

## Local magnetic field distributions: Two-dimensional Ising models

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We show that the statistical mechanics of Ising models can be conveniently reformulated in terms of the local magnetic field probability distribution function  $P(h)$ . It is shown that for arbitrary exchange interactions  $J_{ij}$ , which may or may not be random, both thermodynamic quantities such as magnetization, specific heat, etc., and the neutron scattering law  $S(\vec{k}, \omega)$  can be obtained from  $P(h)$ . Indeed  $S(\vec{k}, \omega)$  provides a direct measurement of the *symmetric* part of  $P(h)$  which also determines the energy, specific heat, etc., while the magnetization can be obtained from the *antisymmetric* part of  $P(h)$ . As an example, specific results for  $P(h)$  are presented for the honeycomb, square, and triangular lattices with constant nearest-neighbor interactions. All three lattices exhibit a pronounced *dip* in the center of  $P(h)$  at the transition temperature.

### I. INTRODUCTION

At various stages in the development of the theory of magnetism, the local-field probability distribution function  $P(h)$  has been used.<sup>1-5</sup> Despite the fact that  $P(h)$  has a simple physical interpretation, it has *not* been widely adopted. This is probably because its usage has been associated with mean-field-type theories and as such it is regarded as an approximation.

In this paper we show that an exact, useful, and complete description of the thermodynamics of a rather general class of Ising models can be obtained in terms of  $P(h)$ . These models have localized spins  $S_i$  associated with sites  $\vec{R}_i$ . The spins can have different magnitudes and the sites  $\vec{R}_i$  do *not* have to form a crystalline lattice. The Hamiltonian involves only the  $S_i^z$  components and contains arbitrary exchange interactions  $J_{ij}$  and external fields  $H_i$ . The range of the  $J_{ij}$  is also quite general. All these results are scattered throughout the literature<sup>1-4</sup> of the early 1960s and are summarized by Southern.<sup>5</sup> We collect them together in this paper.

We show that a measurement of the inelastic-neutron-scattering law  $S(\vec{k}, \omega)$  at a particular temperature provides a direct measurement of the *symmetric* part of  $P(h)$  at that temperature. The total magnetization of the system can be obtained directly from the *antisymmetric* part of  $P(h)$ , although the converse is not true. Finally, the total energy can be obtained from the *symmetric* part of  $P(h)$ , if *all the*  $H_i = 0$ . Other thermodynamic quantities of interest, such as the free energy, specific heat, etc., can be obtained from the energy. The above connections are very powerful because they require a knowledge of *only*  $P(h)$  and the temperature, *no other information about the system*. In the case where the  $H_i \neq 0$ , the ener-

gy, and hence the other thermal thermodynamic quantities, can still be found from  $P(h)$  in simple cases. Such an example would be a uniform field where all the  $H_i = H$ , and a knowledge of  $P(h)$ , the temperature, and  $H$  would lead to the energy.

The layout of this paper is as follows. In the next section we develop the general formalism for  $S = \frac{1}{2}$ . This is for pedagogical reasons, and the rather obvious generalizations to arbitrary spin are given in the Appendix. In Sec. III we illustrate these results for various spin- $\frac{1}{2}$  nearest-neighbor Ising models: the one-dimensional chain, and the honeycomb, square, and triangular nets in two dimensions. These results are exact and could have been obtained at any time in the past 20 years. Surprisingly, they do not appear in the literature. The results in two dimensions are rather interesting as  $P(h)$  changes from a roughly Gaussian shape at high temperatures to develop a pronounced dip in the center at the transition temperature  $T_c$ . It is unclear how general this phenomenon is. We define a quantity that measures the fluctuations in the local field  $h$  and show, not surprisingly, that it has a maximum at  $T_c$ .

The attraction of  $P(h)$  is that it provides an alternative description of a thermodynamic system with perhaps a more intuitive interpretation than the free energy. It contains more information than just the free energy and, for example, the neutron-scattering law  $S(\vec{k}, \omega)$  can also be derived from it. We note that  $S(\vec{k}, \omega)$  cannot be derived from the free energy.

Our original motivation for this work was that computer experiments on spin-glass models at zero temperature often focus on  $P(h)$ . Indeed, it is a "natural" quantity to compute. Such experiments have universally demonstrated a zero-field minimum in spin-glass models with com-

peting interactions in their ground or low-lying metastable states.<sup>6</sup> A similar minimum has been found in simulations of amorphous antiferromagnets.<sup>7,8</sup> Because of the interesting new results found for simple Ising models, we have deferred a discussion of more complex spin systems with competing interactions to a planned, subsequent paper.<sup>9</sup>

## II. GENERAL FORMALISM

We define a spin- $\frac{1}{2}$  Ising system with the Hamiltonian

$$H = -\frac{1}{2} \sum_{i,j} J_{ij} \sigma_i \sigma_j - \sum_i H_i \sigma_i, \quad (1)$$

where the  $J_{ij}$  and  $H_i$  are arbitrary and the factor  $\frac{1}{2}$  is to prevent double counting. This Hamiltonian describes a completely general spin- $\frac{1}{2}$  Ising system with  $\sigma_i = \pm 1$ , an arbitrary range of exchange parameters  $J_{ij}$ , and an external field  $H_i$  that can vary from site to site. We define the  $J_{ii} = 0$ . The sites can be inequivalent and we make no assumptions about the existence of a crystalline lattice or translational invariance. Although we develop these results for spin  $\frac{1}{2}$ , all of the results of this section easily generalize to arbitrary spin, as shown in the Appendix.

There are a number of ways of decomposing the Hamiltonian (1). The most obvious is

$$H = -\sum_i \mathcal{K}_i \sigma_i, \quad (2)$$

where

$$\mathcal{K}_i = \frac{1}{2} \sum_j J_{ij} \sigma_j + H_i. \quad (3)$$

This is not useful in discussing local fields, where it is necessary to decompose (1) as

$$H = -h_i \sigma_i + H', \quad (4)$$

where

$$h_i = \sum_j J_{ij} \sigma_j + H_i. \quad (5)$$

The first term in Eq. (4) contains *all* terms involving  $\sigma_i$ ; other terms are lumped together in  $H'$ . Notice that  $\mathcal{K}_i$  as defined in (3) and  $h_i$  as defined in (5) differ in the factor  $\frac{1}{2}$  in front of the exchange term. This means that some care must be taken in calculating the *energy* of the system later in this section.

