

# Convexity Violations for Noninteger Parameters in Certain Lattice Models

Robert B. Griffiths<sup>1</sup> and P. D. Gujrati<sup>2</sup>

*Received April 27, 1982*

---

The convexity of the free energy is studied for several lattice models in situations in which a parameter which is normally a positive integer takes on noninteger real values. Examples include the number  $n$  of components in the  $n$ -vector model, the number of states in the Potts model, and the dimensionality of the lattice. In a typical case there is a critical value of the parameter such that convexity is preserved when the parameter exceeds the critical value, but can be violated for appropriate Hamiltonians whenever the parameter is less than the critical value, but not a positive integer. In several cases the critical value of the parameter increases with the size of the system, thus raising questions about the significance of a continuous variation of the parameter in the thermodynamic limit.

---

**KEY WORDS:** Convexity; noninteger; analytic continuation;  $n$  vector; Potts.

## 1. INTRODUCTION

In statistical mechanics there are a number of cases in which a lattice model is well defined when a certain parameter is a positive integer, but it is also convenient to consider, at least in a formal sense, what happens when this parameter is a real number not limited to positive integers. Examples of such parameters are: the space dimensionality  $d$  of a lattice, the number of components  $n$  in the  $n$ -vector model,<sup>3</sup> the number  $q$  of states in the Potts

---

<sup>1</sup> Department of Physics, Carnegie-Mellon University, Pittsburgh, Pennsylvania 15213.

<sup>2</sup> Present address: James Franck Institute, University of Chicago, 5640 Ellis Ave., Chicago, Illinois 60637.

<sup>3</sup> It is standard practice in renormalization group studies to treat  $d$  and  $n$  as continuous variables. See, for example, Refs. 1–4. Specific reference to cases in which  $n$  is not a positive integer will be found in Refs. 5–7 (and in numerous other papers).

model,<sup>4</sup> and the number  $n$  of replicas in the replica approach to random magnets.<sup>(11)</sup>

Even a casual inspection of the relevant literature will show that theoretical physicists tend to ascribe a certain “mathematical reality” to properties of such models when these parameters are not integers. Thus, for example, we are told that the crossover or critical dimensionality for a fourth-order multicritical point<sup>(12)</sup> is  $d = 8/3$ ; that the critical value of  $n$  (in the  $n$ -vector model) for stability of the cubic fixed point for  $d = 3$  is approximately<sup>(13)</sup>  $n = 3.128$ ; and that for  $d = 3$  and  $q$  greater than  $2.6 \pm 0.1$ , the Potts model has a first-order transition.<sup>(10)</sup>

Such examples (and many others could be given) raise an important issue: is it really possible to say unambiguously what one means when talking about the dependence of various “physical” quantities on noninteger values of these parameters? Are there specific mathematical models associated with these noninteger values? And if so, do they possess a thermodynamic limit and a convex free energy<sup>(17,18)</sup> (and possibly other properties), as do models with integer parameters? These are interesting and important questions which—so far as we know—have received little attention in the literature.<sup>5</sup>

One very plausible suggestion is that one should use an analytic continuation of the partition function, correlation functions, etc. to extend results which can be calculated for positive integers to other real values of a parameter.<sup>6</sup> In this paper we adopt this approach, using a particular condition (Section 2.2) which ensures that the analytic continuation is unique, and then discuss the convexity of the resulting free energy.

Our interest was aroused by some controversies arising from the application of this procedure to the  $n$ -vector model. The case  $n = 0$  is of interest because it provides a model of self-avoiding walks or “polymers” on a lattice.<sup>(5,14)</sup> In the  $\epsilon = 4 - d$  expansion<sup>(1,3,4)</sup> (which, incidentally, ascribes a certain reality to noninteger dimensions between 3 and 4), it is possible under some circumstances to obtain negative susceptibilities<sup>(15)</sup> for  $n < 1$ . Also, negative specific heats have been found in a one-dimensional model for  $n < 1$ .<sup>(16)</sup> Such violations of convexity are surely not possible when  $n$  is a positive integer!

We shall, in fact, show that *whenever  $n$  is not a positive integer* it is possible to construct a Hamiltonian using dot products of pairs of  $n$  vectors at different sites for which there are violations of convexity. The interac-

<sup>4</sup> References 8–10 are a small selection of the many papers in which  $q$  (also denoted by  $r$  and  $Q$ ) is treated as a continuous variable.

<sup>5</sup> The discussion of the replica method in Ref. 11 is a noteworthy exception.

<sup>6</sup> Such extensions have often been tacitly employed in the literature. Explicit references to analytic continuation will be found in Refs. 7, 19, and 20. A particularly careful discussion (for the case of replicas) will be found in Ref. 11.

tions required are (in most cases) not of the simple, standard “ferromagnetic” type, which is the reason that these violations have not been noted previously. Very similar convexity violations occur in the  $q$ -state Potts model, and in another model which we call the “axis model” (Section 3).

Convexity violations can also occur when  $n$  or  $q$  is a positive integer but the interactions involve (in a formal sense) more than  $n$  components. (Examples will be found in Sections 3 and 4.) In addition, violations of convexity can arise in lattice models of dimensionality  $d$  when  $d$  is not an integer.

There is a close connection between such convexity violations and the existence of negative “probabilities” for certain events whose probabilities are well defined (and, of course, nonnegative) on the positive integers, when these probabilities are analytically continued to noninteger  $n$  (or  $q$  or  $d$ , as the case may be). Such unphysical probabilities can arise even when there is nothing peculiar about the interaction Hamiltonian.

The contents of this paper are as follows. In Section 2.1 we discuss the problem of nonconvexity in general terms and indicate its connection with negative “probabilities.” Section 2.2 states our scheme for analytic continuation. While it is certainly not the only possible scheme, it does seem to coincide with what is done in practice in many cases.<sup>7</sup> In Section 3 we consider two models in which the “spin” variables take on a finite number of values: the Potts model and the axis model.<sup>(21)</sup> These discrete models are technically simpler than the  $n$ -vector model, which is considered in Section 4 for spins of fixed length and in Section 5 for spins of variable length. Noninteger dimensionality  $d$  is considered briefly in Section 6. In this paper we do *not* discuss the issues associated with noninteger  $n$  in the replica method, as these involve some technical complications.

We wish to emphasize that this paper is *not* to be considered as an attack on the use of noninteger values of parameters, a usage which seems (to us) to be justified, at the very least as a heuristic procedure, in terms of the numerous insights which it has provided. More detailed comments will be found in the conclusion, Section 7.

## 2. GENERAL FORMALISM

### 2.1. Convexity and Positive Probabilities

The usual convexity or stability condition for a classical (nonquantum) system in statistical mechanics arise in the following way.<sup>(17,18)</sup> Let  $\langle \rangle$

<sup>7</sup> As, for example, Refs. 2, 7, 16, and 19.

denote the average with respect to some probability measure, and let  $g$  and  $h$  be real-valued functions on the sample space of interest to us. If  $\lambda$  is a real parameter, the convexity of

$$f(\lambda) = \ln \langle e^{g+\lambda h} \rangle \quad (2.1)$$

can be established by looking at its second derivative:

$$f''(\lambda) = d^2f/d\lambda^2 = E(h^2) - [E(h)]^2 = E([h - E(h)]^2) \quad (2.2)$$

Here  $E$  is an average defined by

$$E(k) = \langle ke^{g+\lambda h} \rangle / \langle e^{g+\lambda h} \rangle \quad (2.3)$$

Now we know that if  $k$  is nonnegative function,  $\langle k \rangle$  will be nonnegative, and hence  $E(k)$  will also be nonnegative. Consequently the right side of (2.2), which is the average of the square of a real-valued function, cannot be negative, and thus  $f$  is a convex function of  $\lambda$ . (Naturally we must assume that certain technical restrictions, such as the integrability of the appropriate functions, are satisfied. We believe that these give no difficulties in the examples considered later in this paper.)

In the cases of interest to us, the sample space will consist of configurations of a finite number of "spins" on a lattice,  $\langle \rangle$  will be an average with respect to an appropriate measure in the absence of interactions,  $g + \lambda h$  will be a dimensionless Hamiltonian (i.e., the Hamiltonian divided by  $-kT$ ) containing a real parameter  $\lambda$ , and  $f$  will be a corresponding dimensionless free energy. The convexity of  $f$  for integer values of  $n$ , where  $n$  stands for whichever of the parameters of Section 1 is under investigation, is then an immediate consequence of the fact that  $\langle \rangle$  is associated with a probability measure in the standard way.

To define  $\langle \rangle$  when  $n$  is not a positive integer, we proceed as follows. We consider a class  $\mathcal{K}$  of real-valued functions such that each  $k$  in  $\mathcal{K}$  is defined on the sample space when  $n$  is any positive integer (i.e.,  $k$  is defined on the union of the sample spaces for  $n = 1, 2, \dots$ ), and we let  $\langle k \rangle_n$  be the average of  $k$  restricted to the sample space specified by  $n$ . If  $\mathcal{K}$  has been appropriately chosen, there will be a "natural" extension of  $\langle k \rangle_n$  to all real values of  $n$ , or perhaps real values of  $n$  greater than some constant, or real values of  $n$  with the exclusion of some singular values. For the cases we shall consider there is a sense in which this extension is unique (see Section 2.2).

