sigma_B \sigma_C \rangle / \partial J_A \geq |\langle \sigma_B \rangle \partial \langle \sigma_C \rangle / \partial J_A - \langle \sigma_C \rangle \partial \langle \sigma_B \rangle / \partial J_A| \quad (8)$$

for all $B, C \subset \Lambda$.

Remark. While the inequalities (7a)–(7c) and thus Lemma 1 and the Corollary clearly remain valid in the limit (suitably defined) $\Lambda \nearrow \mathbb{Z}^v$, the limiting correlation functions may not be differentiable, for some values of the potentials $\{J_K\}$, in that limit. The inequality (8) will then still be valid (in a suitable sense) whenever $J_A > 0$ but will hold only for the right-sided derivative when $J_A = 0$.

3. INFINITE-VOLUME EQUILIBRIUM STATES

We shall now use the inequalities derived in the last section to obtain information about the number of equilibrium states for infinite-Ising systems. To do this we assume that the interactions are translation invariant, $J_A = \beta \Phi_{A+x}$, where $A+x$ is the set A translated by a lattice vector x . In particular, for the one-point sets, $A = i \in \mathbb{Z}^v$, $\beta \Phi_i = h$, the magnetic field (times β), and for $|A| = 2$, $J_{\{i,j\}} = \beta \varphi(i-j)$, etc. The energy of a spin configuration σ_Λ in $\Lambda \subset \mathbb{Z}^v$ will depend on the specified values of the spins outside Λ , i.e., we consider the spins outside Λ to be fixed and act as boundary conditions for the spins in Λ .⁽³⁻⁵⁾ A particular boundary condition (b.c.) “ b ” then corresponds to a lattice spin configuration σ^b such that $\sigma_i = \sigma_i^b$ for $i \in \Lambda_c$. (Generally $\sigma_i^b = \pm 1$; $\sigma_i^0 = 0$ correspond to zero b.c.) We then have, corresponding to Eq. (1),

$$H(\sigma_\Lambda; b) = - \sum_{B \supset \{0\}} \sum_x \Phi_B \sigma_{B+x}, \quad \Phi_B \geq 0 \quad (9)$$

where $\{0\}$ designates the origin and the sum over x goes over all x such that $\{B+x\} \cap \Lambda$ is not empty, i.e., at least some of the sites in $B+x$ are in Λ . We assume from now on that the $\Phi_B \geq 0$, i.e., positive ferromagnetic interactions. It is then clear that $H(\sigma_\Lambda; +)$ corresponding to plus b.c., $\sigma_i^+ = 1$, “dominates” all other b.c. in the sense of (5). Hence, defining $\langle \sigma_\Lambda \rangle(\beta, h; b, \Lambda)$ as the expectation value of σ_A , $A \subset \Lambda$, for the Hamiltonian (9) at reciprocal temperature β and magnetic field h , we can identify $\langle \sigma_A \rangle$ of Section 2 with

$\langle \sigma_A \rangle(\beta, h; +, \Lambda)$ and $\langle \sigma_A \rangle'$ with $\langle \sigma_A \rangle(\beta, h; b, \Lambda)$ for any other boundary condition. (Our notation implies the “physicist” point of view, where β and $h = \{\beta\Phi_i\}$ are independent, “externally controlled” variables while $\Phi_K, |K| \geq 2$, are “given” interactions.)

It follows from the GKS inequalities^(1,11) that

$$\lim_{\Lambda \nearrow \mathbb{Z}^v} \langle \sigma_A \rangle(\beta, h; +, \Lambda) = \langle \sigma_A \rangle(\beta, h; +) \tag{10}$$

exist and are translation invariant,

$$\langle \sigma_{A+x} \rangle(\beta, h; +) = \langle \sigma_A \rangle(\beta, h; +) \tag{11}$$

To avoid unnecessary complications we assume that the interactions are of “finite range,” $\Phi_B = 0$, unless $B \subset N, N$ bounded. The thermodynamic free energy per site $\Psi(\beta, h) = \lim\{|\Lambda|^{-1} \ln \text{Tr} \exp[-\beta H(\sigma_A; b)]\}$ then exists and is independent of b .