We consider the thermal average  $\langle O \sigma_i \rangle$  where  $O$  is any operator not involving site  $i$ ; we write

$$\begin{aligned} \langle O \sigma_i \rangle &= \langle \text{Tr}_i [O \sigma_i \exp(\beta h_i \sigma_i)] / \text{Tr}_i [\exp(\beta h_i \sigma_i)] \rangle \\ &= \langle O \tanh(\beta h_i) \rangle. \end{aligned} \quad (6)$$

Setting  $O$  equal to the unit operator, we find that<sup>2,3</sup>

$$\begin{aligned} \langle \sigma_i \rangle &= \tanh(\beta h_i) \\ &= \left\langle \tanh \left[ \beta \left[ \sum_j J_{ij} \sigma_j + H_i \right] \right] \right\rangle. \end{aligned} \quad (7)$$

We note in passing that replacing the thermal average of the tanh in (7) by the tanh of the thermal average leads to mean-field theory.<sup>2</sup> Setting 0 equal to  $h_i$  in (6) leads to

$$\begin{aligned} \langle h_i \sigma_i \rangle &= \left\langle \sum_j J_{ij} \sigma_i \sigma_j + H_i \sigma_i \right\rangle \\ &= \langle h_i \tanh(\beta h_i) \rangle. \end{aligned} \quad (8)$$

It is *not* possible to obtain the energy from (8) alone for  $H_i \neq 0$ , because of the missing factor  $\frac{1}{2}$  in front of the exchange, as required for the decomposition in Eqs. (2) and (3). However, the energy can be obtained as

$$\begin{aligned} E_i &= -\langle \mathcal{K}_i \tanh(\beta h_i) \rangle \\ &= -\frac{1}{2} \langle (h_i + H_i) \tanh(\beta h_i) \rangle. \end{aligned} \quad (9)$$

The magnetization  $M$  and the energy  $E$  are given by

$$M = \sum_i \langle \sigma_i \rangle, \quad E = \sum_i E_i. \quad (10)$$

We introduce the probability distribution  $P_i(h)$  for the local magnetic field at site  $i$  by

$$P_i(h) = \langle \delta(h - h_i) \rangle, \quad (11)$$

where both the "internal" and external fields are included in  $h_i$  via Eq. (5). It is, of course, possible to define a similar quantity  $P'_i(h)$  counting only the internal-field contribution, namely

$$P'_i(h) = \left\langle \delta \left[ h - \sum_j J_{ij} \sigma_j \right] \right\rangle = P_i(h - H_i). \quad (12)$$

For the rest of this paper we shall use (11). From the definition of  $P_i(h)$ , we see that

$$\int P_i(h) dh = 1, \quad (13)$$

$$\left\langle \left[ \sum_j J_{ij} \sigma_j + H_i \right]^n \right\rangle = \int h^n P_i(h) dh, \quad (14)$$

and, from (7) and (9),

$$\langle \sigma_i \rangle = \int \tanh(\beta h) P_i(h) dh, \quad (15)$$

$$E_i = -\frac{1}{2} \int h \tanh(\beta h) P_i(h) dh - \frac{1}{2} H_i \langle \sigma_i \rangle. \quad (16)$$

The distribution function  $P(h)$  for the entire system with  $N$  sites is obtained from (11) via

$$P(h) = \frac{1}{N} \sum_i P_i(h). \quad (17)$$

It can be seen from (15) that a knowledge of  $P(h)$  and the temperature is sufficient to determine the magnetization,

$$M = N \int \tanh(\beta h) P(h) dh. \quad (18)$$

It is not necessary to know anything else about the system; in particular, it is not necessary to know the  $J_{ij}$  or the  $H_i$ . It is this sense in which  $P(h)$  provides a description of the system in the same way as the free energy does. Because  $\tanh(\beta h)$  is an odd function of  $\beta h$ , only the *antisymmetric* part  $P_a(h)$  of  $P(h)$  contributes to  $M$ ,

$$P_a(h) = \frac{1}{2} [P(h) - P(-h)], \quad (19)$$

$$M = N \int \tanh(\beta h) P_a(h) dh. \quad (20)$$

In general, the energy *cannot* be obtained directly from  $P(h)$ . However, if all the  $H_i$  are known to be *zero*, then

from (10) and (16),

$$E = -\frac{N}{2} \int h \tanh(\beta h) P(h) dh, \quad (21)$$

and  $E$  can be calculated directly from  $P(h)$  without any knowledge of the  $J_{ij}$ . Because  $h \tanh(\beta h)$  is an even function of  $h$ , only the symmetric part  $P_s(h)$  of  $P(h)$  contributes to  $E$ ,

$$P_s(h) = \frac{1}{2} [P(h) + P(-h)], \quad (22)$$

$$E = -\frac{N}{2} \int h \tanh(\beta h) P_s(h) dh. \quad (23)$$

In this case, the free energy  $F$  is given by

$$\beta F = -N \ln 2 + \int_0^\beta E(\beta') d\beta'. \quad (24)$$

If the  $H_i$  are sufficiently simple, the free energy can still be found. For example, if the magnetic field is constant at every site  $H_i = H$ , the energy given in (9) becomes

$$E = -\frac{N}{2} \int (h + H) \tanh(\beta h) P(h) dh, \quad (25)$$

and the free energy  $F(H, T)$  is given by (24) with the integration done at constant  $H$ .

It can be seen that under appropriate conditions the local magnetic field probability distribution  $P(h)$  leads to the magnetization  $M$  and the energy  $E$ . All other thermodynamic quantities, such as the free energy, specific heat, etc., have to be found by integrating or differentiating  $M$  or  $E$ . This is because  $M$  and  $E$  are determined from the expectation values of *local operators*, whereas other thermodynamic functions are not. Thus  $M$  and  $E$  are particularly important when the statistical mechanics is done via  $P(h)$ . This point appears not to have been appreciated by Klein and Brout,<sup>4</sup> who attempted to write the free en-

ergy as an integral over  $P(h)$  [see their Eq. (2.5)].

