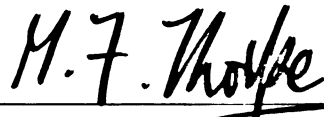This is to certify that the

thesis entitled

PROBLEMS IN ORDERED AND

DISORDERED ISING SYSTEMS

presented by

JOHN MARSHALL THOMSEN

has been accepted towards fulfillment
of the requirements for

___Ph.D.___ degree in __Physics__

Major professor
M. F. Thorpe

Date_18 May 1984_

PROBLEMS IN ORDERED AND DISORDERED ISING SYSTEMS

By

John Marshall Thomsen

A DISSERTATION

Submitted to
Michigan State University
in partial fulfillment of the requirements
for the degree of

DOCTOR OF PHILOSOPHY

Department of Physics and Astronomy

1984

ABSTRACT

PROBLEMS IN ORDERED AND DISORDERED ISING SYSTEMS

By

John Marshall Thomsen

A wide range of Ising systems are studied. In one dimension,
attention is focussed on calculating the transverse susceptibility.
By combining transfer matrix techniques with linear response theory,
it is shown that $\chi_\perp$ can be calculated for pure and dilute spin S
Ising chains. The low temperature behavior in the presence of
a parallel field is discussed. The temperature dependent probability
distribution of internal fields, P(h), is defined, and it is shown
to yield several exact thermodynamic results. This function is
studied on a variety of Ising ferromagnets, with exact results
available in one and two dimensions as well as on the Bethe lattice.
Three and four dimensional lattices are studied with Monte Carlo
simulations. It is shown that P(h) is very sensitive to short
range order. This order is in turn sensitive more to the lattice
dimension and less to the coordination number. P(h) is also studied
for the Sherrington-Kirkpatrick infinite range spin glass model. An
analytic result is available in the paramagnetic phase while Monte

Carlo simulations are employed in the spin glass phase. The development of the dip at $h = 0$ is investigated in some detail. Finally, some speculations are made on the possibility of extending the $P(h)$ formalism to non-Ising systems.

ACKNOWLEDGMENTS

Finally, I should like to thank Amelia Hefferlin whose encouragement and assistance have helped bring this project to completion. No less important have been her occasional reminders that Physics is not all there is to life (which is easy for an Ecologist to say).

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1. Introduction

A fundamental and much studied problem in condensed matter physics is the explanation on a microscopic level of the magnetic properties of various materials. As might be expected, there is frequently a competition between building a model Hamiltonian that describes a system with accuracy, and building a model Hamiltonian which is tractable. Fortunately, there exist a variety of systems which are described reasonably well by a simple spin Hamiltonian.

For a system of well localized effective moments, one general form a spin-spin interaction may take is

$$H_{12} = -\vec{S}_1 \cdot \overleftrightarrow{J} \cdot \vec{S}_2 \qquad (1)$$

where $\overleftrightarrow{J}$ is a 3×3 interaction matrix and $\vec{S}_1$ and $\vec{S}_2$ are three component operators describing spins located at sites 1 and 2. The matrix elements of $\overleftrightarrow{J}$ are related to the overlap of the electronic wave functions associated with the two spins. (For a justification of this Hamiltonian, see White 1983.) In certain cases, the J_{zz} term may dominate the matrix, reducing the interaction to the Ising (1925) form

$$H_{12} = -J S_1^z S_2^z \qquad . \qquad (2)$$

Systems well described by this form over at least a restricted temperature range include $CoCl_2 \cdot 2NC_5H_5$, a one dimensional ferromagnet (Takeda et. al. 1971), $COCs_3Br_5$, a two dimensional antiferromagnet (Mess et. al. 1967), and $DyPO_4$, a three dimensional

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antiferromagnet (Wright et. al. 1971).

The advantage of working with Hamiltonians built with Ising interactions in the absence of a field is that every piece of the Hamiltonian commutes with every other piece. In the presence of external fields, the most general Ising Hamiltonian considered in this work includes one non-commuting piece:

$$H = -\tfrac{1}{2} \sum_{i,j} J_{ij} S_i^z S_j^z - \mu_\| h^z \sum_i S_i^z - \mu_\perp h^x \sum_i S_i^x \quad , \qquad (3)$$

where the $\vec{S}_i$ are taken to be quantum spin operators. The matrix of J_{ij}'s is assumed to be symmetric with vanishing diagonal elements. The fact that the S_i^x terms do not commute with the rest of the Hamiltonian will in general cause problems; however h^x will be taken either to be zero, in which case the problems are eliminated, or infinitessimal, in which case one can work around the commutation problems.

