Journal of Statistical Physics, Vol. 23, No. 3, 1980

Nonconcavity of the Magnetization in Ising Ferromagnets

James L. Monroe[1]

Received December 17, 1979

Some Ising ferromagnets having nonconcave magnetization are presented as counterexamples to the often assumed case of concave magnetization.

KEY WORDS: Ising ferromagnet; magnetization; GHS inequality.

In 1968 Kelly and Sherman[1] in a paper on correlation inequalities listed a number of open questions, one being: Prove or disprove that for ferromagnetic Ising systems the average magnetization per spin M is a concave function of the external magnetic field H for $H > 0$. By ferromagnetic systems we mean systems with positive interactions between spins. Two years later, Griffiths *et al.*[2] gave a proof for ferromagnetic Ising systems having only pair interactions and H. The proof was based on the following correlation inequality:

$$\langle\sigma_i\sigma_j\sigma_k\rangle - \langle\sigma_i\rangle\langle\sigma_j\sigma_k\rangle - \langle\sigma_j\rangle\langle\sigma_i\sigma_k\rangle - \langle\sigma_k\rangle\langle\sigma_i\sigma_j\rangle + 2\langle\sigma_i\rangle\langle\sigma_j\rangle\langle\sigma_k\rangle \leqslant 0 \quad (1)$$

where the σ's are Ising spin variables, $\sigma = \pm 1$, and where the subscripts i, j, and k label the ith, jth, and kth spins.

The restriction to pair interactions is an essential restriction in the proof of the inequalities. Kelly and Sherman[1] gave a counter example to this inequality using a system of Ising spins with a three-body interaction. The inequality is, however, only a sufficient condition for the concavity of the magnetization, not a necessary condition. We know of no results on the actual concavity or lack of concavity of M for ferromagnetic Ising systems other than those for systems with pair interactions[2] and those for systems containing only one spin.[3]

Since the concavity of M is used in proving certain thermodynamic

[1] Physics Department, Beaver Campus, The Pennsylvania State University, Monaca, Pennsylvania 15061.

0022-4715/80/0900-0315$03.00/0

inequalities for critical point exponents[4,5] and generally is considered a plausible conjecture for ferromagnetic Ising systems,[1] examples of positive interaction systems with nonconcave M are of interest. In the remainder of the paper we give examples of such systems. First we begin with some notation and definitions.

The average magnetization per spin M for a system of N spins is

$$M = \frac{1}{N} \sum_{i=1}^{N} \langle \sigma_i \rangle \tag{2}$$

where $\langle \sigma_i \rangle$ is the thermal average of σ_i. It is given by

$$\langle \sigma_i \rangle = \sum_{\{\sigma\}} \sigma_i \exp[-\mathscr{H}(\{\sigma\})] \Big/ \sum_{\{\sigma\}} \exp[-\mathscr{H}(\{\sigma\})] \tag{3}$$

where $\{\sigma\}$ is the set of allowed configurations of the system and $\mathscr{H}(\{\sigma\})$ is the Hamiltonian of the system.

The first example is a slight generalization of the three-body interaction system of Kelly and Sherman[1] used as a counterexample to inequality (1). The Hamiltonian of the system is

$$\mathscr{H}(\{\sigma\}) = -K\sigma_1\sigma_2\sigma_3 - J(\sigma_1\sigma_2 + \sigma_2\sigma_3 + \sigma_3\sigma_1) - H(\sigma_1 + \sigma_2 + \sigma_3) \tag{4}$$

where we take $J \geqslant 0$, $H \geqslant 0$, and $K \geqslant 0$. Then M is easily found to be

$$M = \frac{X^4 \operatorname{sh}(3H + K) + \operatorname{sh}(H - K)}{X^4 \operatorname{ch}(3H + K) + 3 \operatorname{ch}(H - K)} \tag{5}$$

where $X \equiv e^J$. The second derivative of M with respect to H evaluated to lowest order in H is

$$\frac{\partial^2 M}{\partial H^2} = \frac{8[(24X^4 - 8X^8)(V^3 - 1/V^3) + (9 - 3X^4 + 19X^8 - 9X^{12})(V - 1/V)}{[(3 + X^4)(V + 1/V)]^3} \tag{6}$$

where $V \equiv e^K$. Both the numerator and denominator are positive for certain values of X and V, e.g., $X^4 < 2$ and $V > 1$. Therefore in the region of small H, M is convex for a range of values of X and V.