The function  $P(h)$  contains more than just thermodynamic information; it is directly related to the inelastic-neutron-scattering cross section,<sup>10</sup>

$$S(\vec{k}, \omega) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt e^{-i\omega t} \sum_{i,j} \exp[i\vec{k} \cdot (\vec{R}_i - \vec{R}_j)] \times \langle \sigma_i^x \sigma_j^x(t) \rangle, \quad (26)$$

where  $x$  is any direction perpendicular to the  $z$  axis. In the previous part of this section we suppressed the  $z$  superscript on the  $\sigma_i^z$  operators. This cross section is  $\vec{k}$  independent because Ising systems have no dynamics, so that transforming to raising and lowering operators,<sup>11</sup>

$$S(\vec{k}, \omega) = \frac{1}{8\pi} \int_{-\infty}^{+\infty} dt e^{-i\omega t} \sum_i \langle [\sigma_i^+ \sigma_i^-(t) + \sigma_i^- \sigma_i^+(t)] \rangle. \quad (27)$$

The time dependence of these operators is given by

$$\sigma_i^\pm(t) = \exp(iHt) \sigma_i^\pm \exp(-iHt) = \sigma_i^\pm \exp(2ith_i \sigma_i), \quad (28)$$

where the  $h_i$  are given by (5). Combining (27) and (28) we find that

$$\begin{aligned} S(\vec{k}, \omega) &= \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt e^{-i\omega t} \sum_i \langle \exp(2ith_i \sigma_i) \rangle \\ &= \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt e^{-i\omega t} \sum_i \langle [\cos(2th_i) \\ &\quad + i\sigma_i \sin(2th_i)] \rangle. \end{aligned}$$

With the use of Eq. (6), this can be rewritten as

$$\begin{aligned} S(\vec{k}, \omega) &= \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt e^{-i\omega t} \sum_i \langle [\cos(2th_i) + i \tanh(\beta h_i) \sin(2th_i)] \rangle \\ &= \frac{1}{2\pi} \int dh \int_{-\infty}^{+\infty} dt e^{-i\omega t} \sum_i [\cos(2th) + i \tanh(\beta h) \sin(2th)] P_i(h) \\ &= \frac{N}{2} \frac{P(\omega/2) + P(-\omega/2)}{1 + \exp(-\beta\omega)}, \end{aligned} \quad (29)$$

which shows that the neutron-scattering law provides a direct measurement of the *symmetric* part  $P_s(h)$  of  $P(h)$ ,

$$S(\vec{k}, \omega) = N \frac{P_s(\omega/2)}{1 + \exp(-\beta\omega)}. \quad (30)$$

The thermal factor  $[1 + \exp(-\beta\omega)]^{-1}$  ensures detailed balance.

From the properties of  $P(h)$ , it is easy to show that

$$\frac{1}{2N} \int S(\vec{k}, \omega) [1 + \exp(-\beta\omega)] d\omega = 1, \quad (31)$$

and if all the  $H_i = 0$ ,

$$\frac{1}{8} \int S(\vec{k}, \omega) [1 - \exp(-\beta\omega)] \omega d\omega = -E. \quad (32)$$

Both (31) and (32) hold for arbitrary  $J_{ij}$ . Expression (31) could be useful in normalizing neutron data taken at different temperatures, if this data were to be used to find  $E$ .

### III. TWO-DIMENSIONAL ISING MODELS

In this section we present results for  $P(h)$  for some pure two-dimensional Ising systems.<sup>12</sup> This presentation is rather straightforward, but does serve to illustrate some of the points made in the preceding section and provides some interesting results.

It is convenient to redefine the Hamiltonian (1) with only a nearest neighbor  $J_{ij}$  which is set equal to 1,

$$H = -\frac{1}{2} \sum_{i,j} \sigma_i \sigma_j, \quad (33)$$

where the sum goes over nearest-neighbor pairs only, and the factor  $\frac{1}{2}$  is to prevent double counting. In what follows we use a slightly modified form of the notation of Choy and Sherrington.<sup>13</sup> As all sites are equivalent, we can ignore the distinction between  $P_i(h)$  and  $P(h)$ . Therefore,

$$P(h) = \left\langle \delta \left[ h - \sum_{j=1}^z \sigma_j \right] \right\rangle, \quad (34)$$

where the sum over  $j$  goes over the  $z$  nearest neighbors of atom  $i$ . This can be conveniently rewritten as

$$\begin{aligned} P(h) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\theta \exp(-ih\theta) \left\langle \exp \left[ i\theta \sum_{j=1}^z \sigma_j \right] \right\rangle \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\theta \exp(-ih\theta) \left\langle \prod_{j=1}^z (1 + i\sigma_j \tan\theta) \right\rangle \\ &\quad \times \cos^z \theta, \end{aligned} \quad (35)$$

where we have used the integral representation of the Dirac  $\delta$  function with the usual convergence factors implied at  $\pm\infty$ . Multiplying out the product in the angular brackets, this becomes

$$P(h) = \frac{1}{2^z} \sum_{s=-z}^z \sum_{r=0}^z a_{rs}^z c_r \delta(h-s), \quad (36)$$

where the  $r$  sum is in steps of 1 and the  $s$  sum is in steps of 2. The final result has the form

$$P(h) = \sum_{s=-z}^z w_s \delta(h-s), \quad (37)$$

with

$$w_s = \frac{1}{2^z} \sum_{r=0}^z a_{rs}^z c_r, \quad (38)$$

and the  $a_{rs}^z$  are given by the generating function

$$\begin{aligned} \frac{1}{2\pi} \int_{-\infty}^{\infty} d\theta \exp(-ih\theta) \cos^z -r\theta \sin^r \theta i^r \\ = \frac{1}{2^z} \sum_{s=-z}^z a_{rs}^z \delta(h-s). \end{aligned} \quad (39)$$

