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CONCAVITY OF MAGNETIZATION AS A FUNCTION OF EXTERNAL FIELD STRENGTH FOR ISING FERROMAGNETS

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ABSTRACT

For an Ising ferromagnet with n spins $\sigma_1, \sigma_2, \ldots, \sigma_n$, let the Hamiltonian be $-\sum_{i<j} J_{ij}\sigma_i\sigma_j - \sum_{i=1}^{n} J_i\sigma_i$ (with $J_{ij} \geq 0$, $J_i \geq 0$ for all i, j). Define $s = \sigma_1 + \sigma_2 + \ldots + \sigma_n$. Then $\langle s^3\rangle - 3\langle s\rangle\langle s^2\rangle + 2\langle s\rangle^3 \leq 0$. As a consequence: when $J_1 = J_2 = \ldots = J_n = H$, the magnetization $\langle s\rangle$ is a concave function of the external field strength H.

1. Introduction.

The Ising model we consider here is the following: let N denote the index set $\{1,2,\ldots,n\}$; we consider the space of all 2^n spin configurations $\sigma = (\sigma_1, \ldots, \sigma_n)$, where each σ_i is allowed the values $+1$ ("up") or -1 ("down").

Suppose that we are given extended real numbers J_i for each i in N and J_{ij} for each pair (i,j) of distinct members of N, satisfying

(1) $$0 \leq J_{ij} = J_{ji} \leq \infty, \quad 0 \leq J_i \leq \infty.$$

The Hamiltonian is the real-valued function on configurations whose value at σ is

(2) $$H_\sigma = -\sum_{1\leq i<j\leq n} J_{ij}\sigma_i\sigma_j - \sum_{i=1}^{n} J_i\sigma_i.$$

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The <u>Gibbs probability</u> on the space of configurations is defined by

(3) $$P(\sigma) = Z^{-1}\exp(-\beta H_\sigma),$$

where

(4) $$\beta = (kT)^{-1} > 0,$$

k being Boltzmann's constant and T the (absolute) temperature, and where the <u>partition function</u> Z is defined by

(5) $$Z = \sum_\sigma \exp(-\beta H_\sigma).$$

The expected value of a random variable X on this space is called its <u>thermal average</u> and is indicated by angular brackets:

(6) $$\langle X\rangle = Z^{-1}\sum_\sigma X(\sigma)\exp(-\beta H_\sigma).$$

The <u>average magnetization per spin</u> is defined by

(7) $$M = n^{-1}\langle s\rangle,$$

where

(8) $$s = \sigma_1 + \sigma_2 + \dots + \sigma_n.$$

It has been conjectured that in the special case in which all J_i are equal to H, M is a concave function of H; that is, $\frac{\partial^2 M}{\partial H^2} \le 0$. In a paper[1] of the author and S. Sherman, hereafter referred to as (KS), we saw (section 7) that concavity of M(H) is equivalent to

(9) $$D = \langle s^3\rangle - 3\langle s\rangle\langle s^2\rangle + 2\langle s\rangle^3 \le 0$$

and also that

(10) $$D = \sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{n} D_{ijk},$$

where

(11) $$D_{ijk} = \langle\sigma_i\sigma_j\sigma_k\rangle - \langle\sigma_i\rangle\langle\sigma_j\sigma_k\rangle - \langle\sigma_j\rangle\langle\sigma_i\sigma_k\rangle - \langle\sigma_k\rangle\langle\sigma_i\sigma_j\rangle + 2\langle\sigma_i\rangle\langle\sigma_j\rangle\langle\sigma_k\rangle.$$

In this paper we prove the following

<u>Theorem</u>. In the Ising model described by (1), (2), and (3), $D_{ijk} \le 0$

for all triples (i,j,k) of (not necessarily distinct) members of N.

It is of course a corollary that $M(H)$ is concave in H when $J_1 = \ldots = J_n = H$.

Note: in section 7 of (KS) we observed that D_{ijk} is never positive when i, j, and k are not all distinct. So from now on we assume that i, j, and k are fixed distinct members of N.