We shall write $\langle \sigma_i \rangle(\beta, h; +) = m(\beta, h; +)$, the magnetization per site with plus b.c. For more general boundary conditions (including a superposition, with specified weights, of different σ^b) the limit $\Lambda \nearrow \mathbb{Z}^v$ might have to be taken along subsequences to obtain infinite-volume correlation functions $\langle \sigma_A \rangle(\beta, h; b)$ which need not, in general, be translation invariant.⁽¹²⁾ It is, however, always possible to average over translations to obtain translation-invariant correlation functions. The set of correlations $\langle \sigma_A \rangle(\beta, h; b), A \subset \mathbb{Z}^v$, obtained from $\langle \sigma_A \rangle(\beta, h; b, \Lambda)$ as $\Lambda \nearrow \mathbb{Z}^v$ defines an infinite-volume Gibbs measure. These measures are identical to the ones that satisfy the DLR equations and the translation-invariant ones are identical to the solutions of a variational principle (minimizing the free energy per unit volume).⁽³⁻⁵⁾ We shall denote by $G(T, T \subset G)$ the set of all infinite-volume Gibbs (translation-invariant Gibbs) measures μ . We shall sometimes write $\langle \sigma_A \rangle_\mu$ for $\int \sigma_A \mu(d\sigma)$, $\mu \in G$, and $\langle \sigma_A \rangle_+$ for $\int \sigma_A \mu_+(d\sigma), \mu_+ \in T$, the measure obtained with plus b.c.

These considerations also lead to an identification of the $\langle \sigma_A \rangle_\mu, \mu \in T$, with derivatives of the free energy density $\Psi(\mathbf{J})$ with respect to $J_A (= \beta\Phi_A)$,⁽³⁻⁵⁾

$$\Psi(\mathbf{J}) = \lim_{\Lambda \nearrow \mathbb{Z}^v} |\Lambda|^{-1} \ln Z(\mathbf{J}; b, \Lambda) \tag{12}$$

and we have used \mathbf{J} for the argument of Ψ to emphasize that Ψ can be thought of as a function of “all possible” potentials J_K . Since $\Psi(\mathbf{J})$ is a convex function of each J_A , it will be differentiable for almost all values of J_A (keeping the other interactions fixed).

We are now ready to state our first theorem about the number of possible equilibrium states.

Theorem 1. Let $\Psi(\beta, h)$ be the infinite-volume free energy per site of an Ising spin system with translation-invariant interactions; $\Phi_K = \Phi_{K+x} \geq 0$,

$x \in \mathbb{Z}^v, \beta\Phi_{(0)} = h$. If the derivative of Ψ with respect to h exists (is continuous) and is positive, $\partial\Psi(\beta, h)/\partial h > 0$, then there is a unique translation-invariant Gibbs state. In particular $\langle \sigma_A \rangle(\beta, h; b) = \langle \sigma_A \rangle(\beta, h; +) = \partial\Psi/\partial J_A$ for all boundary conditions b .

Proof. Given any $\mu \in T, \langle \sigma_A \rangle_\mu = \partial\Psi/\partial J_A$, when the latter exists⁽³⁻⁵⁾ and the theorem then follows from the Corollary to Lemma 1 with $\langle \sigma_i \rangle = \partial\Psi/\partial h$.

Remark. Theorem 1 states that differentiability of Ψ with respect to h implies differentiability of Ψ with respect to *all* interactions. It thus generalizes to ferromagnetic, many-spin interactions the results of Lebowitz and Martin-Löf⁽¹¹⁾ for the case when the interactions are such that the Fortuin, Kasteleyn, and Ginibre (FKG) inequalities hold, e.g., when only pair interactions are present, $\Phi_K = 0, |K| > 2$.⁽¹³⁾ In that case, however, the results are stronger; there is a unique Gibbs state (and so $T = G$) whenever $\partial\Psi(\beta, h)/\partial h$ exists. For pair interactions this is true for all $h \neq 0$, and is always true at sufficiently high temperatures.^(1,3)