The factor  $1/2^z$  is included so that the  $a_{rs}^z$  are integers. They are easily obtained for a given  $z$  by doing the simple integrals involved in (39) and are given in Table I. The  $c_r$  are correlation functions<sup>13</sup> defined by

$$c_r = \sum_{(ij \dots l)} \langle \sigma_i \sigma_j \dots \sigma_l \rangle, \quad (40)$$

where the parentheses around the summation indices denote that only the *distinct* products of  $r$  operators among the  $z$  nearest neighbors are to be taken. If we label the  $z$  nearest neighbors of an atom *cyclically* from 1 to  $z$ , then for the linear chain,

$$\begin{aligned} c_0 &= 1, \\ c_1 &= \sum_{(i)} \langle \sigma_i \rangle = 2 \langle \sigma_1 \rangle, \\ c_2 &= \sum_{(ij)} \langle \sigma_i \sigma_j \rangle = \langle \sigma_1 \sigma_2 \rangle. \end{aligned} \quad (41)$$

For the honeycomb lattice ( $z=3$ ),

$$\begin{aligned} c_0 &= 1, \\ c_1 &= \sum_{(i)} \langle \sigma_i \rangle = 3 \langle \sigma_1 \rangle, \\ c_2 &= \sum_{(ij)} \langle \sigma_i \sigma_j \rangle = 3 \langle \sigma_1 \sigma_2 \rangle, \\ c_3 &= \sum_{(ijk)} \langle \sigma_i \sigma_j \sigma_k \rangle = \langle \sigma_1 \sigma_2 \sigma_3 \rangle. \end{aligned} \quad (42)$$

For the square net ( $z=4$ ),

TABLE I. Coefficients  $a_{rs}^z$  defined in Eq. (39) are given for  $z=2, 3, 4$ , and 6.

$z=2$					$z=3$					
$s$	$r$	0	1	2	$s$	$r$	0	1	2	3
2		1	1	1	3		1	1	1	1
0		2	0	-2	1		3	1	-1	-3
-2		1	-1	1	-1		3	-1	-1	3
					-3		1	-1	1	-1

$z=4$							$z=6$								
$s$	$r$	0	1	2	3	4	$s$	$r$	0	1	2	3	4	5	6
4		1	1	1	1	1	6		1	1	1	1	1	1	1
2		4	2	0	-2	-4	4		6	4	2	0	-2	-4	-6
0		6	0	-2	0	6	2		15	5	-1	-3	-1	5	15
-2		4	-2	0	2	-4	0		20	0	-4	0	4	0	-20
-4		1	-1	1	-1	1	-2		15	-5	-1	3	-1	-5	15
							-4		6	-4	2	0	-2	4	-6
							-6		1	-1	1	-1	1	-1	1

$$\begin{aligned}
c_0 &= 1, \\
c_1 &= \sum_{(i)} \langle \sigma_i \rangle = 4 \langle \sigma_1 \rangle, \\
c_2 &= \sum_{(ij)} \langle \sigma_i \sigma_j \rangle = 4 \langle \sigma_1 \sigma_2 \rangle + 2 \langle \sigma_1 \sigma_3 \rangle, \\
c_3 &= \sum_{(ijk)} \langle \sigma_i \sigma_j \sigma_k \rangle = 4 \langle \sigma_1 \sigma_2 \sigma_3 \rangle, \\
c_4 &= \sum_{(ijkl)} \langle \sigma_i \sigma_j \sigma_k \sigma_l \rangle = \langle \sigma_1 \sigma_2 \sigma_3 \sigma_4 \rangle.
\end{aligned} \tag{43}$$

For the triangular net ( $z=6$ ),

$$\begin{aligned}
c_0 &= 1, \\
c_1 &= \sum_{(i)} \langle \sigma_i \rangle = 6 \langle \sigma_1 \rangle, \\
c_2 &= \sum_{(ij)} \langle \sigma_i \sigma_j \rangle = 6 \langle \sigma_1 \sigma_2 \rangle + 6 \langle \sigma_1 \sigma_3 \rangle + 3 \langle \sigma_1 \sigma_4 \rangle, \\
c_3 &= \sum_{(ijk)} \langle \sigma_i \sigma_j \sigma_k \rangle = 6 \langle \sigma_1 \sigma_2 \sigma_3 \rangle + 12 \langle \sigma_1 \sigma_2 \sigma_4 \rangle \\
&\quad + 2 \langle \sigma_1 \sigma_3 \sigma_5 \rangle, \\
c_4 &= \sum_{(ijkl)} \langle \sigma_i \sigma_j \sigma_k \sigma_l \rangle = 6 \langle \sigma_1 \sigma_2 \sigma_3 \sigma_4 \rangle + 6 \langle \sigma_1 \sigma_2 \sigma_3 \sigma_5 \rangle \\
&\quad + 3 \langle \sigma_1 \sigma_2 \sigma_4 \sigma_5 \rangle, \\
c_5 &= \sum_{(ijklm)} \langle \sigma_i \sigma_j \sigma_k \sigma_l \sigma_m \rangle = 6 \langle \sigma_1 \sigma_2 \sigma_3 \sigma_4 \sigma_5 \rangle, \\
c_6 &= \sum_{(ijklmn)} \langle \sigma_i \sigma_j \sigma_k \sigma_l \sigma_m \sigma_n \rangle = \langle \sigma_1 \sigma_2 \sigma_3 \sigma_4 \sigma_5 \sigma_6 \rangle.
\end{aligned} \tag{44}$$

From the  $a_{rs}^z$  and the  $c_r$ , the amplitudes of the various fields  $w_s$  occurring in (37) can be calculated using (38). Many of these correlation functions  $c_r$  can be obtained from the literature for two-dimensional lattices. No exact calculations of the  $c_r$  exist in higher dimensions. We include the linear chain only because it is very simple. In what follows,  $K = \beta J$ , where  $J$  has previously been set equal to 1.