2. Notation.

First we adopt the notation of (KS), in which the model, more general than that above, is as follows. Suppose that for each subset A of N a constant J_A is given, with

(12) $$0 \leq J_A \leq \infty.$$

Let the Hamiltonian be

(13) $$H_\sigma = -\sum_{A \subseteq N} J_A \sigma^A,$$

where

(14) $$\sigma^A = \prod_{i \in A} \sigma_i.$$

Again define probabilities by (3), (4), and (5). Then equation (9.2) of (KS) gives

(15) $$Z\langle\sigma^R\rangle = 2^n \sum_{k=0}^{\infty} \frac{1}{k!} \Sigma J_{A_1} \cdots J_{A_k},$$

the inner sum being taken over all ordered k-tuples $(A_1,\ldots,A_k)$ of (not necessarily distinct) subsets of N which satisfy $A_1 \Delta \ldots \Delta A_k = R$. (Here Δ denotes symmetric difference: $A \Delta B = (A \cup B) - (A \cap B)$.)

The expression we shall use for $\langle\sigma^R\rangle$ is based on the notion of multiplicity functions on the subsets of N; that is, functions assigning a nonnegative integer $\mu(A)$ to each subset A of N. For such a function μ, define

(16) $$J_\mu = \prod_{A \subseteq N} J_A^{\mu(A)} \geq 0;$$

(17) $$\mu! = \prod_{A \subseteq N} (\mu(A)!);$$

(18) $$\Delta\mu = \mathop{\Delta}_{A \subseteq N} A^{\mu(A)};$$

this last expression denotes the symmetric difference of all the subsets of N, each subset A being taken $\mu(A)$ times.

With this notation, define, for subsets R of N,

(19) $$\Pi_R = \sum_{\Delta\mu = R} \frac{1}{\mu!} J^{\mu}$$

the sum being over all multiplicity functions μ satisfying $\Delta\mu = R$. Then equations (9.7) and (9.8) of (KS) give that

(20) $$\frac{\Pi_R}{\Pi_\phi} = \langle\sigma^R\rangle; \ \Pi_\phi = 2^{-n}Z \geq 0.$$

(Note: Π_R is an infinite series, which converges as long as all J_A are finite. But $\frac{\Pi_R}{\Pi_\phi}$ is always between 0 and 1, and is increasing in each of the J_A. So the quotient in (20) always makes sense.)

In the model given by (1), (2), and (3), all the J_A are zero except for those A having one or two elements. So the multiplicity functions which we will consider will be multiplicity functions only on the one- and two-element subsets of N; that is, on the vertices and edges of the complete graph on $\{1,2,\ldots,n\}$.

It will be helpful to regard such a function μ graphically by drawing $\mu(\{a,b\})$ bounds between each pair (a,b) of vertices and circling vertex a $\mu(\{a\})$ times. For example, the function μ defined for $n = 4$ by

$$\mu(\{1\}) = 2, \ \mu(\{2\}) = 1,$$

$$\mu(\{1,2\}) = 2, \ \mu(\{1,3\}) = 3, \ \mu(\{2,4\}) = 1,$$

$$\mu(A) = 0 \text{ for all other } A \subseteq N,$$

would be pictured as in diagram 1.

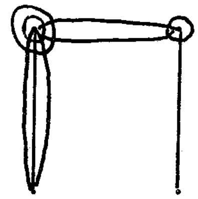

Diagram 1. "Graphic" representation of μ in the example.

For this example, we would also have

$$J_\mu = J_1^2 J_2 J_{12}^2 J_{13}^3 J_{24};$$

$$\mu! = 2!1!2!3!1! = 24;$$

$$\Delta\mu = \{1,3,4\}.$$

3. Reduction of the proof.

In what follows we shall abbreviate $\Pi_{\{i,j,k\}}$, say, by Π_{ijk}, and Π_ϕ by Π_o. We shall also take "$\Delta\mu = ijk$" to mean "$\Delta\mu = \{i,j,k\}$," etc.

