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Magnetization Concavity in Ferromagnets

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We investigate the conjecture that in Ising ferromagnets, single-site magnetization $\langle \sigma_x \rangle$ is a jointly concave function of the magnetic field variables. We present partial results favoring the conjecture, including a numerical survey, although we do not prove it in full generality. We also point out some implications of concavity.

KEY WORDS: Ising model; magnetization; concavity; correlation inequality.

1. INTRODUCTION

In a finite classical spin-1/2 Ising ferromagnet with pair interactions,[(6)] we study the dependence on magnetic field variables of the single-site magnetization $m_x = \langle \sigma_x \rangle$ and total magnetization $M = \sum_x \langle \sigma_x \rangle$. Specifically, we investigate the concavity of the magnetizations m_x and M as functions of $\mathbf{h}$. (Here we have assembled the field variables h_y into a vector $\mathbf{h}$.) It follows from the G.H.S. inequality[(4)] that m_x has a restricted type of concavity in the ferromagnetic orthant $\{\mathbf{h} \geqslant 0\}$: it is concave along any line whose direction vector has nonnegative components. Our purpose in this paper is to analyze the conjecture that m_x is (jointly) concave in $\{\mathbf{h} \geqslant 0\}$, without restriction:

Conjecture 1. In a finite classical spin-1/2 Ising ferromagnet with arbitrary pair interactions, any single-site magnetization $m_x = \langle \sigma_x \rangle$ is a jointly concave function of the magnetic field variables $\mathbf{h}$ throughout the ferromagnetic orthant $\{\mathbf{h} \geqslant 0\}$.

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This conjecture may be restated as negative semidefiniteness of the Hessian matrix $\partial^2 m_x/\partial h_y \partial h_z$, whose entries are third-order Ursell functions $u_3(\sigma_x, \sigma_y, \sigma_z)$. Alternately, since

$$\sum_{y,z} c_y c_z u_3(\sigma_x, \sigma_y, \sigma_z) = \frac{\partial}{\partial h_x}\left(\left\langle\left(\sum_y c_y \sigma_y\right)^2\right\rangle - \left\langle\sum_y c_y \sigma_y\right\rangle^2\right) \tag{1}$$

another equivalent version of the conjecture is that the variance of any linear combination $\sum_y c_y \sigma_y$ of the spins decreases in the field variables h_x. This is a quantitative expression of the idea that increasing the fields drives the spins toward $+1$. A natural weakening of the conjecture replaces single-site magnetization m_x by total magnetization M.

We are unable to prove Conjecture 1 in full generality. This paper is devoted to partial results establishing it in many special cases. In Section 2 we demonstrate some form of concavity for simple examples: two-site models, mean-field models, and one-dimensional nearest-neighbor models. In Section 3 we summarize the results of a numerical study, which supports Conjecture 1. We conclude in Section 4 with a few implications of the conjecture. An Appendix contains some sample numerical data, and several formulas invoked in Section 2.

We use the common notation $\langle f \rangle$ for the thermal average of an observable f (see Ref. 6) and take inverse temperature $\beta = 1$.

2. CONCAVITY IN SIMPLE MODELS

In this section we examine two-site, mean-field, and one-dimensional Ising ferromagnets by means of inequalities and explicit calculations. To obtain tractable formulas for the thermal averages in mean-field and one-dimensional ferromagnets, we require translation invariance.

The site-0 magnetization Hessian $f_{yz} = \partial^2 \langle \sigma_0 \rangle / \partial h_y \partial h_z$ of a two-site model (sites labeled 0, 1) is a 2×2 symmetric matrix with negative entries (G.H.S. inequality). It will be negative definite if its determinant is positive. Computing,

$$\det(f) = 4\langle \sigma_0 \rangle (\langle \sigma_0 \sigma_1 \rangle - \langle \sigma_0 \rangle \langle \sigma_1 \rangle)(\langle \sigma_1 \rangle - \langle \sigma_0 \rangle \langle \sigma_0 \sigma_1 \rangle) \tag{2}$$

which is positive by the Griffiths inequalities.[3] Note that since more sites can be added without changing this computation, it follows in ferromagnets of arbitrary size that m_x is concave when restricted to the two-dimensional quadrants $\{h_x \geqslant 0, h_y \geqslant 0;$ all other h_z fixed$\}$.