For the linear chain,<sup>14</sup>

$$c_0 = 1, \quad c_1 = 0, \quad c_2 = \tanh^2 K, \tag{45}$$

so that from (38) we have

$$w_0 = \frac{1}{2}(1 - \tanh^2 K), \quad w_2 = w_{-2} = \frac{1}{4}(1 + \tanh^2 K). \tag{46}$$

There is no phase transition in the linear chain, and so at all temperatures  $c_1 = 0$  and  $P(h)$  is symmetric. At infinite temperature ( $K=0$ ), we have  $w_0 = \frac{1}{2}$  and  $w_2 = w_{-2} = \frac{1}{4}$ , while at zero temperature ( $K = \infty$ ), we have  $w_0 = 0$  and  $w_2 = w_{-2} = \frac{1}{2}$ .

For the *honeycomb lattice* all of the  $c_r$  can be expressed in terms of the reduced energy  $\epsilon$  and the reduced magnetization  $m$

$$\epsilon = \langle \sigma_0 \sigma_1 \rangle, \quad m = \langle \sigma_0 \rangle, \tag{47}$$

where  $\sigma_0$  is the spin at the site of interest. This is achieved by rewriting (6) as<sup>15-18</sup>

$$\langle O \sigma_0 \rangle = A \langle O(\sigma_1 + \sigma_2 + \sigma_3) \rangle + B \langle O \sigma_1 \sigma_2 \sigma_3 \rangle, \tag{48}$$

where

$$A = \frac{1}{4} [\tanh(3K) + \tanh K], \tag{49}$$

$$B = \frac{1}{4} [\tanh(3K) - 3 \tanh K].$$

Setting  $O=1$  yields

$$\langle \sigma_1 \sigma_2 \sigma_3 \rangle = m(1 - 3A)/B, \tag{50}$$

and setting  $O = \sigma_1$  yields

$$\langle \sigma_1 \sigma_2 \rangle = (\epsilon - A)/(2A + B). \tag{51}$$

Combining all of these results, we find that<sup>19</sup>

$$\begin{aligned}
w_{\pm 1} &= \frac{1}{2} \left[ \frac{3[\tanh(3K) - \epsilon]}{3 \tanh(3K) - \tanh K} \right. \\
&\quad \left. \pm \frac{3m[\tanh(3K) - 1]}{\tanh(3K) - 3 \tanh K} \right], \\
w_{\pm 3} &= \frac{1}{2} \left[ \frac{3\epsilon - \tanh K}{3 \tanh(3K) - \tanh K} \right. \\
&\quad \left. \pm \frac{m(1 - 3 \tanh K)}{\tanh(3K) - 3 \tanh K} \right].
\end{aligned} \tag{52}$$

The reduced energy  $\epsilon$  can be written as an elliptic integral,<sup>12,18</sup> and the reduced magnetization  $m$  is a known function<sup>20</sup> of  $K$ . These results are illustrated in Fig. 1.

For any lattice at high temperatures,  $P(h)$  obeys a binomial distribution. The field is  $h$  if  $\frac{1}{2}(z+h)$  nearest-neighbor spins are up and  $\frac{1}{2}(z-h)$  are down. This occurs with probability  ${}^z C_{(z+h)/2} / 2^z$ , so that at infinite temperature,

$$P(h) = \sum_{s=-z}^z \frac{1}{2^z} {}^z C_{(z+s)/2} \delta(h-s).$$

As  $z$  becomes large,  $P(h)$  approaches closer to a Gaussian distribution.

When the temperature is lowered  $P(h)$  at first flattens and then develops a pronounced dip just above  $T_c$  for the

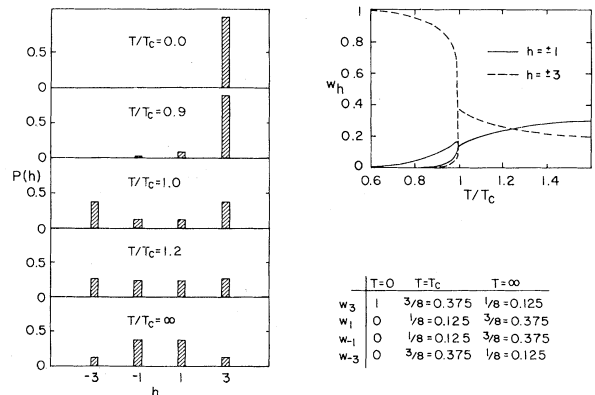


FIG. 1. For the honeycomb lattice, the bar graph at the left and the line graph in the upper right show the behavior of  $P(h)$  as a function of temperature. The ordinate gives the weight  $w_h$  in the  $\delta$  functions. The table in the lower right gives the value of  $w_h$  [defined in Eq. (37)] at special temperatures.

honeycomb lattice as shown in Fig. 1. At  $T_c$ , the values of  $w_s$  can be obtained by setting  $\epsilon_c = 4\sqrt{3}/9$ ,  $m_c = 0$ , and  $\exp(2K_c) = 2 + \sqrt{3}$  in (52). The distribution function rapidly develops an asymmetry below  $T_c$  as the magnetization increases from zero as  $(T_c - T)^\beta$  with  $\beta = \frac{1}{8}$ . At zero temperature there is a single peak at  $h = 3$ , as we would expect when the alignment is complete.

Note that  $P(h)$  contains the critical exponents  $\alpha$  (through  $\epsilon$ ) and  $\beta$  (through  $m$ ) in Eqs. (52). All the critical exponents of interest can be obtained from these two equations.<sup>21</sup>

As the coordination increases, so does the number of correlation functions that must be known. For the *square net*, the three spin correlation function is still proportional to the reduced magnetization via a relationship similar to (50).<sup>15-18</sup> However, it is necessary to compute two other independent, even spin correlation functions, as they *cannot* all be reduced to just  $\epsilon$  via relations such as (48) and (49). Computation of these functions involve evaluating elliptic integrals. For the *triangular net* the situation is much more complex, but a similar reduction to elliptic integrals for even spin correlations can be made starting from the Pfaffian form given by Stephenson.<sup>22</sup> The details are complicated and are given elsewhere.<sup>23</sup> While the magnetization is given by Potts,<sup>24</sup> the remaining odd spin correlations can be found using the methods of Barry, Múnera, and Tanaka.<sup>25</sup> However, we found their results to contain errors and have not pursued this further. Consequently, Fig. 3 for the triangular net is not complete for  $T < T_c$ .