The positivity requirement on $\partial\Psi/\partial h$ is, however, not as restrictive as it might appear. First, by GKS, $\langle \sigma_i \rangle(\beta, h; +) > 0$ if $h > 0$ and hence $\partial\Psi(\beta, h)/\partial h = 0 \Rightarrow h = 0$. Second, if the interactions are such that $\langle \sigma_E \rangle(\beta, h = 0; +) > 0$ for $|E|$ even, e.g., when the nearest neighbor pair interaction is positive, then it is easy to show⁽¹⁴⁾ that $\langle \sigma_i \rangle(\beta, 0; +) = 0 \Rightarrow \langle \sigma_Q \rangle(\beta, 0; +) = 0$ for all $|Q|$ odd. This implies, by GKS, that $\Phi_K = 0$ for all $|K|$ odd. These facts in turn imply that the odd correlations vanish for all b.c. since, by (7), for $|Q|$ odd,

$$0 = \langle \sigma_Q \rangle(\beta, 0; +) \geq \langle \sigma_Q \rangle(\beta, 0; b) = -\langle \sigma_Q \rangle(\beta, 0; -b) \tag{13}$$

where $-b$ is the b.c. obtained from b by reflection; $\sigma_i^{-b} = -\sigma_i^b$. We are therefore left, when $\partial\Psi(\beta, h)/\partial h = 0$ at $h = 0$, only with the possible non-uniqueness of the even correlation functions. We shall now consider this problem, which is also, as we shall see, the central problem when $\partial\Psi(\beta, h)/\partial h$ is discontinuous at $h = 0$ and there are only even interactions, e.g., in the Ising model with ferromagnetic pair interactions.

Definition. We call a (finite) collection of bounded sets $\{K_\alpha\}, K_\alpha \ni \{0\}$ all α , generating for the even sets, $\{K_\alpha\} = \bar{G}$, iff, given any bounded set $E \subset \mathbb{Z}^v, |E|$ even, we can write

$$\sigma_E = \prod_{n=1}^m \sigma_{\{K_{\alpha_i} + x_n\}}$$

m finite, with $K_{\alpha_i} \in G$, and x_n a lattice vector (we may have $K_{\alpha_i} = K_{\alpha_j}$).

By the proof of part (ii) of the Corollary to Lemma 1, \bar{G} will be generating iff it generates all the sets consisting of pairs of sites $\{i, j\}$. Letting e_α be the unit vector in the α th direction, it is now easy to see that the ν nearest neighbor sets, $K_\alpha = \{0, e_\alpha\}$, $\alpha = 1, \dots, \nu$, are generating, e.g., the product $(\sigma_0 \sigma_{e_1})(\sigma_{e_1} \sigma_{e_1+e_2}) = \sigma_0 \sigma_{e_1+e_2}$, where $e_1 + e_2$ is one of the next nearest neighbor sites of the origin, etc.

It follows from part (ii) of the Corollary to Lemma 1 that if the expectation values of σ_{K_α} in a translation-invariant state μ are positive and equal to $\langle \sigma_{K_\alpha} \rangle(\beta, h; +) > 0$, for all $K_\alpha \in \bar{G}$, then all the even correlation functions of μ are the same as in the plus state. This will be the case for all translation-invariant μ whenever Ψ is differentiable with respect to J_{K_α} , for all $K_\alpha \in K$ and $\partial\Psi/\partial J_{K_\alpha} > 0$. We now show that this is equivalent to having $\Psi(\beta, h)$ differentiable with respect to β .

Theorem 2. Let the conditions of Theorem 2 hold and let $\Phi_{K_\alpha} > 0$ for all $K_\alpha \in \bar{G}$. If $\partial\Psi(\beta, h)/\partial\beta$ exists, i.e., the energy per site (apart from the magnetic field contribution) is continuous in β , then the expectation value of σ_E , $|E|$ even, is the same in all translation-invariant states: $\langle \sigma_E \rangle_\mu = \langle \sigma_E \rangle_+$ for $\mu \in T$.