(11) and (20) give

(21) $$\Pi_o^3 D_{ijk} = \Pi_o^2 \Pi_{ijk} - \Pi_o \Pi_i \Pi_{jk} - \Pi_o \Pi_j \Pi_{ik} - \Pi_o \Pi_k \Pi_{ij} + 2\Pi_i \Pi_j \Pi_k.$$

From (19) we have, for any subsets R, S, T of N,

(22) $$\Pi_R \Pi_S \Pi_T = \sum_{\Delta\mu=R} \sum_{\Delta\nu=S} \sum_{\Delta\eta=T} \frac{J_\mu J_\nu J_\eta}{\mu!\nu!\eta!}$$

$$= \sum_{\Delta\mu=R\Delta S\Delta T} \sum_{\substack{\nu\leq\mu \\ \Delta\nu=R}} \sum_{\substack{\eta\leq\mu-\nu \\ \Delta\eta=S}} \frac{1}{\eta!\nu!(\mu-\nu-\eta)!} .$$

Thus

(23) $$\Pi_o^3 D_{ijk} = \sum_{\Delta\mu=ijk} A_\mu J_\mu,$$

where

(24) $$A_\mu = \sum_{\substack{\nu\le\mu \\ \Delta\nu=\phi}} \sum_{\substack{\eta\le\mu-\nu \\ \Delta\eta=\phi}} F_{\mu\nu\eta} - \sum_{\substack{\nu\le\mu \\ \Delta\nu=\phi}} \sum_{\substack{\eta\le\mu-\nu \\ \Delta\eta=i}} F_{\mu\nu\eta} - \sum_{\substack{\nu\le\mu \\ \Delta\nu=\phi}} \sum_{\substack{\eta\le\mu-\nu \\ \Delta\eta=j}} F_{\mu\nu\eta}$$

$$- \sum_{\substack{\nu\le\mu \\ \Delta\nu=\phi}} \sum_{\substack{\eta\le\mu-\nu \\ \Delta\eta=k}} F_{\mu\nu\eta} + \sum_{\substack{\nu\le\mu \\ \Delta\nu=i}} \sum_{\substack{\eta\le\mu-\nu \\ \Delta\eta=j}} F_{\mu\nu\eta} + \sum_{\substack{\nu\le\mu \\ \Delta\nu=i}} \sum_{\substack{\eta\le\mu-\nu \\ \Delta\eta=k}} F_{\mu\nu\eta}$$

and

(25) $$F_{\mu\nu\eta} = \frac{1}{\eta!\,\nu!\,(\mu-\nu-\eta)!} .$$

Regrouping:

(26) $$A_\mu = \sum_{\substack{\nu\le\mu \\ \Delta\nu=\phi}} \frac{R_{\mu\nu}}{\nu!} - \sum_{\substack{\nu\le\mu \\ \Delta\nu=j \text{ or } k}} \frac{R_{\mu\nu}}{\nu!}$$

where

(27) $$R_{\mu\nu} = \sum_{\substack{\eta\le\mu-\nu \\ \Delta\eta=\phi}} \frac{1}{\eta!(\mu-\nu-\eta)!} - \sum_{\substack{\eta\le\mu-\nu \\ \Delta\eta=i}} \frac{1}{\eta!(\mu-\nu-\eta)!} .$$

Let

(28) $$B_\lambda(A) = \{\kappa \le \lambda : \Delta\kappa = A\}$$

for an arbitrary subset A of N and multiplicity function λ. Then proposition 1 in section 9 of (KS), which is our main lemma, provides that

(29) $$R_{\mu\nu} = \begin{cases} 0 \quad \text{if } B_{\mu-\nu}(i) \ne \phi \\ \displaystyle\sum_{\substack{\eta\le\mu-\nu \\ \Delta\eta=\phi}} \frac{1}{\eta!(\mu-\nu-\eta)!} \text{ if } B_{\mu-\nu}(i) = \phi \end{cases}$$