The translation-invariant mean-field Hamiltonian with N sites (labeled from 0) is

$$-H = \frac{J}{2N} \sum_{y,z} \sigma_y \sigma_z + h \sum_y \sigma_y, \qquad J, h > 0 \tag{3}$$

The negated Hessian $-F_{yz} = -\partial^2 M/\partial h_y \partial h_z$ of the total magnetization has only two distinct entries:

$$D = -F_{yy} = 2\langle\sigma_0\rangle(1 - N\langle\sigma_0\rangle^2 + [N-1]\langle\sigma_0\sigma_1\rangle), \qquad 0 \leqslant y \leqslant N-1 \tag{4}$$

$$E = -F_{yz} = D - (N-2)(\langle\sigma_0\sigma_1\sigma_2\rangle - \langle\sigma_0\rangle\langle\sigma_0\sigma_1\rangle) - 2\langle\sigma_0\rangle(1 - \langle\sigma_0\sigma_1\rangle), \qquad y \neq z \tag{5}$$

Since

$$-\sum_{y,z} c_y c_z F_{yz} = E\Big(\sum_y c_y\Big)^2 + (D-E)\sum_y (c_y)^2 \tag{6}$$

and $D > E > 0$ by the G.H.S. and Griffiths inequalities, the Hessian F of total magnetization is negative definite. Local joint concavity of M in $\mathbf{h}$ (for $\mathbf{h}$ approximately uniform) now follows trivially by continuity.

The negated Hessian $-f_{yz} = -\partial^2\langle\sigma_0\rangle/\partial h_y \partial h_z$ of the site-0 magnetization of the mean-field model (3) has three distinct entries:

$$u = -f_{00} = 2\langle\sigma_0\rangle(1 - \langle\sigma_0\rangle^2) \tag{7}$$

$$v = -f_{0y} = -f_{yy} = 2\langle\sigma_0\rangle(\langle\sigma_0\sigma_1\rangle - \langle\sigma_0\rangle^2), \qquad 0 \neq y \tag{8}$$

$$w = -f_{yz} = v - (\langle\sigma_0\sigma_1\sigma_2\rangle - \langle\sigma_0\rangle\langle\sigma_0\sigma_1\rangle), \qquad 0, y, z \text{ distinct} \tag{9}$$

Since $u > v > w > 0$ by the G.H.S. and Griffiths inequalities, the identity

$$-\sum_{y,z} c_y c_z f_{yz} = \Big(\sqrt{u}\, c_0 + \frac{v}{\sqrt{u}} \sum_1^{N-1} c_y\Big)^2 + \Big(w - \frac{v^2}{u}\Big)\Big(\sum_1^{N-1} c_y\Big)^2 + (v - w)\sum_1^{N-1}(c_y)^2 \tag{10}$$

shows the inequality $uw \geqslant v^2$, if true, would imply that f is negative definite. In terms of correlations, the proposed inequality for mean-field models becomes

$$-u_3(\sigma_0, \sigma_1, \sigma_2) \geqslant \langle\sigma_0\rangle(2\langle\sigma_0\sigma_1\rangle^2 - \langle\sigma_0\rangle\langle\sigma_0\sigma_1\sigma_2\rangle - \langle\sigma_0\rangle^2\langle\sigma_0\sigma_1\rangle) \tag{11}$$

We are unable to prove (11), which is a comparison of two positive quantities. However, a numerical check of (11) in a thousand mean-field models with 3 to 15 sites yields no counterexamples. Sample data appear in the Appendix.

A by-product of this survey concerns mean-field bounds.[7] Although the magnetization $\langle\sigma_0; N\rangle$ of an N-site model appears to increase monotonically in N to its limiting and bounding self-consistent value $\langle\sigma_0;\infty\rangle$, the two-point function $\langle\sigma_0\sigma_1;N\rangle$ for finite N may exceed its limiting value $\langle\sigma_0\sigma_1;\infty\rangle$. Thus, a mean-field bound on the two-point function analogous to the known magnetization bound appears problematic.

The translation-invariant one-dimensional nearest-neighbor Hamiltonian with N sites (labeled from 0) is

$$-H = J\sum_y \sigma_y\sigma_{y+1} + h\sum_y \sigma_y, \qquad J, h > 0 \tag{12}$$

The boundary condition is periodic: $\sigma_N \equiv \sigma_0$. All expectations in this model —in particular, the entries of the magnetization Hessian—can be conveniently calculated by transfer-matrix methods.[6]

The Hessian $F_{yz} = \partial^2 M/\partial h_y \partial h_z$ of the total magnetization is a Töplitz matrix. It is therefore diagonalized by the finite Fourier transform, with eigenvalues

$$\lambda_p = \sum_x F_{0x} e^{ipx}, \qquad p = \frac{2\pi k}{N}, \qquad 0 \leqslant k \leqslant N-1 \tag{13}$$

The lowest eigenvalue λ_0 is negative by the G.H.S. inequality. A somewhat lengthy calculation yields a formula for the other eigenvalues:

$$\begin{aligned}\lambda_p = -\alpha_p\Big\{&(1-r^{2N})\big(1+2r-2\big[1+2c_p\big]r^2+2r^3+r^4\big)\\ &-\big(1-2c_p r + r^2\big)(1-r^2)2Nr^N\Big\}\end{aligned} \tag{14}$$