The extended definition of  $\langle \rangle_n$  can be used to define a free energy  $f$  by means of (2.1) when  $n$  is not a positive integer provided  $\mathcal{K}$  contains  $\exp(g + \lambda h)$ , and for  $f$  to be convex it is sufficient that  $\langle k \rangle_n$  be nonnegative whenever  $k$  is nonnegative. Actually, convexity follows from a somewhat

weaker condition, namely, that for every  $k \in \mathcal{H}$ ,

$$\langle k^2 \rangle_n \geq 0 \quad (2.4)$$

since, see (2.3),

$$E_n(k^2) = \langle [ke^{(1/2)(g+\lambda h)}]^2 \rangle_n / \langle [e^{(1/2)(g+\lambda h)}]^2 \rangle_n \quad (2.5)$$

We are here assuming that  $\exp[(1/2)(g + \lambda h)]$ , and this function multiplied by  $k$ , are elements of  $\mathcal{H}$ .

We shall always assume that the class  $\mathcal{H}$  contains the identity function and is closed under the addition or product of two members, and under multiplication by real constants, so that it forms an algebra. In some cases in which the sample spaces are discrete, a convenient  $\mathcal{H}$  is generated by characteristic or indicator functions for certain events, functions taking the value +1 or 0 depending on whether the event does or does not occur. In this case one can speak of extending probability distributions to noninteger  $n$ , and convexity will be preserved provided the extended probabilities are nonnegative. When the sample space is not discrete it is often convenient to look at the extended probability distribution density. Provided the latter is positive and provided  $\langle k \rangle_n$  can be evaluated by integration, convexity will, of course, be preserved. However, it may turn out that (2.4) is valid for a particular algebra  $\mathcal{H}$  even when the extended probability distribution density is not always positive.

In any case, as will be clear from the examples in the remainder of this paper, violations of (2.4) when  $n$  is not a positive integer do depend on the choice of the algebra  $\mathcal{H}$ . Usually there is a "natural" choice for  $\mathcal{H}$ , depending on the type of Hamiltonian under consideration. Even if violations of (2.4) occur for  $k$  in this  $\mathcal{H}$  it does not, of course, mean that for the actual Hamiltonians of interest  $f$  will fail to be convex. It does mean that if one sets  $g = 0$  and  $h = k$  in (2.1), then  $f''(0) < 0$ .

## 2.2. Extension off the Integers

Obviously there is no unique way of taking a function  $g(n)$  defined when  $n$  is a positive integer and extending it to a function defined on all, or a large part, of the real  $n$  axis, unless one places very strong restrictions on the extended function. In this paper we shall require that the extension satisfy the conditions given in the next paragraph. We have no fundamental justification for these conditions, but they have the advantage that if there is an extension which satisfies them, it will be unique. In addition, the extensions which are adopted in the relevant literature appear to satisfy this condition. Thus, for example, the theoretical physicist who has employed

some procedure to obtain a function  $(n + 2)/(n + 8)$  when  $n$  is a positive integer will not usually add to it a piece proportional to  $\sin(\pi n)$  when he is considering noninteger  $n$ .

The conditions are as follows. Let there be finite real numbers  $n_0$ ,  $\alpha$ ,  $C$ , and  $\gamma$ , with

$$\gamma < \pi \quad (2.6)$$

such that  $g(n)$  is an analytic function of the complex variable  $n$  in the half-plane,

$$\operatorname{Re}(n) \geq n_0 \quad (2.7)$$

and such that on this domain

$$|e^{-\alpha n} g(n)| < C \exp(\gamma |n|) \quad (2.8)$$

One can use Carlson's theorem<sup>(22)</sup> to show that if there are two functions  $g(n)$  and  $h(n)$  satisfying these conditions with (possibly) different choices of the constants—with of course (2.6) satisfied in both cases—and if  $g$  and  $h$  agree for all integer values of  $n$  greater than some finite  $N$ , then they are identical on the intersection of the two half-planes (2.7). Analytic continuation may then be used to extend the domain in the vicinity of the real axis toward smaller (more negative) values of  $n$ . If this extension is possible, then of course the extended functions  $g$  and  $h$  coincide on the enlarged domain.

In what follows we shall not bother to draw explicit attention to these conditions except in special cases, but they are always what we have in mind when speaking of an extension of a function off the positive integers.

### 3. DISCRETE MODELS

#### 3.1. The $q$ -State Potts Model

For  $i = 1, 2, \dots, N$  let  $S_i$  be a variable which takes on the values  $1, 2, 3, \dots, q$ . In typical applications,  $i$  labels the sites of some finite part of a regular lattice. A typical dimensionless Hamiltonian is of the form

$$H = \sum_{i < j} K_{ij} \delta(S_i, S_j) + \sum_j h_i \delta(S_i, 1) \quad (3.1)$$

where  $\delta(a, b)$ , the Kronecker delta, is 1 when  $a = b$  and 0 otherwise. The Potts model, strictly speaking, corresponds to the case where all the  $h_i$  vanish, but it is often convenient to consider the effect of these single-site terms. The average  $\langle \rangle$  will be associated with a probability distribution in

which the  $S_i$  for different  $i$  are statistically independent, and for each  $i$ ,  $S_i$  takes each possible value with probability  $1/q$ .

Let us first consider the situation in which there is only a single site,  $N = 1$ . For  $q \geq 1$  an integer, one finds that

$$f(h) = \ln \langle e^{h\delta(S_1,1)} \rangle = \ln [(e^h + q - 1)/q] \tag{3.2}$$

has a second derivative:

$$f''(h) = (q - 1)e^h / (e^h + q - 1)^2 \tag{3.3}$$

The right side of this equation is analytic in  $q$  for a fixed  $h$ , except for the pole at  $1 - e^h$ , and is nonnegative for real  $q \geq 1$ . However, for real  $q < 1$  it is negative, indicating a violation of convexity in this region.

To see that everything will be well behaved for  $q \geq 1$ , we compute the probabilities  $P_0$  and  $P_1$  that  $\delta(S_1, 1)$  takes the values 0 and 1, respectively, when  $q$  is a positive integer:

$$P_0 = (q - 1)/q, \quad P_1 = 1/q \tag{3.4}$$

Note that  $P_0$  and  $P_1$  are positive and sum to 1 for all real  $q > 1$ . Consequently (2.4) will be satisfied for  $q \geq 1$  whenever  $k$  is a real-valued function of  $\delta(S_1, 1)$ , and no violations of convexity are to be expected when  $\mathcal{H}$  (Section 2.1) is the algebra generated by  $\delta(S_1, 1)$ .

Since the joint probability distribution (corresponding to  $\langle \rangle$ ) for the  $\delta(S_i, 1)$ ,  $i = 1, 2, \dots, N$  is the product of the individual distributions, the same conclusions hold when  $\mathcal{H}$  is the algebra generated by these quantities. That is, there can be no violations of convexity for any Hamiltonian in  $\mathcal{H}$  as long as  $q \geq 1$ . In particular,  $H$  may involve interactions of the form  $\delta(S_i, 1)\delta(S_j, 1)$  for  $i \neq j$ , as well as the single-site terms in (3.1). However, for any  $q < 1$  it is clear that violations of convexity are possible. For example, with all the  $K_{ij}$  and all the  $h_i$  except  $h_1$  set equal to zero in (3.1), we return to the example already considered in (3.3).

A generalization of  $\mathcal{H}$  is the algebra  $\mathcal{H}_\nu$  generated by  $\delta(S_i, \alpha)$  for  $\alpha = 1, 2, \dots, \nu$  and  $i = 1, 2, \dots, N$ . The argument given above in the case  $\nu = 1$  can be easily extended to show that (2.4) will be satisfied for noninteger  $q$  provided  $q \geq \nu$ . However, violations arise as soon as  $q$  is less than  $\nu$ , as is easily shown by means of examples involving a single site, e.g.,

$$\left\langle \left[ 1 - \sum_{\alpha=1}^{\nu} \delta(S_1, \alpha) \right]^2 \right\rangle = q^{-1}(q - \nu) \tag{3.5}$$

$$\frac{d^2}{dh^2} \left\langle \exp h \sum_{\alpha=1}^{\nu} \delta(S_1, \alpha) \right\rangle = \frac{\nu(q - \nu)e^h}{(q - \nu + \nu e^h)^2} \tag{3.6}$$

When the  $h_i$  in (3.1) are all zero, it is natural to focus attention on the algebra  $\mathcal{K}'$  generated by the  $N(N-1)/2$  quantities

$$\theta_{ij} = \delta(S_i, S_j) \quad (3.7)$$

The probability  $P_\phi$  that *all* of the  $\theta_{ij}$  are zero is easily calculated:

$$P_\phi = \left\langle \prod_{i < j} (1 - \theta_{ij}) \right\rangle = q(q-1)(q-2) \cdots (q-N+1)/q^N \quad (3.8)$$

Obviously  $P_\phi \geq 0$  for all real  $q \geq N-1$ , but it is negative for

$$N-2 < q < N-1 \quad (3.9)$$

That this constitutes a violation of (2.4) follows from (3.8) upon noting that

$$\left[ \prod_{i < j} (1 - \theta_{ij}) \right]^2 = \prod_{i < j} (1 - \theta_{ij}) \quad (3.10)$$

is an element of  $\mathcal{K}'$ .