In the above example the three-body interaction term does not have the spin-flip symmetry usually associated with ferromagnetic interactions, i.e., if we take the negative of all spin values, we do not have the same interaction energy. Because of this lack of symmetry, M is no longer an odd function of H. One might suppose that if we restrict our interactions to being both positive and having this spin-slip symmetry, M would be concave for all $H > 0$. That this is not the case is shown by the next example.

Consider a four-spin system with Hamiltonian

$$\mathscr{H}(\{\sigma\}) = -L\sigma_1\sigma_2\sigma_3\sigma_4 - J(\sigma_1\sigma_2 + \sigma_2\sigma_3 + \sigma_3\sigma_4 + \sigma_4\sigma_1) - H(\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4) \tag{7}$$

The magnetization is found to be

$$M = \frac{X^8 W^2 \operatorname{sh}(4H) + 2X^4 \operatorname{sh}(2H)}{X^8 W^2 \operatorname{ch}(4H) + 4X^4 \operatorname{ch}(2H) + 2X^4 W^2 + W^2} \tag{8}$$

where $X \equiv e^J$ and $W \equiv e^L$. The second derivative of M with respect to H to lowest order in H is

$$\begin{aligned}\frac{\partial^2 M}{\partial H^2} = \{&16X^4H[(4X^4 + 16X^8 + 12X^{12} - 8X^{16} - 8X^{20})W^6 \\ &+ (1 + 4X^4 + 14X^8 + 20X^{12} - 39X^{16})W^4 \\ &- (4X^4 + 8X^8 + 36X^{12})W^2 - 32X^8]\} \\ &\times [(1 + 2X^4 + X^8)W^2 + 4X^4]^{-3}\end{aligned} \tag{9}$$

The denominator is positive; the numerator can be made positive when

$$(1 + 3X^4) > 2X^{12} \tag{10}$$

by choosing W large enough. For example, let $X^4 = 1.2$; then for $W \geqslant 2$ the numerator is positive. Therefore as in the previous example for small H the magnetization is convex.

We conclude with two examples which are variations of the previous system. These illustrate first that one can have the nonconcavity of M in higher spin systems, and second, in the thermodynamic limit. For the first example we replace the σ_i of Eq. (7) with S_i, where $S_i = \pm 1$ or 0. Setting, for simplicity, J equal to zero, M is

$$\begin{aligned}M = {} & [2W^2 \operatorname{sh}(4H) + 6W \operatorname{sh}(3H) + (6W + 4)\operatorname{sh}(2H) + 4W \operatorname{sh}(H)] \\ & \times [2W^2 \operatorname{ch}(4H) + 8W \operatorname{ch}(3H) + (12W + 8)\operatorname{ch}(2H) \\ & + 32W \operatorname{ch}(H) + (6W^2 + 13)]^{-1}\end{aligned} \tag{11}$$

To leading order in H the second derivative of M with respect to H is

$$\frac{\partial^2 M}{\partial H^2} = \frac{H(2048W^6 + 41600W^5 + 171616W^4 - 270210W^3 - 45952W^2 + 7808)}{(8W^2 + 65W + 8)^3} \tag{12}$$

and as before for W large this is positive.