Proof. By the general arguments⁽³⁻⁵⁾ mentioned earlier, $\partial\Psi(\beta, h)/\partial\beta$ continuous implies that for every $\mu \in T$, $\sum_{K \ni \{0\}} \Phi_K \langle \sigma_K \rangle_+ = \sum_{K \ni \{0\}} \Phi_K \langle \sigma_K \rangle_\mu$. By (7), $\langle \sigma_K \rangle_+ \geq \langle \sigma_K \rangle_\mu$; hence the continuity of $\partial\Psi(\beta, h)/\partial\beta$ implies that $\langle \sigma_K \rangle_+ = \langle \sigma_K \rangle_\mu$ for all $\mu \in T$ and all K such that $\Phi_K > 0$. In particular $\Phi_{K_\alpha} > 0$ for all $K_\alpha \in \bar{G}$ and by GKS, $\langle \sigma_{K_\alpha} \rangle_+ > 0$, so part (ii) of the Corollary to Lemma 1 implies that $\langle \sigma_E \rangle_+ = \langle \sigma_E \rangle_\mu$ for all $|E|$ even.

The interest of Theorem 1 lies primarily in what it tells us about the number of extremal translation-invariant Gibbs states for a system with even ferromagnetic interactions, when $h = 0$, and $\Psi(\beta, h)$ not differentiable at $h = 0$. Since $\Psi(\beta, h)$ is now symmetric (and convex) in h , the nondifferentiability of Ψ at $h = 0$ corresponds to the existence of a spontaneous magnetization with⁽¹¹⁾

$$m^*(\beta) = \lim_{h \searrow 0} \frac{\partial\Psi(\beta, h)}{\partial h} = -\lim_{h \nearrow 0} \frac{\partial\Psi(\beta, h)}{\partial h} = \langle \sigma_i \rangle(\beta, h = 0; +) = -\langle \sigma_i \rangle(\beta, h = 0; -) \quad (14)$$

Here $\langle \sigma_A \rangle(\beta, -h; -) = (-1)^{|A|} \langle \sigma_A \rangle(\beta, h; +)$ is the expectation of σ_A in the infinite-volume Gibbs state μ_- obtained, as $\Lambda \nearrow \mathbb{Z}^\nu$, with "minus" boundary conditions (translation invariance is assured if $h \geq 0$). As already mentioned, there are cases, i.e., only pair interactions (ferromagnetic), when $h = 0$ is the only place where a phase transition is possible. With more general even interactions only the symmetry $h \rightarrow -h$ is known a priori.

In a recent paper⁽¹⁴⁾ we were able, using the GKS inequalities, to obtain some information about the Gibbs states of such a system at $h = 0$. The following theorem greatly extends those results.

Theorem 3. Let the conditions of Theorem 1 hold and let $\Phi_K = 0$ for all $|K|$ odd and $\Phi_{K_\alpha} > 0$ for all $K_\alpha \in \bar{G}$. If $\partial\Psi(\beta, h = 0)/\partial\beta$ exists, then there are at most two extremal translation-invariant Gibbs states μ_+ and μ_- . These states coincide if $\partial\Psi(\beta, h)/\partial h$ exists at $h = 0$.

Proof. By Theorem 2 the differentiability of $\Psi(\beta, 0)$ implies that the $\langle\sigma_E\rangle_\mu$, $|E|$ even, are the same in all $\mu \in T$. If, furthermore, $\partial\Psi(\beta, h)/\partial h = 0$ at $h = 0$, then, by the remarks following Theorem 1, the odd correlations vanish for all $\mu \in G$ and the state $\mu \in T$ is then unique. (When the FKG inequalities hold, differentiability with respect to h implies differentiability with respect to β .) When Ψ is not differentiable at $h = 0$, $m^*(\beta) > 0$, there are at least two extremal translation-invariant Gibbs states μ_+ and μ_- .⁽¹¹⁾ Let $\mu(\beta, 0; b)$ be an invariant state; then $\bar{\mu}(\beta, 0; b) \equiv \frac{1}{2}[\mu(\beta, 0; b) + \mu(\beta, 0; -b)]$ is an invariant state in which all the odd correlations vanish by symmetry. Hence $\bar{\mu}(\beta, 0; b) = \frac{1}{2}(\mu_+ + \mu_-)$, which, since invariant Gibbs states form a simplex, i.e., each state has a unique decomposition into extremal states, implies that $\mu(\beta, 0; b) = \gamma\mu_+ + (1 - \gamma)\mu_-$, $0 \leq \gamma \leq 1$. This completes the proof. (The last part of the argument, which is also used in Refs. 7 and 8, I heard originally from Ruelle.)