Of course one can calculate the analog of (3.8) for any subset of the  $N$  sites. If this subset contains  $N'$  sites, (3.8) holds with  $N$  replaced by  $N'$ . This shows that negative "probabilities" and violations of (2.4) are also possible for  $q$  between  $N'-2$  and  $N'-1$ . Since  $N'$  can be as small as 2 this means that such violations are possible for any real, positive  $q$  less than  $N-1$ , with the exception of integer values. Furthermore, a direct calculation shows that

$$(d^2/dK^2)\ln\langle \exp K\theta_{12} \rangle = (q-1)e^K/(e^K + q-1)^2 \quad (3.11)$$

and hence violations of convexity can occur for any real  $q < 1$ .

It is not difficult to show that the probability that a specific subset of the  $\theta_{ij}$  are equal to 1 and the rest are equal to zero is either zero or given by the right side of (3.8) with  $N$  replaced by a smaller positive integer. Since such quantities are nonnegative for  $q \geq N-1$ , we conclude that no violations of convexity will occur when  $q$  is an arbitrary real number not less than  $N-1$ .

We conclude that for the algebra  $\mathcal{K}'$  generated by the  $\theta_{ij}$  there is a critical value

$$q_c = N-1 \quad (3.12)$$

for  $q$  such that violations of (2.4) cannot occur for  $q \geq q_c$ , but can occur for any  $q < q_c$  unless this  $q$  is a positive integer. The fact that violations of convexity *can* occur does not mean they actually *will* occur for a specific Hamiltonian and a particular linear parameter. But even in those cases in which no "observable" violations of convexity occur, one can still expect that for  $q$  less than  $q_c$  and not a positive integer there will be certain events with negative "probabilities." Also note that since  $q_c$ , (3.10), increases with



$N$ , in the thermodynamic limit when  $N$  goes to infinity the only “safe” values of  $q$  are the positive integers.

### 3.2. The Axis Model

For  $i = 1, 2, \dots, N$ , let  $\mathbf{S}_i$  be a vector with components  $S_i^\alpha$ ,  $\alpha = 1, 2, \dots, n$ , and suppose that all of these components are zero except for one, which takes the values  $+1$  or  $-1$ . That is,  $\mathbf{S}_i$  is a unit vector parallel or antiparallel to one of the  $n$  coordinate axes (whence the name “axis model”). Each of these  $2n$  possibilities is given equal weight and the  $\mathbf{S}_i$  are independent in the probability distribution which determines  $\langle \rangle$ .

The analog of (3.1) is

$$H = \sum_{i < j} K_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + \sum h_i S_i^1 \tag{3.13}$$

where  $\mathbf{S}_i \cdot \mathbf{S}_j$  is the usual dot product,  $\sum_\alpha S_i^\alpha S_j^\alpha$ . This suggests a study of the algebras  $\mathcal{K}$ , generated by the  $S_i^1$  for  $i = 1, 2, \dots, N$ , and  $\mathcal{K}'$  generated by the  $N(N - 1)/2$  quantities

$$\theta_{ij} = \mathbf{S}_i \cdot \mathbf{S}_j \tag{3.14}$$

The results obtained are similar to those for the Potts model in Section 3.1. In particular, we have

$$\frac{d^2}{dh^2} \ln \langle \exp h S_1^1 \rangle = \frac{1 + (n - 1) \cosh h}{(n - 1 + \cosh h)^2} \tag{3.15}$$

Thus for any  $n < 1$  it is possible to produce violations of convexity by making  $h$  sufficiently large. On the other hand, the probabilities  $P_0$ ,  $P_+$ , and  $P_-$  that  $S_1^1$  takes the values  $0$ ,  $+1$ , and  $-1$ , respectively, are

$$P_0 = (n - 1)/n, \quad P_+ = P_- = 1/2n. \tag{3.16}$$

Since these are nonnegative for all real  $n \geq 1$ , we conclude that violations of convexity are only possible for  $n < 1$  in the case of the algebra  $\mathcal{K}$ .

As in the case of the Potts model, we can extend  $\mathcal{K}$  to the algebra  $\mathcal{K}_\nu$ , generated by the  $S_i^\alpha$  for  $1 \leq \alpha \leq \nu$  and  $1 \leq i \leq N$ . (This is of some interest in view of the fact that the  $n \rightarrow 0$  limit of a partition function using

$$H = \sum_{i < j} K_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + \sum_i h_i \sum_{\alpha=1}^\nu S_i^\alpha \tag{3.17}$$

with  $|\mathbf{S}_i|$  equal to  $\sqrt{\nu}$  rather than  $1$ , describes an assembly of  $\nu$  different kinds of self-avoiding walks.<sup>8</sup> In the following equations we will, however,

<sup>8</sup> The method of Hilhorst<sup>(21)</sup> can be extended to  $\nu > 1$  using the methods proposed in Ref. 25.

assume that  $|\mathbf{S}_i| = 1$ , not  $n$ .) Violations of convexity arise as soon as  $n$  is less than  $\nu$ , as is evident from examples involving one site:

$$\frac{d^2}{dh^2} \ln \left\langle \exp h \sum_{\alpha=1}^{\nu} S_1^{\alpha} \right\rangle = \frac{\nu + (n - \nu) \cosh h}{(n - \nu + \nu \cosh h)^2} \quad (3.18)$$

$$\left\langle \left[ 1 - \sum_{\alpha=1}^{\nu} (S_1^{\alpha})^2 \right] \right\rangle = \left\langle \sum_{\alpha=\nu+1}^n (S_1^{\alpha})^2 \right\rangle = n^{-1}(n - \nu) \quad (3.19)$$

Once again, it is not difficult to show that (2.4) will be satisfied for all  $n \geq \nu$ . Thus the results are quite analogous to those for the Potts model.

In the case of  $\mathcal{H}'$  we note that the probability  $P_{\phi}$  that all the  $\theta_{ij}$  are zero is given by

$$P_{\phi} = n(n-1)(n-2) \cdots (n-N+1)/n^N \quad (3.20)$$

which is the same as (3.8) if  $q$  is changed to  $n$ . Thus the same argument as in Section 3.1 shows that violations of convexity are possible for any real, noninteger  $n$  between 0 and  $N-1$ . In addition, direct calculation shows that

$$\frac{d^2}{dK^2} \ln \langle \exp K\theta_{12} \rangle = \frac{1 + (n-1) \cosh K}{(n-1 + \cosh K)^2} \quad (3.21)$$

and hence violations of convexity can occur for any  $n < 1$ . On the other hand, by an argument similar to that in Section 3.1, one can show that the probability of any event in which all the  $\theta_{ij}$  have specified values must be nonnegative, and hence violations of convexity are impossible, for real  $n \geq N-1$ .

## 4. THE $n$ -VECTOR MODEL: SPINS OF FIXED LENGTH

### 4.1. Introduction

For  $j = 1, 2, \dots, N$ , let  $\mathbf{S}_j$  be a ("spin") vector whose  $n$  components  $S_j^{\alpha}$ ,  $\alpha = 1, 2, \dots, n$ , are real and satisfy

$$\sum_{\alpha=1}^n (S_j^{\alpha})^2 = a \quad (4.1)$$

Throughout this part of the paper we shall assume that  $a = 1$ , so the  $\mathbf{S}_j$  are of unit length. It is nonetheless convenient to leave  $a$  in various formulas as a parameter; in particular, this will facilitate the discussion in Section 5.

A typical dimensionless Hamiltonian is of the form

$$H = \sum_{i < j} K_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + \sum_i h_i S_i^1 \quad (4.2)$$

where  $\mathbf{S}_i \cdot \mathbf{S}_j$  is the usual dot product,  $\sum_{\alpha} S_i^{\alpha} S_j^{\alpha}$ , and  $h_i$  is a (dimensionless) magnetic field at the  $i$ th site.

The average  $\langle \rangle$  corresponds to a probability distribution in which the  $\mathbf{S}_i$  for different  $i$  are statistically independent, and for each  $i$  a uniform weight is assigned to the sphere defined by (4.1). Consider a single site, say,  $i = 1$ , and for convenience define

$$x_{\alpha} = S_1^{\alpha} \tag{4.3}$$

Then for this site the probability distribution may be thought of as arising from a probability density

$$\rho(x_1, x_2, \dots, x_n) = \delta\left(a - \sum_{\alpha=1}^n x_{\alpha}^2\right) / \int_{-\infty}^{\infty} dx_1 \dots dx_n \delta\left(a - \sum_{\alpha=1}^n x_{\alpha}^2\right) \tag{4.4}$$

where  $\delta(\ )$  is the Dirac delta function. The moments of the distribution can be easily calculated in the manner shown in Appendix A. In particular, if  $p$  is a vector whose components,  $p_{\alpha}$ , are nonnegative integers, then

$$\left\langle \prod_{\alpha=1}^n (x_{\alpha})^{p_{\alpha}} \right\rangle = \frac{a^{|p|/2} \prod_{j=1}^n [1.3.5 \dots (p_j - 1)]}{n(n+2) \dots (n+|p|-2)} \tag{4.5}$$

where

$$|p| = \sum_{\alpha} p_{\alpha} \tag{4.6}$$

and all the  $p_{\alpha}$  are *even*. If one or more of the  $p_{\alpha}$  is an odd integer, the left side of (4.5) vanishes.