The results for the square net and the triangular net are shown in Figs. 2 and 3, respectively. They are very similar to those for the honeycomb lattice given in Fig. 1, showing a rather universal behavior for  $P(h)$  for all two-dimensional lattices.

Results have been published previously<sup>13</sup> by two of us for the *antiferromagnetic* triangular net, which show that there is very little change in  $P(h)$  between  $T = \infty$  and  $T = 0$ , apart from some flattening. This is related to the fact that this model does not have a phase transition and has a finite entropy at zero temperature. The antiferromagnetic honeycomb and square lattices map on to

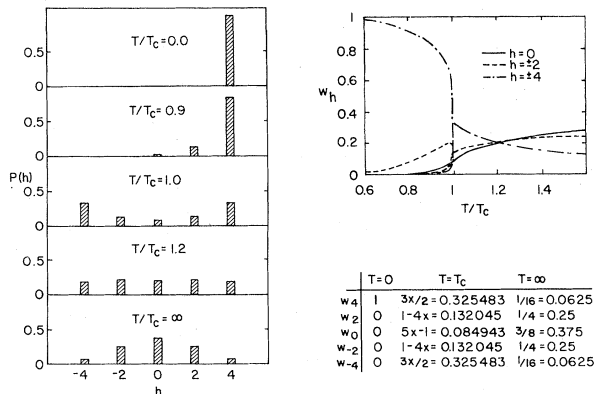


FIG. 2. Same as Fig. 1 except for the square net. The parameter  $x = 1/\pi - 1/\pi^2$ .

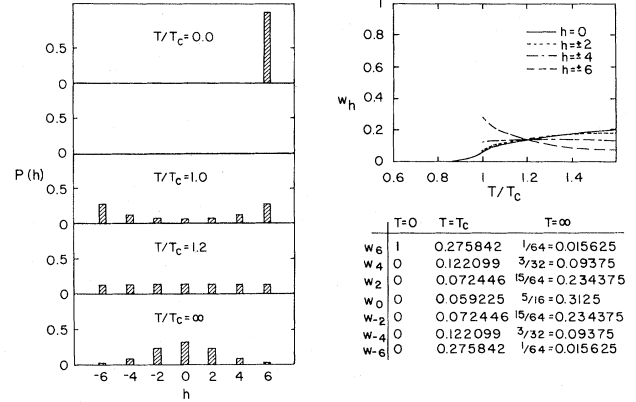


FIG. 3. Same as Fig. 1 except for the triangular net. The results for  $T < T_c$  are not complete as we have not been able to compute the required odd spin-correlation functions.

their ferromagnetic counterparts as they are both bi-chromatic. With the use of the definition (11) for  $P_i(h)$ , these functions will be identical above  $T_c$  for both sublattices and equal to the ferromagnetic counterparts. However, below  $T_c$ , the asymmetry will develop on opposite sides of  $h = 0$  for the two sublattices, and thus  $P(h)$  for the entire system is just the symmetric part  $P_s(h)$  of  $P(h)$  defined in (22) for the ferromagnetic counterpart. This leads to zero net magnetization via (18), as expected. In order to obtain the staggered magnetization it would be necessary to know  $P_i(h)$  at the up and down sites *separately*, and not just the average.

The one-dimensional Ising model can also be regarded as having a dip in  $P(h)$  at  $T_c$  if  $T_c$  is identified with zero temperature. At zero temperature  $w_0 = 0$  and  $w_2 = w_{-2} = \frac{1}{2}$ , from (46).

If the distribution  $P(h)$  is to be characterized by a single parameter, the most useful is

$$v = [\overline{h^2} - (\overline{h})^2] / z, \quad (53)$$

where the overbar denotes an average over  $P(h)$ . From the definition of the  $c_r$ , this can be rewritten as

$$v = 1 + (2c_2 - c_1^2) / z, \quad (54)$$

and is shown in Fig. 4 for *ferromagnetic* interactions in the honeycomb, square net, and triangular net. At high temperatures,  $v \rightarrow 1$  for all lattices as the correlation functions  $c_1, c_2$  become zero. Not surprisingly, this quantity, which measures the local fluctuations, has a maximum at  $T_c$  and then decreases rapidly to zero as the temperature goes to zero. The increase in  $v$  as the temperature is lowered from infinity towards  $T_c$  is due to the flattening and then the dip in  $P(h)$ . The rapid drop in  $v$  below  $T_c$  is due to the asymmetry caused by  $c_1$  and, hence, the magnetization.

For *antiferromagnetic* interactions, the quantity  $v$  keeps going up as the temperature is lowered. For two sublattice antiferromagnetics, such as the honeycomb and square net, the local magnetic field distribution function is given by the symmetric part [see Eq. (22)] of the distribution for the corresponding ferromagnet (i.e., all exchange interactions changing sign). Thus  $v$  increases

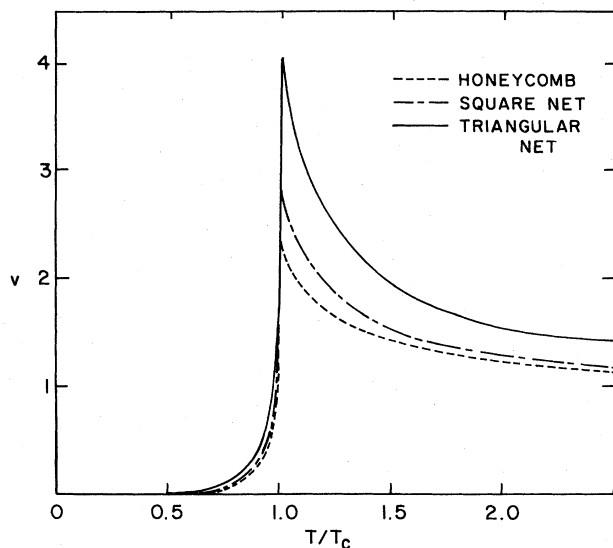


FIG. 4. Fluctuation  $v$  in the local field as a function of reduced temperature  $T/T_c$  for ferromagnetic interactions in the honeycomb, square net, and triangular net.