Remarks. (i) It follows⁽¹⁾ from GKS that there exists a unique β_c such that

$$m^*(\beta) \begin{cases} = 0, & \beta < \beta_c \\ > 0, & \beta > \beta_c \end{cases}$$

We always have^(1,15) $\beta_c \geq \beta_0 > 0$ and for $\nu \geq 2$ (with nonvanishing Φ_K), $\beta_c \leq \beta_p < \infty$, by the Peierls argument (or the more recent method of Frohlich *et al.*⁽¹⁶⁾ for $\nu \geq 3$). Using the convexity of $\Psi(\beta, 0)$ it follows from Theorem 3 that with the possible exception at a countable number of values of β , there is a unique $\mu \in T$ for $\beta < \beta_c$ and two extremal states $\mu \in T$ for $\beta > \beta_c$. In particular there are no triple or higher order points at $h = 0$ when the energy is continuous in β .

(ii) The state at $h = 0$ obtained with "zero" (or periodic) b.c. μ_0 (μ_p) is translation invariant and has vanishing odd correlations.^(1,15) Hence $\mu_0 = \mu_p = \frac{1}{2}(\mu_+ + \mu_-)$. This implies in particular the existence of "long-range order" in these states for $\beta > \beta_c$, i.e.,

$$\langle\sigma_i\sigma_j\rangle_{\mu_0} \xrightarrow{|i-j|\rightarrow\infty} [m^*(\beta)]^2 > 0$$

for $\beta > \beta_c$. (The converse of this statement, long-range order $\Rightarrow m^*(\beta) > 0$, is also true.⁽¹⁾)

(iii) Setting $B = \{i\}$ and $C = \{i, j\}$ in (7c), we find that for $\beta > 0$ and $h \geq 0$

$$[1 + \langle \sigma_i \sigma_j \rangle(\beta + \delta, h + \epsilon; +)] [m(\beta + \delta, h + \epsilon; +) - m(\beta, h; +)] \\ \geq m(\beta + \delta, h + \epsilon; +) [\langle \sigma_i \sigma_j \rangle(\beta + \delta, h + \epsilon; +) - \langle \sigma_i \sigma_j \rangle(\beta, h; +)] \quad (15)$$

with $\epsilon \geq 0$ for $h = 0$. We shall use (15), and forms related to it, to derive various interesting inequalities in the next section. We mention here one. Letting $h = 0$ and $\delta = 0$ and noting that $\langle \sigma_i \sigma_j \rangle \leq 1$, we obtain, for $\beta > \beta_c$,

$$m^*(\beta + \delta) - m^*(\beta) \geq \frac{1}{2} m^*(\beta) [\langle \sigma_i \sigma_j \rangle(\beta + \delta, 0; +) - \langle \sigma_i \sigma_j \rangle(\beta, 0; +)] \quad (16a)$$

We see from (16a) that continuity of the spontaneous magnetization $m^*(\beta)$ implies continuity of the pair correlation $\langle \sigma_i \sigma_j \rangle(\beta, 0; +)$. By similar arguments we obtain continuity of all $\langle \sigma_B \rangle(\beta, 0; +)$ and also continuity of the energy. Hence, $m^*(\beta)$ continuous implies, for $\beta > \beta_c$, the existence of only two extremal invariant states.