Thus

(30) $$A_\mu = \sum_{\substack{\nu\le\mu \\ \Delta\nu=\phi \\ B_{\mu-\nu}(i)=\phi}} \sum_{\substack{\eta\le\mu-\nu \\ \Delta\eta=\phi}} \frac{1}{\nu!\eta!(\mu-\nu-\eta)!} - \sum_{\substack{\nu\le\mu \\ \Delta\nu=j \text{ or } k \\ B_{\mu-\nu}(i)=\phi}} \sum_{\substack{\eta\le\mu-\nu \\ \Delta\eta=\phi}} \frac{1}{\nu!\eta!(\mu-\nu-\eta)!}$$

Replacing $\mu - \nu$ by λ, we get

(31)
$$A_\mu = \sum_{\substack{\lambda\leq\mu \\ \Delta\lambda=ijk \\ B_\lambda(i)=\phi}} \sum_{\substack{\eta\leq\lambda \\ \Delta\eta=\phi}} \frac{1}{(\mu-\lambda)!\eta!(\lambda-\eta)!}$$

$$- \sum_{\substack{\lambda\leq\mu \\ \Delta\lambda=ij \text{ or } ik \\ B_\lambda(i)=\phi}} \sum_{\substack{\eta\leq\lambda \\ \Delta\eta=\phi}} \frac{1}{(\mu-\lambda)!\eta!(\lambda-\eta)!}$$

Reversing the order of summation:

(32)
$$A_\mu = \sum_{\substack{\eta\leq\mu \\ \Delta\eta=\phi}} \frac{1}{\eta!} \sum_{\substack{\eta\leq\lambda\leq\mu \\ \Delta\lambda=ijk \\ B_\lambda(i)=\phi}} \frac{1}{(\mu-\lambda)!(\lambda-\eta)!}$$

$$- \sum_{\substack{\eta\leq\lambda\leq\mu \\ \Delta\lambda=ij \text{ or } ik \\ B_\lambda(i)=\phi}} \frac{1}{(\mu-\lambda)!(\lambda-\eta)!} .$$

So to prove $D_{ijk} \leq 0$ (which is our theorem), it suffices to show that for every μ with $\Delta\mu = ijk$ and every $\eta \leq \mu$ with $\Delta\eta = \phi$, we have

(33)
$$\sum_{\substack{\eta\leq\lambda\leq\mu \\ \Delta\lambda=ijk \\ B_\lambda(i)=\phi}} \frac{1}{(\mu-\lambda)!(\lambda-\eta)!} \leq \sum_{\substack{\eta\leq\lambda\leq\mu \\ \Delta\lambda=ij \text{ or } ik \\ B_\lambda(i)=\phi}} \frac{1}{(\mu-\lambda)!(\lambda-\eta)!} .$$

Now if $B_\eta(i) \neq \phi$, then $\lambda \geq \eta$ implies $B_\lambda(i) \neq \phi$, so that both sums in (33) are empty sums. So we assume that $B_\eta(i) = \phi$. Because of this, we can rewrite (33), letting $\nu = \lambda - \eta$, as

(34)
$$\sum_{\substack{0\leq\nu\leq\mu-\eta \\ \Delta\nu=ijk \\ B_\nu(i)=\phi}} \frac{1}{\nu!(\mu-\eta-\nu)!} \leq \sum_{\substack{0\leq\nu\leq\mu-\eta \\ \Delta\nu=ij \text{ or } ik \\ B_\nu(i)=\phi}} \frac{1}{\nu!(\mu-\eta-\nu)!} .$$

Finally, replacing $\mu - \lambda$ with μ, we see that it is sufficient to prove that for any μ with $\Delta\mu = ijk$, we have

(35)
$$\sum_{\nu\varepsilon L} \frac{1}{\nu!(\mu-\nu)!} \leq \sum_{\nu\varepsilon R} \frac{1}{\nu!(\mu-\nu)!}$$

where

$$L = \{\nu: \nu \leq \mu, \Delta\nu = ijk, B_\nu(i) = \phi\},$$

$$R = \{\nu: \nu \leq \mu, \Delta\nu = ij \text{ or } ik, B\nu(i) = \phi\}.$$

4. Proof of (35).

Now we view multiplicity functions graphically as in section 2 above. We will say that μ has a singleton at vertex a if a is circled, i.e. if $\mu(\{a\}) \geq 1$; and that μ has a bond $\{a,b\}$ if $\mu(\{a,b\}) \geq 1$. In fact, μ has $\mu(\{a,b\})$ bonds between a and b.