monotonically from 1 at high temperatures to  $z$  at zero temperature. For the triangular net, antiferromagnet  $v$  increases from 1 at high temperatures to 1.097 809 at zero temperature.<sup>13</sup>

Finally, in this section, we consider the neutron-scattering law, Eqs. (26) and (30). The scattering only takes place at discrete energies. In Table II we have included the thermal factor in (30) to give  $S(\vec{k}, \omega)$  for the square net. At very low temperatures, only the "spin-wave peak" is seen at  $\omega=8$ .<sup>10</sup> This corresponds to flipping a spin where all its nearest neighbors are parallel. As the temperature is raised, other peaks have nonzero weights.<sup>26</sup> Even at  $T_c$ , we note that 63% of the weight is still in the spin-wave peak. However, there is some weight at  $\omega=4$ , which corresponds to a spin flip where three nearest neighbors are up and one is down. The peak at  $\omega=0$  will combine with the elastic peak and the peaks at negative frequencies are related to those at positive frequencies by detailed balance factors. At infinite temperature the thermal factor is  $\frac{1}{2}$  for all frequencies and the neutron-scattering law becomes symmetric. There is a useful sum rule for spin  $\frac{1}{2}$  [in addition to (31) and (32)] which shows that the total integrated intensity is indepen-

TABLE II. Inelastic-neutron-scattering intensity per site,  $S(\vec{k}, \omega)/N$ , at various special temperatures for the square net. The frequency is in units of  $J$  and the numbers in the table give the weights  $2w_s/[1 + \exp(-\beta\omega)]$  of the five  $\delta$  functions.

$\omega$	$T = 0$	$T_c$	$\infty$
8	1	0.6324	0.0625
4	0	0.2254	0.25
0	0	0.0849	0.375
-4	0	0.0387	0.25
-8	0	0.0186	0.0625

dent of temperature, as is clear from Table II,

$$\int S(\vec{k}, \omega) d\omega = 1. \quad (55)$$

This is easily proved from the definition (26).

#### IV. CONCLUSIONS

We have shown that the statistical mechanics of Ising models can be described through the local magnetic field probability distribution function  $P(h)$ . This function determines both the neutron-scattering law  $S(\vec{k}, \omega)$  and the thermodynamic quantities of interest for a large class of Ising systems. We have calculated  $P(h)$  for the ferromagnetic honeycomb, square net, and triangular net, and have shown that in all cases a pronounced dip develops at  $T_c$ .

In a subsequent paper, we plan to extend these results to random spin systems and spin-glass models and also to look at systems described by classical rather than Ising spins.

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#### APPENDIX

The results of Sec. II can be generalized to case of arbitrary spins  $S_i$  whose magnitude can vary from site to site. We will adopt a numbering scheme for equations such that equations in the text and the Appendix correspond. The Hamiltonian is

$$H = -\frac{1}{2} \sum_{i,j} J_{ij} S_i^z S_j^z - \sum_i H_i S_i^z. \quad (1')$$

Note that this  $J_{ij}$  differs from the  $J_{ij}$  in the main text by a factor of 4 in the limit when the spin becomes  $\frac{1}{2}$ . This is because we found it more convenient to use Pauli operators in the main text. In a similar way there is a factor-of-2 difference in the definition of  $H_i$ . Rather than redefine these quantities, we prefer to start from (1'). The reader will easily discover places where factors of 2 appear between equations in the main text and the corresponding equations in the Appendix. In order to proceed it is necessary to insist that the  $J_{ii}=0$ . The most obvious decomposition of (1') is

$$H = -\sum_i \mathcal{H}_i S_i^z, \quad (2')$$

where

$$\mathcal{H}_i = \frac{1}{2} \sum_j J_{ij} S_j^z + H_i, \quad (3')$$

but the most useful for our purposes is

$$H = -\sum_i h_i S_i^z + H', \quad (4')$$

where

$$h_i = \sum_j J_{ij} S_j^z + H_i \quad (5')$$

Note that it is important that  $H$  be *linear* in all the  $S_i^z$  so that terms such as  $(S_i^z)^2$ ,  $(S_i^z)^2 S_j^z$ ,  $(S_i^z S_j^z)^2$ , etc., are *not* allowed in the Hamiltonian if the present formalism is to be used.

The thermal average  $\langle OS_i^z \rangle$ , where  $O$  is any operator not involving site  $i$  is given by

$$\begin{aligned} \langle OS_i^z \rangle &= \langle \text{Tr}_i [OS_i^z \exp(\beta h_i S_i^z)] / \text{Tr}_i [\exp(\beta h_i S_i^z)] \rangle \\ &= \langle O \mathcal{B}_{S_i}(\beta h_i) \rangle, \end{aligned} \quad (6')$$

where the modified Brillouin function<sup>27</sup> is defined by

$$\mathcal{B}_S(x) = (S + \frac{1}{2}) \coth[(S + \frac{1}{2})x] - \frac{1}{2} \coth(\frac{1}{2}x),$$

and hence

$$\mathcal{B}_{1/2}(x) = \frac{1}{2} \tanh(\frac{1}{2}x).$$

Setting  $O$  equal to the unit operator in (6'), we find that

$$\langle S_i^z \rangle = \langle \mathcal{B}_{S_i}(\beta h_i) \rangle, \quad (7')$$

and setting  $O$  equal to  $h_i$  leads to

$$\begin{aligned} \langle h_i S_i^z \rangle &= \left\langle \sum_j J_{ij} S_i^z S_j^z + H_i S_i^z \right\rangle \\ &= \langle h_i \mathcal{B}_{S_i}(\beta h_i) \rangle. \end{aligned} \quad (8')$$

There is the same problem with the factor of  $\frac{1}{2}$  in obtaining the energy as before, and we have

$$\begin{aligned} E_i &= -\langle h_i \mathcal{B}_{S_i}(\beta h_i) \rangle \\ &= -\frac{1}{2} \langle (h_i + H_i) \mathcal{B}_{S_i}(\beta h_i) \rangle. \end{aligned} \quad (9')$$

The magnetization  $M$  and the energy  $E$  are given by (10), as before.