### 4.2. The Case of $\nu$ Explicit Components

We shall begin our study of convexity of the  $n$ -vector model by considering the algebra  $\mathcal{H}$  (Section 2.1) generated by the first  $\nu$  components of the vectors  $\mathbf{S}_j$ , i.e., by  $\{S_j^{\alpha}\}$  with  $\alpha = 1, 2, \dots, \nu$ . Here  $\nu$  will be a positive integer which is held fixed when  $n$  is varied. The case  $\nu = 1$  arises in a natural way if one sets  $K_{ij} = 0$  in (4.2), and corresponds to the first situation considered in the Potts model and the axis model (Section 3). It is actually sufficient, as we shall see, to work out the results for a single site, and for this purpose we use the notation (4.3).

As long as  $n \geq \nu$  is an integer, the joint probability distribution density for  $x_1, x_2, \dots, x_{\nu}$  can be obtained integrating (4.4) over  $x_{\nu+1}, x_{\nu+2}, \dots, x_n$ . The result (Appendix A) is

$$\tilde{\rho}(x_1, x_2, \dots, x_{\nu}) = \frac{\Gamma(n/2)(a - \tilde{x}^2)^{(n-\nu)/2-1}}{\pi^{\nu/2} \Gamma\left[\frac{1}{2}(n-\nu)\right] a^{n/2-1}} \tag{4.7}$$

where

$$\tilde{x}^2 = \sum_{\alpha=1}^{\nu} x_{\alpha}^2 \quad (4.8)$$

lies between 0 and  $a$ ; when  $\tilde{x}^2$  is outside this range,  $\tilde{\rho}$  vanishes. (For present purposes,  $a$  may be replaced by 1.)

Although (4.7) has been derived for  $n$  an integer, it is evident that when  $\tilde{x}^2$  has a value less than  $a$ , the right-hand side of this equation defines a function of  $n$  which is analytic in the entire complex  $n$  plane except for some poles on the real axis for  $n \leq \nu$ . The function satisfies the conditions of Section 2.2, and in this sense is a unique extension of the probability density off the positive integers  $n > \nu$ . Furthermore, for real  $n > \nu$  it is a nonnegative probability density.

On the other hand, the right side of (4.7) is negative in the range

$$\nu - 2 < n < \nu \quad (4.9)$$

for  $\nu \geq 2$ , or  $0 < n < 1$  when  $\nu = 1$ . Thus one is not surprised to discover that

$$a^{-2} \langle (a - \tilde{x}^2)^2 \rangle = \frac{(n - \nu)(n + 2 - \nu)}{n(n + 2)} \quad (4.10)$$

is negative in the same interval. (This formula can be obtained either from (4.7) or by the use of (4.5).) Furthermore, upon replacing  $\tilde{x}^2$  by the sum of the squares of the first  $\nu'$  of the  $x_{\alpha}$ , with  $\nu' < \nu$ , one obtains (4.10) with  $\nu$  replaced by  $\nu'$ . Consequently, violations of condition (2.4) will occur for any  $n$  between 0 and  $\nu$ . They also occur for all  $n < 0$ , since, by (4.5),

$$\langle x_1^2 \rangle = a/n \quad (4.11)$$

In the case  $\nu = 1$  it is helpful to look at an explicit example, that of a spin at one site in a magnetic field. One can show that

$$Z = \langle e^{hx_1} \rangle = \Gamma(n/2)(h/2)^{1-n/2} I_{n/2-1}(h) \quad (4.12)$$

where  $I_{\nu}$  is a modified Bessel function, and thus (see Appendix B):

$$m(h) = d \ln Z / dh = I_{n/2}(h) / I_{n/2-1}(h) \quad (4.13)$$

For convexity to be satisfied,  $m(h)$  must be monotone increasing in  $h$ . However, for any  $n < 1$  (see Appendix B),  $dm/dh$  is negative when  $h$  is sufficiently large. When  $n = 0$ ,  $dm/dh$  decreases as  $-2/h^2$  for large  $h$ .

If one has  $\nu > 1$  and considers a dimensionless Hamiltonian

$$H = (h/\sqrt{\nu}) \sum_{\alpha=1}^{\nu} S_1^{\alpha} \quad (4.14)$$

it is easy to show by means of a rotation that the corresponding partition function is identical to that in (4.12). Hence for this particular example, unlike its analogs in the Potts and axis models [Section 3; see (3.6) and (3.18)] a violation of convexity sets in at  $n = 1$  and not at  $n = \nu$ .

The conclusion is that for a single site and the algebra  $\mathcal{H}$  generated by  $x_1, x_2, \dots, x_\nu$ , convexity is preserved for any real  $n \geq \nu$ , but violations can occur for any real  $n < \nu$ . The results for  $N$  sites are the same as for a single site. Thus for  $n > \nu$  the joint probability distribution density associated with  $\langle \rangle$  for  $N$  sites is simply a product of positive densities of the form (4.7). On the other hand, violations of (2.4) for  $n < \nu$  using functions which depend only on the  $S_1^\alpha$  for  $\alpha = 1, 2, \dots, \nu$  are obviously still present for  $N > 1$ . Note the resemblance between this result for the  $n$ -vector model and what we obtained for the algebra  $\mathcal{H}$  in the Potts and axis models, Section 3, where we only considered  $\nu = 1$ .

### 4.3. The Algebra of Dot Products

With the  $h_i = 0$  in (4.2), we are naturally led to consider the algebra  $\mathcal{H}'$  generated by the  $N(N - 1)/2$  dot products

$$M_{ij} = \mathbf{S}_i \cdot \mathbf{S}_j \tag{4.15}$$

Actually it will be convenient to regard the  $M_{ij}$  as elements of a real, symmetrical, positive semidefinite matrix  $M$  whose diagonal elements, in accordance with (4.15) and (4.1), are all equal to  $a$ . It can then be shown, Appendix A, that for  $n$  an integer greater than or equal to  $N$ , the joint probability distribution density for the  $M_{ij}$  with  $i < j$  is given by the expression

$$\rho(M) = \frac{\pi^{N(1-N)/4}}{a^{N(n-1)}} \left\{ \prod_{j=1}^{N-1} \frac{\Gamma(n/2)}{\Gamma[\frac{1}{2}(n-j)]} \right\} (\det M)^{(n-N-1)/2} \tag{4.16}$$

Here  $\det M$  stands for the determinant of the matrix, and it is understood that (4.16) holds only when  $M$  is positive (semi-) definite, as otherwise  $\rho = 0$ .

When  $M$  is fixed and  $\det M$  is positive, the right side of (4.16) is an analytic function of  $n$  in the entire complex plane with the (possible) exception of poles on the negative real axis. Since the conditions of Section 2.2 are satisfied, we can speak of a unique extension off the integers  $n \geq N$ . Furthermore the coefficient in curly brackets is positive as long as  $n$  is real and exceeds the critical value of

$$n_c = N - 1 \tag{4.17}$$

On the other hand, the right side of (4.16) is negative for  $n_c - 1 < n < n_c$ , suggesting that violations of convexity might be possible in this interval.

A direct calculation, Appendix D, shows that

$$\langle (\det M)^m \rangle = \prod_{j=1}^{N-1} \frac{\Gamma(n/2)\Gamma[\frac{1}{2}(n-j) + m]}{\Gamma(n/2 + m)\Gamma[\frac{1}{2}(n-j)]} \tag{4.18}$$

where  $m$  is real and positive, and thus in particular,

$$\langle (\det M)^2 \rangle = \prod_{k=1}^{N-1} \frac{(n - N + k)(n - N + k + 2)}{n(n + 2)} \tag{4.19}$$

The right side of (4.19) is negative for  $n_c - 1 < n < n_c$ , and since  $\det M$  belongs to  $\mathcal{H}'$ , this is a violation of (2.4). By restricting ourselves to the subalgebra obtained from dot products of some subset of the  $S_i$  and repeating the above argument, we can produce violations of (2.4) for  $n$  between  $n_c - 2$  and  $n_c - 1$ , or  $n_c - 3$  and  $n_c - 2$ , etc. That is to say, violations of convexity can occur for *any noninteger*  $n$  in the interval  $0 < n < n_c$ .

In addition, a direct calculation (Appendix B) shows that for  $a = 1$ ,

$$d \ln \langle \exp(K S_1 \cdot S_2) \rangle / dK = I_{n/2}(K) / I_{(n/2-1)}(K) \tag{4.20}$$

The right side is the same as (4.13) with  $h$  replaced by  $K$ . Hence for any  $n < 1$  violations of convexity will occur when  $K$  is sufficiently large.

Thus we conclude that for the algebra  $\mathcal{H}'$  of dot products, violations of convexity or negative “probabilities” must be anticipated for any real  $n$  less than the critical value of  $n_c = N - 1$ , *except* when  $n$  is a positive integer. Just as in the cases of the Potts and axis models, one has the troublesome feature that  $n_c$  increases to infinity in the thermodynamic limit.