A chain beginning at a and ending at b (or vice versa) is a finite sequence of distinct bonds $\{a,a_1\}$, $\{a_1,a_2\}$, $\ldots,\{a_{n-1},a_n\},\{a_n,b\}$. A cycle is a chain between a and a passing through at least one other vertex.

A subset of N is connected (with respect to a given μ) if there is a chain between every pair of vertices in the subset; it is a component of μ if it is not a proper subset of any connected set. The components of μ are of course disjoint.

Now the condition $B_\mu(i) \neq \phi$ means that there is a function $\lambda \leq \mu$ with $\Delta\lambda = i$; this means μ has either a singleton at i or a chain beginning at i with a singleton at one of its vertices.

So if $\Delta\nu = ijk$ and $B_\nu(i) = \phi$, then ν has a component containing i, and this component cannot have a singleton (or else $B_\nu(i) \neq \phi$). But i appears an odd number of times among the singletons and bonds of ν, so μ must contain a chain beginning at i and ending at some other vertex,which chain cannot be lengthened. Since $\Delta\nu = ijk$, this other vertex must be j or k. Suppose for definiteness that it is j.

Then this component cannot contain k; for in order that $\Delta\nu = ijk$, there must be either a singleton at k or a chain beginning at k and having a singleton at one of its vertices. (This is because ν already has a chain from i to j which cannot be lengthened.)

Summing up the results of the last three paragraphs: if $\Delta\nu = ijk$ and $B_\nu(i) = \phi$, then ν has a component ν_m containing i and either j or k, with no singletons; we call this the <u>main component</u>. ν also has a component ν_o containing k or j and a singleton; we call this the <u>odd component</u>. ν will in general have other components ν_n, all satisfying $\Delta\nu_n = \phi$; we call them <u>null components</u>.

In similar fashion we see that if $\Delta\nu = ij$ or ik and $B_\nu(i) = \phi$, then ν has a main component containing i and either j or k, with no singletons; all other components are null.

Now for any fixed ν in L, with main component ν_m, let L_ν be the set of all functions in L with main component ν_m, and let R_ν be the set of functions in R with main component ν_m. To prove (35) it suffices to show that for every ν in L,

$$(36) \qquad \sum_{\lambda\varepsilon L_\nu} \frac{1}{\lambda!(\mu-\lambda)!} \leq \sum_{\lambda\varepsilon R_\nu} \frac{1}{\lambda!(\mu-\lambda)!}$$

Suppose for definiteness again that $j \varepsilon \nu_m$, $k \notin \nu_m$. Then every λ in L_ν is of the form $\lambda = \nu_m + \eta$, where $\eta \leq \lambda - \nu_m$ and $\Delta\eta = k$; the requirement $B_\eta(i) = \phi$ is vacuously satisfied for $\eta \leq \lambda - \nu_m$ (since ν_m contains i).

Similarly, every λ in R_ν is of the form $\lambda = \nu_m + \eta$, where $\eta \leq \lambda - \nu_m$ and $\Delta\eta = \phi$.

Thus (36) can be written

$$(37) \quad \frac{1}{\nu_m!} \sum_{\substack{\eta\leq\lambda-\nu_m \\ \Delta\eta=k}} \frac{1}{\eta!(\lambda-\nu_m-\eta)!} \leq \frac{1}{\nu_m!} \sum_{\substack{\eta\leq\lambda-\nu_m \\ \Delta\eta=\phi}} \frac{1}{\eta!(\mu-\nu_m-\eta)!} .$$

But this follows immediately from proposition 1 of section 9 of (KS). End of proof.

REFERENCES

1. D. G. Kelly and S. Sherman, J. Math. Phys. 9, 466-484 (1968). See also R. B. Griffiths, J. Math. Phys. 8, 478-483 and 484-489 (1967).