Here $c_p = \cos(p)$, r lies in $(0,1)$ and is the ratio of smallest to largest eigenvalues in the transfer matrix, and $\alpha_p > 0$ is a positive factor given explicitly in the Appendix. The sign of λ_p is thus controlled by the factor $\{\cdot\}$ in curly brackets, which we claim is positive for all $c_p \in [-1,1]$. To show this, we underestimate the term $(1-r^{2N})$ in (14) by the inequality

$$1 - r^{2n} \geqslant N(1-r^2)r^{N-1}, \qquad 0 \leqslant r \leqslant 1 \tag{15}$$

whose proof we temporarily defer. [A simple worst-case analysis with $c_p = +1$ demonstrates that the term multiplying $(1-r^{2N})$ is nonnegative.] Using (15) in (14) and performing some cancellations, we find

$$\lambda_p \leqslant -\alpha_p N r^{N-1}(1-r^2)^3, \qquad 0 < r < 1 \tag{16}$$

Thus the Hessian is negative definite, and the total magnetization jointly concave, for approximately uniform fields $\mathbf{h}$.

It remains to establish (15). By convexity of the exponential function $f(x) = r^{2x}$,

$$\sum_{j=0}^{N-1} r^{2j} \geqslant N r^{N-1} \tag{17}$$

Since $0 \leqslant r \leqslant 1$,

$$(1 - r^{2N}) = (1 - r^2) \sum_0^{N-1} r^{2j} \geqslant N(1 - r^2) r^{N-1} \tag{18}$$

as claimed.

3. NUMERICAL STUDY

We studied Conjecture 1 numerically. The investigation had two parts: a broad survey of examples, and a purposeful search for a counterexample.

In the survey, we examined several thousand Ising ferromagnets chosen at random. The randomly selected parameters were the exponentiated fields and couplings $\exp(-2h_y)$ and $\exp(-2J_{yz})$, taken independently and uniformly from (0, 1). Site number N ranged from 3 to 10, inclusive. After a preliminary transformation to tridiagonal form, we applied the usual determinant criterion to test the site-0 magnetization Hessian $f_{yz} = \partial^2 m_0 / \partial h_y \partial h_z$ for definiteness. One must take some care to compute f_{yz} accurately, as it can be a nearly singular matrix if fields or couplings become too large or too small.

All examples in the survey were consonant with Conjecture 1; the site-0 magnetization Hessian f_{yz} was negative definite in every instance. Sample data appear in the Appendix.

We used a nonlinear optimization routine[1] to seek a counterexample actively. The routine altered fields h_y and couplings J_{yz} so as to maximize the algebraically largest eigenvalue of the site-0 magnetization Hessian f. We considered ferromagnets with site number N between 3 and 6, inclusive. For each N, we randomly picked 50 sets of fields and couplings as starting points.

We found no counterexamples to Conjecture 1. In each case, the optimization routine merely drove fields and couplings to the boundary of the ferromagnetic region, and the maximum eigenvalue of the Hessian to 0.

4. IMPLICATIONS

We summarize a few of the consequences Conjecture 1 would have, if true. To simplify the language, we write as if the conjecture had been proved.

Conjecture 1 extends at once by Griffiths' "analog system" approximation scheme[3] to ferromagnet models with certain other *a priori* spin distributions. Higher-spin models, models with uniform spin distribution, and lattice ϕ^4 fields are examples of this type.

Another corollary of Conjecture 1 follows by differentiating the site-x magnetization Hessian f with respect to external field h_w at $\mathbf{h}=0$. Since $f(0)=0$, the resulting matrix f', with entries

$$f'_{yz} = \langle \sigma_w \sigma_x \sigma_y \sigma_z \rangle - \langle \sigma_x \sigma_w \rangle \langle \sigma_y \sigma_z \rangle - \langle \sigma_x \sigma_y \rangle \langle \sigma_w \sigma_z \rangle - \langle \sigma_x \sigma_z \rangle \langle \sigma_w \sigma_y \rangle \quad (19)$$

is negative semidefinite for any choice x and w. This matrix inequality holds for all $\mathbf{h} \geqslant 0$ by the "ghost spin" method of Ref. 2. It may have implications for the triviality of the ϕ_4^4 field theory; see Ref. 5.

In translation-invariant models, the reinterpretation (1) implies that the amplitudes $\langle |\sum_y \sigma_y e^{ipy}|^2 \rangle$ with $p \neq 0$ decrease in all external field variables (see Section 2 for notation).