## 5. THE $n$ -VECTOR MODEL: SPINS OF VARIABLE LENGTH

### 5.1. The Case of $\nu$ Explicit Components

We employ the notation of Section 4.1, but drop the requirement (4.1). We shall assume that at a single site the probability density is given by [compare with (4.4)]

$$\rho(x_1, x_2, \dots, x_n) = w\left(\sum_{\alpha=1}^n x_\alpha^2\right) / \int_{-\infty}^{\infty} dx_1 \dots dx_n w\left(\sum_{\alpha=1}^n x_\alpha^2\right) \tag{5.1}$$

where  $w(t)$  is a nonnegative function for  $t \geq 0$ . The density for a system of  $N$  spins is then a product of functions of the type (5.1). The marginal distribution density for the first  $\nu \leq n$  components is then [compare with

(4.7)]:

$$\tilde{\rho}(x_1, \dots, x_\nu) = \psi_n(\tilde{x}^2) = \frac{\Gamma(n/2) \int_0^\infty w(t + x^2) t^{(1/2)(n-\nu)-1} dt}{\pi^{\nu/2} \Gamma[\frac{1}{2}(n-\nu)] \int_0^\infty w(t) t^{(1/2)n-1} dt} \quad (5.2)$$

Provided  $w(t)$  is suitably “well behaved”—in particular, decays sufficiently rapidly as  $t \rightarrow \infty$ —the right side of (5.2) is defined and positive for all real  $n > \nu$ , and for fixed  $\tilde{x}^2$  is an analytic function of  $n$  of the type discussed in Section 2.2. This means that no violations of (2.4) will occur for  $n \geq \nu$ .

The situation for  $n < \nu$  depends on  $w$ , and it is useful to consider two examples. For a Gaussian weight,

$$w(t) = e^{-\beta t} \quad (5.3)$$

one finds that

$$\psi_n(\tilde{x}^2) = (\beta/\pi)^{\nu/2} \exp(-\beta \tilde{x}^2) \quad (5.4)$$

is independent of  $n$ . This means (2.4) will be satisfied for all  $n$ . On the other hand,

$$w(t) = te^{-\beta t} \quad (5.5)$$

gives rise to

$$\psi_n(\tilde{x}^2) = (\beta/\pi)^{\nu/2} [1 - \nu/n + 2\beta \tilde{x}^2/n] \exp(-\beta \tilde{x}^2) \quad (5.6)$$

As soon as  $n$  is less than  $\nu$ , the quantity in square brackets is negative when  $\tilde{x}^2$  is sufficiently small. A violation of (2.4) is, therefore, possible for any positive  $n < \nu$  for the algebra  $\mathcal{H}$  generated by the  $x_\alpha$  for  $\alpha = 1, 2, \dots, \nu$ . For example, one can construct a polynomial in  $\tilde{x}^2$  which is finite at  $\tilde{x}^2 = 0$  and then drops to a very small value until  $\tilde{x}^2$  is much larger than  $1/\beta$ .

In order to understand the behavior exhibited by the two previous examples it is helpful to write the integral  $Y$  appearing in the numerator of (5.2) in the case  $\tilde{x}^2 = 0$  as the sum of three terms:

$$Y_1 = w(0) \int_0^b t^{(n-\nu)/2-1} dt = \frac{2w(0)b^{(n-\nu)/2}}{n-\nu} \quad (5.7)$$

$$Y_2 = \int_0^b [w(t) - w(0)] t^{(n-\nu)/2-1} dt \quad (5.8)$$

$$Y_3 = \int_b^\infty w(t) t^{(n-\nu)/2-1} dt \quad (5.9)$$

where  $b > 0$  is some constant. We shall consider the analytic continuation of each of these integrals to  $n < \nu$ .

As long as  $w(t)$  is well behaved,  $Y_3$  will be an entire analytic function of  $n$  which is positive when  $n$  is real. The analytic continuation of  $Y_1$  is

given by the right side of (5.7); note that the pole at  $n = \nu$  will be canceled by the corresponding pole in the denominator of (5.2). The behavior of  $Y_2$  depends on the behavior of  $w$  near  $t = 0$ . If we assume that for  $0 \leq t \leq b$ ,

$$|w(t) - w(0)| \leq At^p \quad (5.10)$$

for some  $p > 0$ , then (5.8) defines a function of  $n$  which is analytic as long as

$$\operatorname{Re}(n) > \nu - 2p \quad (5.11)$$

and hence has a unique analytic continuation to values of  $n$  somewhat less than  $\nu$ .

For  $w(0) > 0$ ,  $Y$  is dominated by  $Y_1$  near  $n = \nu$ , and will therefore be negative for  $n$  slightly less than  $\nu$ . As the  $\Gamma$  function in the denominator of (5.2) also changes sign at  $n = \nu$ ,  $\psi_n(0)$  remains positive. When  $w(0) = 0$ , on the other hand,  $Y$  is the sum of  $Y_2$  and  $Y_3$ , both of which are positive for  $n > \nu - 2p$ . Consequently,  $\psi_n(0)$  will be negative for

$$\nu - 2p < n < \nu \quad (5.12)$$

or at least that portion of this interval on which  $n$  is positive. Note that these conclusions agree with the previous examples, and indicate an important difference between the cases  $w(0) = 0$ , and  $w(0) > 0$ , a difference noted previously (in another connection) by Jasnow and Fisher.<sup>(20)</sup>

As another example, suppose that  $w(0) > 0$ , and that  $w(t)$  is increasing at  $t = 0$  and has the form

$$w(t) \simeq w(0) + At^p \quad (5.13)$$

with  $A > 0$  and  $p > 0$ , for small  $t$ . Then  $Y_2$ , (5.8), will diverge to  $+\infty$  as  $n$  decreases to  $\nu - 2p$ , which means that  $Y$  must be positive for  $n$  slightly larger than  $\nu - 2p$ . If, in addition,  $p \leq 1$  and  $\nu \geq 2p$ ,  $\Gamma[\frac{1}{2}(n - \nu)]$  will be negative and  $\Gamma(n/2)$  positive for  $n$  between  $\nu - 2p$  and  $\nu$ , so that  $\psi_n(0)$  will be negative for  $n$  in some open interval whose infimum is  $\nu - 2p$ . In particular, if both  $w$  and its first derivative are positive at  $t = 0$ , one can expect violations of convexity for  $\nu \geq 2$  to occur for  $n$  someplace in the interval between  $\nu - 2$  and  $\nu$ .

By applying the preceding arguments to the function

$$\bar{w}(t) = w(\tilde{x}^2 + t) \quad (5.14)$$

rather than  $w(t)$ , one can analyze the analytic continuation of  $\psi_n(\tilde{x}^2)$  for  $\tilde{x}^2 > 0$ . We shall omit the details and merely mention two results:

If  $w(0) = 0$  and  $w(t)$  is continuous near  $t = 0$ , then for  $n$  slightly less than  $\nu$  there is an  $\epsilon_n > 0$  such that  $\psi_n(\tilde{x}^2)$  is negative for  $\tilde{x}^2 < \epsilon_n$ . This means [see the discussion which follows (5.6)] that violations of (2.4) can be anticipated for suitable elements of  $\mathcal{K}$  when  $n$  is slightly less than  $\nu$ .



If at some  $t_0 > 0$ ,  $w$  has a positive first derivative, then—see the discussion following (5.13)— $\psi_n(\hat{x}^2 = t_0)$  is negative for  $n$  slightly larger than  $\nu - 2$ , assuming  $\nu \geq 2$ .

### 5.2. The Algebra of Dot Products

We follow the notation of Sections 5.1 and 4.3. As shown in Appendix A, the joint probability distribution density for  $M_{ij}$ ,  $i \leq j$ , [see (4.15)] is

$$\hat{\rho}(M) = R(n, N, w) \left[ \prod_{j=1}^N w(M_{ij}) \right] (\det M)^{(n-N-1)/2} \tag{5.15}$$

with

$$R(n, N, w) = \frac{\prod_{j=1}^N \{ \Gamma(\frac{1}{2}n) / \Gamma[\frac{1}{2}(n-j)] \}}{\left[ \pi^{(N-1)/4} \int_0^\infty t^{n/2-1} w(t) dt \right]^N} \tag{5.16}$$

The density  $\hat{\rho}$  is zero when  $M$  is not positive definite.

Formula (5.15) has a strong resemblance to (4.16). In particular for a suitably well-behaved  $w(t)$  decreasing rapidly as  $t \rightarrow \infty$  and bounded near  $t = 0$ , the right side of (5.15) can be extended to noninteger  $n$ , at least in the region  $\text{Re}(n) > 0$ , and it is positive for  $n > N - 1$  and becomes negative for  $n$  between  $N - 2$  and  $N - 1$ . Hence we can anticipate violations of convexity for the algebra  $\hat{\mathcal{K}}$  generated by  $\mathbf{S}_i \cdot \mathbf{S}_j$  for  $i \leq j$ . Indeed, as shown in Appendix A,

$$\langle (\det M)^m \rangle_w = \left[ \frac{\int_0^\infty t^{n/2+m-1} w(t) dt}{\int_0^\infty t^{n/2-1} w(t) dt} \right]^N \langle (\det M)^m \rangle_1 \tag{5.17}$$

where  $\langle \rangle_w$  refers to an average carried out using (5.15), i.e., corresponding to the weight  $w$ , and  $\langle \rangle_1$  is the corresponding average for spins of fixed length equal to 1, and is given by (4.18). Since the quantity in square brackets in (5.17) is positive, we find that our conclusions of Section 4.3 apply essentially unchanged: violations of convexity are to be expected for  $0 < n < n_c$ , where  $n_c = N - 1$ , with the exception of the integers.