(iv) For the two-dimensional Ising system with nearest neighbor pair interactions the continuity of $\partial \Psi(\beta, h = 0) / \partial \beta$ follows from Onsager's^(1,17) exact computation of $\Psi(\beta, 0)$. Hence Theorem 3 establishes the existence of exactly two extremal states for all $\beta > \beta_c$ [β_c being here the place where the second derivative of $\Psi(\beta, 0)$ diverges logarithmically⁽¹⁸⁾]. This result for the square lattice was proven earlier, using duality, by Messager and Miracle-Sole.⁽⁷⁾ For more general Ising systems with even ferromagnetic interactions this result is known at low temperatures (not all the way to T_c) from the work of Gallavotti and Miracle-Sole and of Slawny.⁽⁸⁾ Gallavotti and Miracle-Sole used (for nearest neighbor interactions) a beautiful version of the Peierls argument, while Slawny used the Asano-Ruelle method of locating zeros of the partition function to prove analyticity of $\Psi(\mathbf{J})$ in the even interactions at sufficiently large β . Using the above theorem, it is sufficient to establish that $\Psi(\beta, 0)$ is C^1 . This can be done readily if the correlation function in the plus state clusters sufficiently well for⁽¹⁸⁾

$$\sum_x [\langle \sigma_A \sigma_{B+x} \rangle(\beta, 0; +) - \langle \sigma_A \rangle(\beta, 0; +) \langle \sigma_{B+x} \rangle(\beta, 0; +)] < \infty$$

The latter can be easily proven for large β by a Peierls-type argument,⁽¹⁹⁾ which actually establishes exponential clustering.

(v) Theorem 3 can be generalized, in a fairly direct way, using the ideas of Slawny, Gruber, and their co-workers to noneven interactions. One then gets a larger number of extremal states: these are related to the group, acting on the spins, that leaves the Hamiltonian invariant.

4. DIVERGENCE OF GENERALIZED SUSCEPTIBILITIES

AS $\beta \rightarrow \beta_c$

Various authors^(14,20-22) have investigated the asymptotic behavior of higher order correlation functions, e.g., the triplet correlation $\langle \sigma_i \sigma_j \sigma_k \rangle$, as $h \searrow 0$ and $\beta \rightarrow \beta_c$. Some results were obtained by Barber⁽²²⁾ for the triplet correlation in the case of only ferromagnetic pair interactions and by Lebowitz⁽¹⁴⁾ for all odd correlations in the case of even interactions (satisfying the conditions of Theorem 3). The latter results may be summarized as follows: Let

$$\langle \sigma_A \rangle^*(\beta) = \lim_{h \searrow 0} \langle \sigma_A \rangle_+(\beta, h) = \langle \sigma_A \rangle_+(\beta, 0)$$

and let

$$\chi(A, \beta) = \limsup_{h \searrow 0} h^{-1} [\langle \sigma_A \rangle_+(\beta, h) - \langle \sigma_A \rangle^*(\beta)]$$

Then for all $|A|$ odd, $\beta \geq \epsilon$, $\epsilon > 0$ arbitrary,

$$C_1 m^*(\beta) \leq \langle \sigma_A \rangle^*(\beta) \leq C_2 m^*(\beta) \tag{16b}$$

and

$$C_1 \chi(\beta) \leq \chi(A, \beta) \leq C_2 \chi(\beta), \quad \text{for } \beta \leq \beta_c \tag{17}$$

where C_1 and C_2 are positive constants, $0 < C_1, C_2 < \infty$, and $\chi(\beta) = \chi(\{0\}, \beta)$ is the usual susceptibility. In particular, if $m^*(\beta) \sim (\beta - \beta_c)^b$ as $\beta \searrow \beta_c$ (b is "usually" called β , the critical exponent for the spontaneous magnetization), then also $\langle \sigma_A \rangle^*(\beta) \sim (\beta - \beta_c)^b$ for $|A|$ odd. (For $\beta < \beta_c$ we of course have $\langle \sigma_A \rangle^*(\beta) = 0$, $|A|$ odd.) Similarly, if $\chi(\beta)$ diverges as $(\beta - \beta_c)^{-\gamma}$ when $\beta \nearrow \beta_c$, so do all odd $|A|$. Barber also showed, for pair interactions, that $\chi(A, \beta)$ for $|A| = 3$ does not diverge as $\beta \searrow \beta_c$ any faster than $\chi(\beta)$. He could not, however, show that it diverges as fast as $\chi(\beta)$.