It is convenient to define a  $P(h)$  for the entire system as

$$P(h) = \left[ \sum_i \mathcal{B}_{S_i}(\beta h) P_i(h) \right] / \left[ \sum_i \mathcal{B}_{S_i}(\beta h) \right], \quad (11')$$

$$\begin{aligned} S(\vec{k}, \omega) &= \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt e^{-i\omega t} \sum_i \langle [S_i^+ S_i^-(t) + S_i^- S_i^+(t)] \rangle \\ &= 2 \sum_i [P_i(\omega) + P_i(-\omega)] \mathcal{B}_{S_i}(\beta\omega) / [1 - \exp(-\beta\omega)] \\ &= 2N [P(\omega) + P(-\omega)] \mathcal{B}(\beta\omega) / [1 - \exp(-\beta\omega)], \end{aligned} \quad (29')$$

or

$$S(\vec{k}, \omega) = 4NP_s(\omega) \mathcal{B}(\beta\omega) / [1 - \exp(-\beta\omega)]. \quad (30')$$

These lead to the sum rules

$$\frac{1}{2N} \int S(\vec{k}, \omega) \frac{1 - \exp(-\beta\omega)}{2\mathcal{B}(\beta\omega)} d\omega = 1, \quad (31')$$

and if all the  $H_i = 0$ ,

$$\frac{1}{8} \int S(\vec{k}, \omega) [1 - \exp(-\beta\omega)] \omega d\omega = -E. \quad (32')$$

These sum rules are very general and can be proved without introducing  $P(h)$ . The second one is particularly easy to

and, further, an average Brillouin function  $\mathcal{B}(\beta h)$  by

$$\mathcal{B}(\beta h) = \frac{1}{N} \sum_i \mathcal{B}_{S_i}(\beta h).$$

This takes account of a varying spin magnitude. It is only necessary to know the *number* of sites with each spin magnitude in order to know  $\mathcal{B}(\beta h)$ .

From (7) and (9) we have

$$\langle S_i^z \rangle = \int \mathcal{B}_{S_i}(\beta h) P_i(h) dh \quad (15')$$

and

$$E_i = -\frac{1}{2} \int h \mathcal{B}_{S_i}(\beta h) P_i(h) dh - \frac{1}{2} H_i \langle S_i^z \rangle. \quad (16')$$

The magnetization  $M$  is given by

$$M = N \int \mathcal{B}(\beta h) P(h) dh, \quad (18')$$

and, as before, it is *not* necessary to know the  $J_{ij}$  or the  $H_i$  in order to find  $M$  from  $P(h)$ .

Again, as before, the energy cannot be obtained directly from  $P(h)$ . However, if all the  $H_i$  are known to be 0, then from (10) and (16'),

$$E = -\frac{N}{2} \int h \mathcal{B}(\beta h) P(h) dh, \quad (21')$$

the free energy  $F$  is given by

$$\beta F = -\sum_i \ln(2S_i + 1) + \int_0^\beta E(\beta') d\beta', \quad (24')$$

and Eq. (21) generalizes in the obvious way with  $\tanh(\beta h) \rightarrow \mathcal{B}(\beta h)$ .

The inelastic-neutron-scattering cross section is given by

$$\begin{aligned} S(\vec{k}, \omega) &= \frac{2}{\pi} \int_{-\infty}^{+\infty} dt e^{-i\omega t} \sum_{i,j} \exp[i\vec{k} \cdot (\vec{R}_i - \vec{R}_j)] \\ &\quad \times \langle S_i^x S_j^x(t) \rangle, \end{aligned} \quad (26')$$

where  $x$  is any direction perpendicular to  $z$ . Using arguments similar to those in Sec. II, we find that



establish as the magnitude of the spin does not enter explicitly.

Using the identity<sup>28</sup>

$$\langle A(0)B(t) \rangle = \langle B(t - i\beta)A(0) \rangle$$

for any operators  $A, B$ , we see that

$$S(\vec{k}, \omega)[1 - \exp(-\beta\omega)] = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt e^{-i\omega t} \sum_{i,j} \exp[i\vec{k} \cdot (\vec{R}_i - \vec{R}_j)] \langle [S_i^+ S_j^-(t) + S_i^- S_j^+(t) - S_j^-(t) S_i^+ - S_j^+(t) S_i^-] \rangle.$$

Only the diagonal terms contribute for Ising models so that

$$S(\vec{k}, \omega)[1 - \exp(-\beta\omega)] = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt e^{-i\omega t} \sum_i \langle [S_i^+, S_i^-(t)] + [S_i^-, S_i^+(t)] \rangle.$$

Therefore,

$$\begin{aligned} \int S(\vec{k}, \omega)[1 - \exp(-\beta\omega)] \omega d\omega &= -i \sum_i \left\langle \left[ S_i^+, \frac{\partial S_i^-}{\partial t} \right] + \left[ S_i^-, \frac{\partial S_i^+}{\partial t} \right] \right\rangle \\ &= \sum_i \langle [S_i^+, h_i S_i^-] - [S_i^-, h_i S_i^+] \rangle \\ &= 4 \sum_i \langle h_i S_i^z \rangle \\ &= -8E. \end{aligned}$$

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$$\begin{aligned} \int P(h)dh &= 1, \quad \int h \tanh(\beta h) P(h)dh = 3\epsilon, \\ \int hP(h)dh &= 3m, \quad \int \tanh(\beta h) P(h)dh = m. \end{aligned}$$

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$$B_x(x) = \frac{2S+1}{2S} \coth \left[ \frac{2S+1}{2S} x \right] - \frac{1}{2S} \coth \left[ \frac{x}{2S} \right],$$

by including a prefactor of  $S$ , and a factor  $S$  in both arguments so that  $\mathcal{B}_s(x) = SB_s(Sx)$ . This saves having to write many factors  $S_i$  in subsequent formulas.

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