When considering spins of variable length, it is plausible to employ the algebra  $\hat{\mathcal{K}}$  which differs from  $\mathcal{K}'$  (Section 4.3) in that it contains the diagonal products  $\mathbf{S}_i \cdot \mathbf{S}_j$ . One can, of course, ask the question as to whether violations of convexity can be obtained using *only* elements from  $\mathcal{K}'$  in (2.4). We have not studied this situation in detail. Preliminary results or simple examples with  $N = 2$  suggest that for  $w(0) > 0$  an analytic continuation of  $\langle \rangle$  to  $n$  less than  $N - 1$  may be possible without violating convexity. However, we have not found the situation easy to analyze.

## 6. LATTICES OF NONINTEGER DIMENSION

The case of noninteger spatial dimensionality poses more problems than the examples considered earlier in this paper. The free energy of such a system depends on the type of lattice (e.g., body centered or simple cubic) as well as the dimensionality. Also it is somewhat unnatural to ascribe a dimensionality to a *finite* piece of an infinite lattice. In this section we shall not discuss the general problem, but instead restrict ourselves to a particular example: the Ising model ( $n = 1$ ) on a  $d$ -dimensional hypercubic lattice  $Z^d$ , with a particular type of “near-neighbor” interactions.

The sites of the lattice are labeled by ordered  $d$ -tuples of integers,  $a = (a_1, \dots, a_d)$ . We shall say that two sites  $a$  and  $b$  are *near neighbors of class  $\beta$*  provided the vector difference  $a - b$  has  $\beta$  components which are  $+1$  or  $-1$ , and all the other components vanish. Thus neighbors of class 1 are separated by a unit vector parallel to one of the coordinate axes, those of class 2 by the diagonal of a square, etc. The dimensionless Hamiltonian will have the form

$$H = h \sum_a S_a + \sum_{\beta=1}^M K_\beta \sum_{\langle ab \rangle}^\beta S_a S_b \quad (6.1)$$

where  $S_a = \pm 1$  is an Ising variable associated with the site  $a$ ,  $\sum_{\langle ab \rangle}^\beta$  means a sum over all pairs of sites  $a$  and  $b$  belonging to class  $\beta$ , with each pair appearing in the sum precisely once, and  $h$  and the  $K_\beta$  are dimensionless single-site and pair coupling constants. The integer  $M$  may be chosen as large as we please.

When  $d$  is a positive integer, the free energy  $f$  per site for the infinite system possesses a convergent<sup>9</sup> “high-temperature” expansion,<sup>(23)</sup>

$$f = \ln 2 + \frac{1}{2} h^2 + \frac{1}{4} \sum_{\beta=1}^M 2^\beta \binom{d}{\beta} (K_\beta)^2 + \dots \quad (6.2)$$

provided  $h$  and  $K_\beta$  are sufficiently small (the condition depends on  $d$ ). Here  $\dots$  denotes cubic and higher-order terms. Note that  $2^\beta$  times the binomial coefficient is simply the number of possible vector differences  $a - b$  for sites which are neighbors of class  $\beta$ .

The coefficients of the lowest-order terms in (6.2) are polynomials in  $d$ ,

$$\binom{d}{\beta} = d(d-1) \cdots (d-\beta+1) \quad (6.3)$$

and the same is true for all the higher-order terms, for reasons which can be inferred from a paper by Fisher and Gaunt.<sup>(24)</sup> This means that they

<sup>9</sup> See Ref. 17, p. 112, and Ref. 18, p. 48.

possess a “natural” extension to noninteger  $d$ , and this allows one to extend  $f$ , at least formally, to noninteger  $d$ . However, it is not clear that the expansion (6.2) will continue to converge when  $d$  is not a positive integer. [For a given set of coefficients  $h$ ,  $K_1$ , etc., one expects there will be an upper limit to the *integer* dimensionality for which the series converges, unless these coefficients are made to depend explicitly on the dimensionality. But even when  $d$  is less than this upper limit, it might be the case that (6.2) fails to converge for some or all noninteger values.]

Leaving aside the difficulty just mentioned, we can say that if (6.2) does define an extension of  $f$  to noninteger  $d$ , this extension is obviously not a convex function of  $K_\beta$  for  $d$  between  $\beta - 2$  and  $\beta - 1$  when the coupling constants are sufficiently small, since the coefficient of  $(K_\beta)^2$  in (6.2) is negative. Consequently violations of convexity can occur whenever  $d$  is less than  $M - 1$ , with the exception of cases in which  $d$  is a nonnegative integer.

This situation might seem at first sight somewhat analogous to those discussed earlier in this paper. However, there is an important difference: while we have shown that violations of convexity can occur for  $d < M - 1$ , we have not shown they are impossible for  $d > M - 1$ , but only that they are absent at “high temperatures” where  $f$  is dominated by the terms shown explicitly in (6.2). Also note once more that our argument depends on the convergence of (6.2); should this fail, the absence of convexity is probably a minor difficulty compared to the problem of *defining*  $f$  for noninteger  $d$ .

## 7. SUMMARY AND CONCLUSIONS

We have shown that in each of the cases we have studied—the  $n$ -vector model, the  $q$ -state Potts model, the axis model, and the dimensionality  $d$  of the lattice—violations of convexity are possible under suitable circumstances when the parameter of interest ( $n$ ,  $q$ , or  $d$ ) is not a positive integer. In order to “see” such violations it is necessary to use an appropriate Hamiltonian; the fact that typical Hamiltonians are not of the appropriate sort is the reason why these problems seem to have been overlooked previously, except for special cases. However, even in those cases in which the Hamiltonian does not contain interactions which make the violations of convexity explicit, there are likely to be certain configurations of the system to which a suitable analytic continuation from the positive integers will assign a negative “probability.” Both negative probabilities and violations of convexity are, of course, exceptions to the usual principles of statistical mechanics.

In addition we have shown that there are other circumstances in which real noninteger values of these parameters are “safe” in the sense that probabilities (of the configurations or events of interest) are nonnegative

and convexity is not violated. In the examples we have considered, the safe values of the parameter are those in which it is larger than a certain critical value. However, in the case of dot products for the  $n$ -vector model, or the analogous products for the Potts and axis models, the critical value tends to infinity with the size of the system, suggesting that in the thermodynamic limit violations of convexity are to be anticipated whenever the parameter is not a positive integer. In the case of the dimensionality  $d$ , we have not been able to show that there is a critical value above which noninteger values are safe. Violations of convexity can occur in the thermodynamic limit whenever  $d$  is less than  $M - 1$  and not an integer, where  $M$  is the upper limit of the sum in (6.1). As the choice of  $M$  is somewhat arbitrary there is some justification for concluding that in the thermodynamic limit violations of convexity are also possible whenever  $d$  is not a positive integer (or zero).

While the mathematical situation (as far as we have studied it) is clear and unambiguous, its implication for the numerous calculations involving noninteger  $n$ ,  $q$ , and  $d$  which have appeared in recent years—almost all of them based on approximations whose validity is difficult to assess—is far from obvious. On the one hand, our results by themselves need not cast any serious doubts on the conclusions of these calculations. For example, it seems entirely plausible that various critical exponents, which are (presumably) well defined in the  $n$ -vector model for  $d = 3$  and  $n$  a positive integer, should depend on  $n$  in a smooth way, which allows some sort of analytic continuation to noninteger  $n$ , at least near some intervals on the real  $n$  axis. Breakdowns of convexity may turn out to be of no significance for the asymptotic critical behavior for  $n \geq 1$ .

And even if breakdowns of convexity do occur in a region of interest, they may be perfectly consistent with some particular physical application. This is what seems to be the case for  $d = 3$  and  $n = 0$ , where one of us has shown that a proper translation of the  $n$ -vector model at  $n = 0$  into the physically interesting system of self-avoiding walks results in a convex free energy for the latter.<sup>(25)</sup> Negative susceptibilities and the like, while contrary to one's intuition, may merely be a necessary price to pay in order to gain the full benefit of certain powerful theoretical tools.

On the other hand, our results may be pointing to some fundamental limitations in those theoretical procedures which treat  $n$ , etc., as continuous variables. Such procedures often seem to involve the implicit assumption that "there is nothing special about the integers." Our calculations, however, indicate that positive integer values of these parameters *are* special in at least *one* important respect: convexity of the free energy. Could it be that the positive integers are unique in other respects?

As we indicated in the introduction, we think that their undeniable success in terms of physical insight, agreement with experiment, and reasonable correspondence with other approximate and exact calculations is by itself a justification of methods in which  $n$ ,  $d$ , etc. are treated as continuous parameters. Even if one eventually has to conclude—and, in our opinion, the time has not yet arrived—that these procedures lack a firm mathematical foundation and are perhaps even a trifle misleading, the situation need be no worse than what is found in various other areas of statistical mechanics. For example, it is well known that there are severe mathematical problems associated with the proper definition of a metastable state in equilibrium thermodynamics and statistical mechanics.<sup>(26)</sup> Nonetheless, the concept is extremely useful when used in its proper context and is not taken too seriously. Similarly, noninteger parameters of the sort considered here ought to be a fruitful source of insight when used within their proper limits, even if such limits should turn out to be narrower than has hitherto been supposed.