In our final example we consider a collection of $2N$ σ-spins as shown in Fig. 1. As before the σ's take only the values ± 1. The Hamiltonian for the

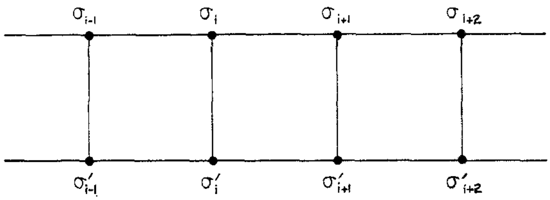

Fig. 1

system is

$$\mathscr{H}(\{\sigma, \sigma'\}) = -L \sum_{i=1}^{N} \sigma_i \sigma_i' \sigma_{i+1} \sigma'_{i+1} - H \sum_{i=1}^{N} (\sigma_i + \sigma_i') \tag{13}$$

where we set $\sigma_{N+1} = \sigma_1$ and $\sigma'_{N+1} = \sigma'_1$. We will be interested in finding M when $N \to \infty$. This can be found by the usual transfer matrix method.[6] After taking $N \to \infty$

$$M = \frac{\mathrm{ch}(H)\,\mathrm{sh}(H)}{[\mathrm{sh}^4(H) + (1/W^4)\,\mathrm{ch}(2H)]^{1/2}} \times \left\{1 - \frac{1 - 1/W^4}{\mathrm{ch}^2(H) + [\mathrm{sh}^4(H) + (1/W^4)\,\mathrm{ch}(2H)]^{1/2}}\right\} \tag{14}$$

where again $W \equiv e^L$. The complexity of M is seen in Fig. 2, where M is plotted as a function of H for various values of W.

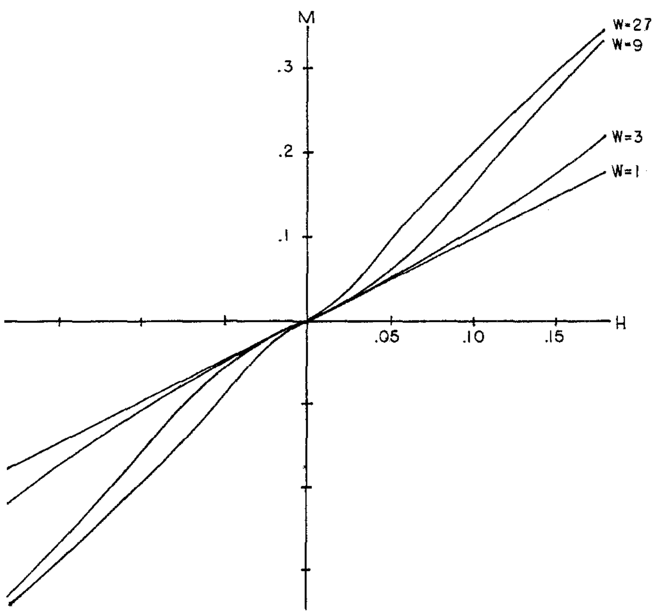

Fig. 2

The above examples illustrate that the concavity of M may not be as ever-present as one might conjecture, since by adding positive four-body interaction to systems with pair interactions we destroy the concavity of M at small H. However, a check of the magnetizations of a six-spin system with only a six-body interaction and an eight-spin system with only an eight-body interaction shows M to be concave for small H. The concavity of M seems to be a subtle feature of the system and we seem to be far from being able to state necessary and sufficient conditions for this concavity.

ACKNOWLEDGMENTS

I would like to thank Profs. R. Griffiths and J. L. Lebowitz for critical readings of the manuscript.

REFERENCES

1. D. G. Kelly and S. Sherman, *J. Math. Phys.* **9**:466 (1968).
2. R. B. Griffiths, C. A. Hurst, and S. Sherman, *J. Math. Phys.* **11**:790 (1970).
3. R. S. Ellis and C. M. Newman, *Trans. Am. Math. Soc.* **237**:83 (1978).
4. R. B. Griffiths, *J. Chem. Phys.* **43**:1958 (1965).
5. R. B. Griffiths, in *Phase Transitions and Critical Phenomena*, Vol. 1, C. Domb and M. S. Green, eds. (Academic Press, London).
6. C. J. Thompson, in *Mathematical Statistical Mechanics* (Macmillan, New York), Chapter 5; K. Huang, *Statistical Mechanics* (Wiley, New York), Chapter 16.