We conclude by applying Conjecture 1 to the problem of locating the extrema of single-site and total magnetization on the simplex of fixed total flux

$$\Phi = \sum_y h_y, \qquad \mathbf{h} \geqslant 0 \quad (20)$$

For any interaction, joint concavity ensures a global minimum at some vertex (all flux at a single site). If the pair interaction has sufficient geometric structure—typically, translation invariance—one can also identify a global maximum of the total magnetization $M(\mathbf{h})$. Specifically, let G be a (finite) group acting linearly on the ferromagnetic orthant $\{\mathbf{h} \geqslant 0\}$, under which M is invariant. Assume that each simplex (20) is invariant under G, and that the uniform configurations (simplex centroids)

$$h_y = \Phi/N, \qquad \forall y \quad (21)$$

are the only fixed points of G. By averaging over G, joint concavity ensures a global maximum of M at the uniform configuration (21). For mean-field interactions, this maximum property may be proved independently of Conjecture 1.

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APPENDIX

We define the factor α_p appearing in (14). We then present sample numerical data.

Let $\tau_+ > \tau_- > 0$ be the eigenvalues and e_+, e_- the corresponding unit eigenvectors of the transfer matrix

$$T = \begin{pmatrix} e^{J-h} & e^{-J} \\ e^{-J} & e^{J+h} \end{pmatrix} \tag{22}$$

Let Σ be the spin matrix

$$\Sigma = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \tag{23}$$

Define the matrix element u by

$$u = e_+^T \sum e_+ \tag{24}$$

Then $0 < u < 1$ for $h, J > 0$. The values of r and α_p in (14) are

$$r = \tau_- / \tau_+ \tag{25}$$

$$\alpha_p = \frac{2u(1-u^2)}{(1+r^N)^2(1-2c_p r + r^2)^2} \tag{26}$$

Data from Mean-Field Survey

Example 1. With $J = 0.2$ and $H = 0.2$, we have the following table. Note that $\langle\sigma_0\rangle$ increases with N, but $\langle\sigma_0\sigma_1\rangle$ and $\langle\sigma_0\sigma_1\sigma_2\rangle$ do not. Data rounded to five digits.

N	$\langle\sigma_0\rangle$	$\langle\sigma_0\sigma_1\rangle$	$\langle\sigma_0\sigma_1\sigma_2\rangle$	$uw - v^2$
3	0.22408	0.11452	$0.49308E-1$	$0.13705E-2$
4	0.22844	0.10182	$0.42662E-1$	$0.90374E-3$
5	0.23121	$0.93880E-1$	$0.38138E-1$	$0.63971E-3$
10	0.23715	$0.77213E-1$	$0.27594E-1$	$0.19844E-3$
15	0.23927	$0.71410E-1$	$0.23549E-1$	$0.95228E-4$

Example 2. With $J = 0.4$, $H = 1.0$, we have the following table. Note that unlike Example 1, $\langle\sigma_0\rangle$, $\langle\sigma_0\sigma_1\rangle$, and $\langle\sigma_0\sigma_1\sigma_2\rangle$ all increase with N. Data rounded to five digits.

N	$\langle\sigma_0\rangle$	$\langle\sigma_0\sigma_1\rangle$	$\langle\sigma_0\sigma_1\sigma_2\rangle$	$uw - v^2$
3	0.83760	0.71674	0.62187	$0.13031E-2$
4	0.84710	0.72758	0.63142	$0.60663E-3$
5	0.85270	0.73445	0.63773	$0.33734E-3$
10	0.86359	0.74883	0.65173	$0.59670E-4$
15	0.86711	0.75377	0.65680	$0.23202E-4$

Data from General Concavity Survey

The Hamiltonian is defined by

$$-H = \sum_{y>z} J_{yz}\sigma_x\sigma_y + \sum h_y\sigma_y \tag{27}$$

Numerical values are rounded to five digits.

Example 3.

Number of sites N:	5				
Magnetic fields h_y :	0.73785	0.46747	0.29512	0.44708	0.6158
Couplings J_{yz} , $y > z$:	1.8363				
	1.6376	0.39675			
	0.93374	0.067699	0.18538		
	0.52510	0.76631	0.13675	0.42623	
Site-0 magnetization $\langle\sigma_0\rangle$:	0.98539				

Hessian $f_{yz} = \partial^2\langle\sigma_0\rangle/\partial h_y\partial h_z$ of site-0 magnetization:

$-5.7174E-2$	$-5.5906E-2$	$-5.5612E-2$	$-4.9168E-2$	$-4.9832E$
$-5.5906E-2$	$-5.5809E-2$	$-5.4527E-2$	$-4.8369E-2$	$-4.9491E$
$-5.5612E-2$	$-5.4527E-2$	$-5.5059E-2$	$-4.8025E-2$	$-4.8692E$
$-4.9168E-2$	$-4.8369E-2$	$-4.8025E-2$	$-4.7614E-2$	$-4.4525E$
$-4.9832E-2$	$-4.9491E-2$	$-4.8692E-2$	$-4.4525E-2$	$-4.9140E$

Number of nonnegative eigenvalues of Hessian: 0.

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