**ACKNOWLEDGMENTS**

Financial support for this research was provided by the National Science Foundation through Grant No. DMR 78-20394.

**APPENDIX A. DERIVATION OF (4.5), (4.7), AND (5.2).**

To obtain (4.5), we use (4.4) and the following integral, in which the  $p_\alpha$  are nonnegative even integers whose sum is  $|p|$ :

$$\int_{-\infty}^{\infty} dx_1 \dots dx_n \delta\left(t - \sum_{\alpha=1}^n x_\alpha^2\right) \prod_{\alpha=1}^n (x_\alpha)^{p_\alpha} = \left\{ t^{(n+|p|)/2-1} / \Gamma\left[\frac{1}{2}(n + |p|)\right] \right\} \sum_{\alpha=1}^n \Gamma\left[\frac{1}{2}(1 + p_\alpha)\right] \quad (\text{A.1})$$

The derivation of (A.1) can be carried out as follows. The exponent of  $t$  on the right side can be obtained by a dimensional argument or by making the substitution  $x_\alpha = y_\alpha \sqrt{t}$  in the integral. To check the remaining factors, multiply both sides of (A.1) by  $e^{-t}$ , integrate over  $t$  from 0 to  $\infty$ , and use that fact that

$$\int_{-\infty}^{\infty} x^p e^{-x^2} dx = \Gamma\left[\frac{1}{2}(1 + p)\right] \quad (\text{A.2})$$

when  $p$  is an even integer. For future reference, we note that when all the  $p_\alpha$

are zero (A.1) reads

$$\int_{-\infty}^{\infty} dx_1 \dots dx_n \delta\left(t - \sum_{\alpha=1}^n x_{\alpha}^2\right) = \frac{\pi^{n/2} t^{n/2-1}}{\Gamma(n/2)} \tag{A.3}$$

Equation (4.7) is a special case of (5.2) obtained by setting  $w(t)$  equal to  $\delta(1-t)$  in the latter. To obtain (5.2), we begin with (5.1) and note that

$$\begin{aligned} &\int_{-\infty}^{\infty} w\left(\sum_{\alpha=1}^n x_{\alpha}^2\right) dx_{\nu+1} dx_{\nu+2} \dots dx_n \\ &= \int_0^{\infty} dt w(\tilde{x}^2 + t) \int_{-\infty}^{\infty} \delta\left(t - \sum_{\alpha=\nu+1}^n x_{\alpha}^2\right) dx_{\nu+1} \dots dx_n \\ &= \frac{\pi^{(n-\nu)/2}}{\Gamma[\frac{1}{2}(n-\nu)]} \int_0^{\infty} dt w(\tilde{x}^2 + t) t^{(n-\nu)/2-1} \end{aligned} \tag{A.4}$$

where

$$\tilde{x}^2 = \sum_{\alpha=1}^{\nu} x_{\alpha}^2 \tag{A.5}$$

and we have used (A.3) to evaluate one of the integrals. The denominator on the right side of (5.1) is given by (A.4) in the special case in which  $\nu$  and  $\tilde{x}^2$  are both zero:

$$\int_{-\infty}^{\infty} w\left(\sum_{\alpha=1}^n x_{\alpha}^2\right) dx_1 \dots dx_n = \frac{\pi^{n/2}}{\Gamma(n/2)} \int_0^{\infty} w(t) t^{n/2-1} dt \tag{A.6}$$

**APPENDIX B. DERIVATION OF (4.12), (4.13), AND (4.20);  $m(h)$  FOR  $n < 1$**

Equation (4.12) can be obtained by expanding the exponential in a power series and comparing the result with the corresponding expansion for the modified Bessel function<sup>(27)</sup>  $I_{\nu}(h)$ . The recursion relation

$$dI_{\nu}/dh = (\nu/h)I_{\nu} + I_{\nu+1} \tag{B.1}$$

allows one to write  $m(h)$  in the form (4.13). The easiest way to obtain (4.20) is to note that by symmetry the average over  $S_1$  cannot depend on the direction of  $S_2$ . Thus the latter can be assumed to be of the form  $(1, 0, \dots, 0)$ , and consequently

$$\langle \exp K S_1 \cdot S_2 \rangle = \langle \exp(Kx_1) \rangle \tag{B.2}$$

The asymptotic behavior of  $I_{\nu}(h)$  for large  $h > 0$  is given by the

formula<sup>(27)</sup>

$$I_\nu(h) \sim \frac{e^h}{(2\pi h)^{1/2}} \left[ 1 - \frac{1}{2}(\nu^2 - \frac{1}{4})h^{-1} + O(h^{-2}) \right] \tag{B.3}$$

Therefore

$$m(h) = I_{n/2}(h)/I_{(n/2-1)}(h) \sim 1 + \frac{1}{2}(1-n)h^{-1} + O(h^{-2}) \tag{B.4}$$

decreases as  $h$  increases when  $h$  is sufficiently large, whenever  $n$  is less than 1.

**APPENDIX C. DERIVATION OF (4.16) AND (5.15)**

Equation (4.16) is our immediate consequence of (5.15) when one replaces  $w(t)$  by  $\delta(1-t)$  and integrates over the  $M_{ij}$ . To derive (5.15), we note that

$$\begin{aligned} \hat{\rho}(M) &= Z^{-1} \int \left[ \prod_{j < k} \delta(M_{jk} - \mathbf{S}_j \cdot \mathbf{S}_k) \right] \prod_j w(\mathbf{S}_j \cdot \mathbf{S}_j) d\mathbf{S}_1 \dots d\mathbf{S}_N \\ &= Z^{-1} \left[ \prod_{j=1}^N w(M_{jj}) \right] J_{n,N}(M) \end{aligned} \tag{C.1}$$

where  $Z$  is a normalization constant and  $J_{n,N}$  is defined by

$$J_{n,N}(M) = \int \prod_{j < k} \delta(M_{jk} - \mathbf{S}_j \cdot \mathbf{S}_k) d\mathbf{S}_1 \dots d\mathbf{S}_N \tag{C.2}$$

In these formulas the matrix  $M$  with components  $M_{jk}$  is assumed to be symmetrical and positive definite. The symbol  $d\mathbf{S}_j$  stands for  $\prod_\alpha dS_j^\alpha$ .

Formula (C.2) can be evaluated recursively by noting that the integrand is invariant under a simultaneous rotation (real orthogonal transformation) of all of the  $\mathbf{S}_j$ . Consequently  $J_{n,N}$  is equal to

$$\int \delta(M_{NN} - \mathbf{S}_N \cdot \mathbf{S}_N) d\mathbf{S}_N = \pi^{n/2} (M_{NN})^{n/2-1} / \Gamma(n/2) \tag{C.3}$$

times the integral over the remaining product of  $\delta$  functions in (C.2) with  $\mathbf{S}_N$  replaced by a vector  $(0, 0, \dots, (M_{NN})^{1/2})$ , i.e.,

$$\int \prod_{j=1}^{N-1} \delta(M_{jN} - S_j^n (M_{NN})^{1/2}) \prod_{j < k}^{N-1} \delta(M_{jk} - \mathbf{S}_j \cdot \mathbf{S}_k) d\mathbf{S}_1 \dots d\mathbf{S}_{N-1} \tag{C.4}$$

The next step is to integrate this expression over  $d\mathbf{S}_1^n d\mathbf{S}_2^n \dots d\mathbf{S}_{N-1}^n$ . If  $\mathbf{S}'_j$  is the vector with  $n-1$  components equal to the first  $n-1$  components of

$\mathbf{S}_j$ , the result can be written in the form

$$\left[ (M_{NN})^{1/2} \right]^{1-N} \int \prod_{j < k} \delta(M'_{jk} - \mathbf{S}'_j \cdot \mathbf{S}'_k) d\mathbf{S}'_1 \dots d\mathbf{S}'_{N-1} \quad (\text{C.5})$$

where  $M'$  is an  $(N-1) \times (N-1)$  matrix with components

$$M'_{jk} = M_{jk} - M_{jN}M_{kN}/M_{NN}$$

Upon comparing (C.5) with (C.2) and putting all the factors together, we have the desired recursion relation:

$$J_{n,N}(M) = \left[ \pi^{n/2} \left[ (M_{NN})^{1/2} \right]^{n-N-1} / \Gamma(n/2) \right] J_{n-1,N-1}(M') \quad (\text{C.6})$$

Now  $M'_{jk}$  can be thought of as consisting of the upper left (first  $N-1$  rows and columns) block of an  $N \times N$  matrix obtained from  $M$  by subtracting the  $N$ th row of  $M$  multiplied by  $M_{jN}/M_{NN}$  from the  $j$ th row, for  $j = 1, 2, \dots, N-1$ . As the  $N$ th column of this new matrix is zero except for the  $NN$  element equal to  $M_{NN}$ , and as it has the same determinant as  $M$ , we conclude that

$$\det M = M_{NN} \det M' \quad (\text{C.7})$$

In the case  $N = 1$  a direct calculation gives

$$J_{n,1}(M) = \pi^{n/2} (\det M)^{n/2-1} / \Gamma(n/2) \quad (\text{C.8})$$

where, of course,  $\det M$  is just  $M_{11}$ . Combining (C.6), (C.7), and (C.8) then yields the formula

$$J_{n,N}(M) = \frac{\pi^{N(2n-N+1)/4} (\det M)^{(n-N-1)/2}}{\prod_{j=0}^{n-1} \Gamma\left[\frac{1}{2}(n-j)\right]} \quad (\text{C.9})$$

To complete the derivation of (5.15), we note that the normalization constant  $Z$  in (C.1) is

$$Z = \int \prod_j w(\mathbf{S}_j \cdot \mathbf{S}_j) d\mathbf{S}_1 \dots d\mathbf{S}_N = \left\{ \left[ \pi^{n/2} / \Gamma(n/2) \right] \int_0^\infty w(t) t^{n/2-1} dt \right\}^N \quad (\text{C.10})$$

where we have made use of (A.6).