It follows, however, directly from Lemma 2 with $C = \{i\}$ that for $h > 0$

$$\frac{\partial \langle \sigma_B \sigma_i \rangle(\beta, h; +)}{\partial h} + m(\beta, h) \frac{\partial \langle \sigma_B \rangle(\beta, h; +)}{\partial h} \geq \langle \sigma_B \rangle(\beta, h; +) \frac{\partial m(\beta, h; +)}{\partial h} \tag{18}$$

Letting $h \searrow 0$ then yields immediately

$$\chi(Q, \beta) + m^*(\beta) \chi(B, \beta) \geq \langle \sigma_B \rangle^*(\beta) \chi(\beta) \tag{19}$$

with $\sigma_Q = \sigma_B \sigma_i$. If $|Q|$ is odd, $|B|$ is even and $\langle \sigma_B \rangle^*(\beta) \geq C > 0$ for $\beta > \beta_c$. Hence if $\chi(Q, \beta)$ does not diverge as fast as $\chi(\beta)$ for some $|Q|$ odd, $\chi(B, \beta)$ has to diverge as $\chi(\beta)/m^*(\beta)$ when $\beta \searrow \beta_c$ [and $m^*(\beta) \rightarrow 0$] for an even $|B|$,

$\sigma_B = \sigma_Q \sigma_i$. It is easy to show that this cannot happen generally, e.g., it follows from Lemma 2 (after some manipulations) that

$$\begin{aligned} \frac{\partial \langle \sigma_B \sigma_i \rangle_+}{\partial J_A} &\leq \epsilon \langle \sigma_B \rangle_+ \frac{\partial \langle \sigma_i \rangle_+}{\partial J_A} \\ &\Rightarrow \frac{\partial}{\partial J_A} \langle \sigma_B \sigma_{B+\{x\}} \sigma_i \rangle_+ \geq (1 - 2\epsilon) \langle \sigma_B \rangle_+^2 \frac{\partial \langle \sigma_i \rangle_+}{\partial J_A} \end{aligned} \quad (20)$$

so at least “many” $\chi(Q, \beta)$, $|Q|$ odd fixed, must diverge as $\chi(\beta)$. I have not, however, been able to find an argument that this is true for all Q , $|Q|$ odd, with general even ferromagnetic interaction.

If we restrict ourselves, however, to pair interactions, then it follows easily from the FKG inequalities⁽¹⁸⁾ that the divergence of $\chi(\beta)$ dominates that of $\chi(A, \beta)$ for all A . To see this, we note that

$$\begin{aligned} \partial \langle \sigma_A \rangle (\beta, h; +) / \partial h &= \sum_{i \in \mathbb{Z}^v} [\langle \sigma_A \sigma_i \rangle_+ - \langle \sigma_A \rangle_+ \langle \sigma_i \rangle_+] \\ &\leq C_A \sum_{i \in \mathbb{Z}^v} \{ \langle \sigma_i \rangle_+ - [m(\beta, h; +)]^2 \} \\ &= c_A \partial m(\beta, h; +) / \partial h \end{aligned} \quad (21)$$

where $c_A < \infty$. Combining (21) with (18) and letting $h \searrow 0$, we obtain the desired result:

Theorem 4. For an Ising system on \mathbb{Z}^v with ferromagnetic pair interactions (such that nearest neighbor correlations do not vanish identically) $\chi(Q, \beta)$ diverges like $\chi(\beta)$ as $\beta \rightarrow \beta_c$ whenever $m^*(\beta) \rightarrow 0$ as $\beta \searrow \beta_c$ for all $|Q|$ odd. Under the more general conditions of Theorem 3 either $\chi(Q, \beta)$ or $\chi(Q', \beta)$ (or both) must diverge at least as fast as $\chi(\beta)$: The set Q' is obtained from Q by the addition or deletion of any site.

Remark. It is clear that many additional relations between singularities in different correlations, e.g., in derivatives with respect to β , or derivatives with respect to h at $\beta = \beta_c$, can be derived from our basic inequality. The results are consistent, but do not prove the assumption, often made, that all even correlations have the same decay near β_c when separated into two odd sets.