#### APPENDIX D. DERIVATION OF (4.18) AND (5.17)

To obtain (5.17), we note that

$$\langle |M|^m \rangle_w = L/Z \quad (\text{D.1})$$

where  $|M|$  denotes the determinant of  $M$ , the matrix with elements  $M_{ij}$



equal to  $\mathbf{S}_i \cdot \mathbf{S}_j$

$$L = \int d\mathbf{S}_1 \dots d\mathbf{S}_N |M|^m \prod_{j=1}^N w(\mathbf{S}_j \cdot \mathbf{S}_j) \tag{D.2}$$

in the notation of Appendix C, and  $Z$  is given by (C.10). Equation (D.2) may be rewritten as

$$L = \int_0^\infty dt_1 \dots dt_N \left[ \prod_{j=1}^N w(t_j) \right] \int d\mathbf{S}_1 \dots d\mathbf{S}_N |M|^m \prod_{j=1}^N \delta(t_j - \mathbf{S}_j \cdot \mathbf{S}_j) \tag{D.3}$$

If we make the substitution

$$\mathbf{S}_j = (t_j)^{1/2} \mathbf{T}_j \tag{D.4}$$

and note that

$$|M| = |N| \prod_j t_j \tag{D.5}$$

where  $N$  is the matrix with elements

$$N_{jk} = \mathbf{T}_j \cdot \mathbf{T}_k \tag{D.6}$$

(D.3) becomes

$$L = \int_0^\infty dt_1 \dots dt_N \left[ \prod_j w(t_j) t_j^{n/2+m-1} \right] \int d\mathbf{T}_1 \dots d\mathbf{T}_N |N|^m \prod_j \delta(1 - \mathbf{T}_j \cdot \mathbf{T}_j) \tag{D.7}$$

Combining (D.7) and (C.10) yields (5.17), where  $\langle \rangle_1$  refers to the case in which  $w(t)$  is  $\delta(1 - t)$ .

To derive (4.18), we obtain a recursion formula for

$$D_{n,N}(m) = \langle |M|^m \rangle_w \tag{D.8}$$

in the special case where

$$w(t) = e^{-t} \tag{D.9}$$

and then use (5.17). When (D.9) is inserted in (D.2), the result can be written as

$$L_{n,N} = \int_0^\infty dt \int d\mathbf{S}_1 \dots d\mathbf{S}_N \delta(t - \mathbf{S}_N \cdot \mathbf{S}_N) |M|^m \exp\left(-\sum_{j=1}^N \mathbf{S}_j \cdot \mathbf{S}_j\right) \tag{D.10}$$

where we have added subscripts to  $L$  for use in (D.13) below. The integrand is invariant under the simultaneous rotation of all the  $\mathbf{S}_j$ , and it is convenient to consider the situation in which

$$\mathbf{S}_N = (0, 0, \dots, 0, \sqrt{t}) \tag{D.11}$$

Let  $S'_j$ , for  $j = 1, 2, \dots, N-1$ , be the  $(n-1)$ -component vector obtained by discarding the  $n$ th component of  $S_j$ , and the  $M'_{ij}$  be the  $(n-1) \times (n-1)$  matrix with elements  $S'_i \cdot S'_j$ . Its determinant  $|M'|$  is related to that of  $M$  through the equation

$$|M| = t|M'| \quad (\text{D.12})$$

which can be obtained in the same manner as (C.7): for  $j = 1, 2, \dots, N-1$ , subtract the  $N$ th row of  $M$  multiplied by  $M'_{jN}/t$  from the  $j$ th row.

Consequently (D.10) may be written in the form

$$\begin{aligned} L_{n,N} &= \int_0^\infty dt e^{-t} t^m \int d\mathbf{S}_N \delta(t - \mathbf{S}_N \cdot \mathbf{S}_N) \\ &\quad \times \int dS_1^n \dots dS_{N-1}^n \exp \left[ - \sum_{j=1}^{N-1} (S_j^n)^2 \right] \\ &\quad \times \int dS'_1 \dots dS'_{N-1} |M'|^m \exp \left( - \sum_{j=1}^{N-1} \mathbf{S}'_j \cdot \mathbf{S}'_j \right) \\ &= \pi^{(N+n-1)/2} [\Gamma(m+n/2)/\Gamma(n/2)] L_{n-1, N-1} \end{aligned} \quad (\text{D.13})$$

where we have used (A.3). Combining (D.13) with (C.10) for the case (D.9), and noting (D.8) and (D.1) yields the desired recursion formula:

$$D_{n,N}(m) = [\Gamma(m+n/2)/\Gamma(n/2)] D_{n-1, N-1}(m) \quad (\text{D.14})$$

The integral (D.2) is elementary when  $N = 1$ , and combining this with (D.14) yields the result

$$D_{n,N}(m) = \prod_{j=0}^{N-1} \frac{\Gamma[m + \frac{1}{2}(n-j)]}{\Gamma[\frac{1}{2}(n-j)]} \quad (\text{D.15})$$

for

$$m > (N - n - 1)/2 \quad (\text{D.16})$$

As a final step, (4.18) is obtained by inserting (D.9) on the right side of (5.17), and noting that in this case the left side is given by (D.15).

## REFERENCES

1. K. G. Wilson and M. E. Fisher, *Phys. Rev. Lett.* **28**:240 (1972).
2. K. G. Wilson, *Phys. Rev. Lett.* **28**:548 (1972).
3. P. Pfeuty and G. Toulouse, *Introduction to the Renormalization Group and Critical Phenomena* (Wiley, London, 1977).
4. C. Domb and M. S. Green, eds. *Phase Transitions and Critical Phenomena*, Vol. 6, (Academic Press, London, 1976).
5. P. G. deGennes, *Phys. Lett.* **38A**:339 (1972).
6. R. Balian and G. Toulouse, *Phys. Rev. Lett.* **30**:544 (1973).

7. M. E. Fisher, *Phys. Rev. Lett.* **30**:679 (1973).
8. P. W. Kasteleyn and C. M. Fortuin, *J. Phys. Soc. Japan (Suppl.)* **26**:11 (1969).
9. B. Nienhuis *et al.*, *Phys. Rev. Lett.* **43**:737 (1979).
10. J. B. Kogut and D. K. Sinclair, *Phys. Lett.* **86A**:38 (1981).
11. J. L. van Hemmen and R. G. Palmer, *J. Phys.* **A12**:563 (1979).
12. G. F. Tuthill, J. F. Nicoll, and H. E. Stanley, *Phys. Rev.* **B11**:4579 (1975).
13. A. Aharony, in *Phase Transitions and Critical Phenomena*, Vol. 6, C. Domb and M. S. Green, eds. (Academic Press, London, 1976), p. 357.
14. J. des Cloizeaux, *J. Phys.* **36**:281 (1975).
15. M. A. Moore and C. A. Wilson, *J. Phys. A* **13**:3501 (1980).
16. R. Balian and G. Toulouse, *Ann. Phys. (N.Y.)* **83**:28 (1974).
17. D. Ruelle, *Statistical Mechanics* (Benjamin, New York, 1969).
18. R. B. Griffiths, in *Phase Transitions and Critical Phenomena*, Vol. 1, C. Domb and M. S. Green, eds., (Academic Press, London, 1972), p. 7.
19. P. R. Gerber and M. E. Fisher, *Phys. Rev. B* **10**:4697 (1974).
20. D. Jasnow and M. E. Fisher, *Phys. Rev. B* **13**:1112 (1976).
21. H. J. Hilhorst, *Phys. Lett.* **56A**:153 (1976).
22. E. C. Titchmarsh, *The Theory of Functions*, 2nd ed. (Oxford, London, 1939), p. 186.
23. C. Domb, in *Phase Transitions and Critical Phenomena*, Vol. 3, C. Domb and M. S. Green, eds., (Academic Press, London, 1974), p. 357.
24. M. E. Fisher and D. S. Gaunt, *Phys. Rev.* **133**:A224 (1964).
25. P. D. Gujrati, *Phys. Rev. A* **24**:2096 (1981).
26. O. Penrose and J. L. Lebowitz, in *Fluctuation Phenomena*, E. W. Montroll and J. L. Lebowitz, eds., (North-Holland, Amsterdam, 1979), p. 293.
27. M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (National Bureau of Standards, Washington, 1964), pp. 374ff.