5. SOME GENERALIZATIONS

(i) The use of cubical lattices is of course not essential. All our results (suitably rephrased) remain valid for any regular ν -dimensional lattice.

(ii) While all our results have been stated for the case of spin-1/2 Ising systems, $\sigma_i = \pm 1$, they remain valid also in the case of “higher” Ising spins,

i.e., when the spin variable at each lattice site S_i takes on the integer values $\{n, n - 2, \dots, -n\}$. The reason for this is the discovery by Griffiths^(1,23) that it is possible to relate the $n > 1$ system to an ordinary Ising system by introducing at each site $\{i\}$, n spin-1/2 variables $\sigma_{i,\alpha}$, $\alpha = 1, \dots, n$. We may then, in equilibrium, use the transcription $S_i = n^{-1} \sum_{\alpha} \sigma_{i,\alpha}$ for obtaining probability distributions of the $\{S_i\}$ variables, provided one introduces additional ferromagnetic pair interactions of the form $j_{\alpha\alpha'} \sigma_{i,\alpha} \sigma_{i,\alpha'}$ at each site i . The $j_{\alpha,\alpha'} \geq 0$ are chosen so as to give equal a priori weights to the different $(n + 1)$ values of each S_i .

The (formal) translation-invariant Hamiltonian of the spin- $\frac{1}{2}n$ system has the form

$$\beta H(\mathbf{S}) = -h \sum S_i - \beta \sum \Phi^{(2)}(i - j) S_i S_j - \beta \sum \Phi^{(3)}(i - j) (S_i^2 S_j + S_i S_j^2) + \dots$$

Since all the Φ 's are nonnegative for ferromagnetic interactions, the basic inequalities (7a)–(7c) clearly remain valid for the $\sigma_{i,\alpha}$. The important observation now is that, identifying plus b.c. with $S_i^+ = n$, it follows from the GKS inequalities (as in the proof of Theorem 2) that $\langle S_i \rangle_+ = \langle S_i \rangle_\mu$ implies $\langle \sigma_{i,\alpha} \rangle_+ = \langle \sigma_{i,\alpha} \rangle_\mu$ and $\langle S_i S_j \rangle_+ = \langle S_i S_j \rangle_\mu$ implies $\langle \sigma_{i,\alpha} \sigma_{j,\alpha'} \rangle_+ = \langle \sigma_{i,\alpha} \sigma_{j,\alpha'} \rangle_\mu$. Here the measure μ on the $\{S_i\}$ induces in a natural way, using the Griffiths interactions $j_{\alpha\alpha'}$, a measure on the $\{\sigma_{i,\alpha}\}$.

All our results therefore remain unchanged as long as n is finite. We have not investigated in detail what happens for continuum spins, which can also sometimes be constructed from spin- $\frac{1}{2}$ Ising systems^(23,24) or can otherwise be shown to satisfy the GKS inequalities. It can be readily shown, however,⁽²⁵⁾ that the inequality (7a) with σ_B replaced by $\prod_{i \in B} S_i^{n_i}$, etc., remains valid for general (continuous or discrete) Ising spin variables whenever the “intrinsic” spin measure $d\nu(S_i)$ satisfies condition Q_3 of Ginibre,⁽⁹⁾ e.g., when

$$d\nu(S) = C \exp(-aS^{2n} + bS^{2n-2} + \dots + cS^2) dS$$

Some of the results of Section 4 therefore also remain valid in this case.

(iii) The results of Section 3 may be restated to say that, under suitable conditions, there is only one translation-invariant state, $\mu \in T$, with a given magnetization $\langle \sigma_i \rangle_\mu = m$. It seems reasonable to conjecture that, under the same conditions, specification of $\langle \sigma_i \rangle_\mu$ for all $i \in \mathbb{Z}^v$ is sufficient to uniquely characterize all Gibbs states, $\mu \in G$.

ACKNOWLEDGMENTS

I would like to thank E. Presutti and D. Ruelle for very valuable discussions and Prof. N. H. Kuiper for his kind hospitality at IHES.

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