The Ising Hamiltonian has been studied in a wide variety of forms, and some of the more relevant studies are reviewed here. When first introduced, the partition function of a pure spin $\tfrac{1}{2}$ chain with uniform nearest neighbor interactions was calculated (Ising 1925). Analytic results for the specific heat and parallel susceptibility are now available for spins up to 3/2 (Suzuki et. al. 1967). The site diluted version has been studied by, among others, Matsubara et. al. (1973) for $S=\tfrac{1}{2}$, and Matsubara and Yoshimura (1973) for S=1 and S=3/2. In both cases, the parallel susceptibility and the specific heat were calculated.

The zero field transverse susceptibility of a pure spin $\tfrac{1}{2}$ infinite chain was calculated by Fisher (1963), while Grest and

Rajagopal (1974) repeated the calculation in a finite <u>parallel</u> field. Chapter 2 focusses on extending the transverse susceptibility calculations to include higher spins and site dilution, both with and without external parallel fields. Unusual effects arising from dilution and from the application of the parallel field will be discussed.

Traditional approaches to studying Ising models focus on determining the free energy of the system and obtaining other thermodynamic quantities by differentiation. The subsequent chapters of this work deal with an alternative approach involving the distribution of local fields. This function, $P(h)$, has been much studied in relation to spin glasses at zero temperature (see for instance Palmer and Pond 1979 or Kirkpatrick and Sherrington 1978). However, it will be shown in Chapter 3 that at all temperatures, the thermodynamics of an Ising system may be reformulated exactly in terms of the temperature dependent $P(h)$. From $P(h)$, one may obtain not only the magnetization and energy (and hence the free energy), but also the inelastic neutron scattering cross section. Furthermore, since $P(h)$ describes what is happening <u>locally</u>, it can give some intuitive feel for what is happening to the system. It was for these reasons that a study of $P(h)$ on various Ising systems was undertaken.

While the original motivation to study $P(h)$ lay in spin glass research, it is useful to first study this function on well understood uniform Ising systems in order to obtain a basic understanding of how it behaves. In Chapter 4, $P(h)$ is calculated for Bethe lattices with nearest neighbor ferromagnetic interactions. The

Bethe lattice allows one to make a fairly smooth transition from a network of small coordination to the mean field limit, and hence may provide some insight into the effect of coordination number (or perhaps dimensionality) on this function.

The Bethe lattice provides well behaved analytic results, but it is not a true lattice and the large fraction of spins residing on its surface makes it unphysical. For this reason, it is useful to look at the two dimensional Ising model. This model takes on a special significance in statistical mechanics as it is one of the few exactly solvable models exhibiting a phase transition at a finite temperature. The partition function of a square net with uniform nearest neighbor interactions was first derived by Onsager (1944). He extended the transfer matrix technique introduced by Kramers and Wannier (1941). Since then, a variety of solutions have been developed. The Pfaffian approach taken by Montroll et. al. (1963) seems to lend itself most readily to calculating correlation functions, although it may not be the quickest way to determine the free energy. This approach has since been generalized to a wide variety of two dimensional lattices (see, e.g., Hurst 1963 and Stephenson 1964). These results are drawn on in Chapter 5 to perform exact calculations of $P(h)$ for several two dimensional Ising systems.

The general features of $P(h)$ on these two dimensional lattices are relatively insensitive to coordination number. However, there is a strong dependence of $P(h)$ on lattice dimension. This dependence is explored in Chapter 6 using Monte Carlo simulations.

Results in three and four dimensions are compared to the mean field limit. The models chosen, nearest neighbor ferromagnetic interactions on diamond, simple cubic, body centered cubic, face centered cubic, and hypercubic lattices, have all been studied in detail with high temperature series. Since these series provide sufficiently accurate estimates of T_c for the purposes of this study (see, e.g., Domb 1974), it is possible to concentrate on P(h) without getting bogged down in details such as locating T_c.

In Chapter 7, attention is turned to a spin glass model, the Sherrington-Kirkpatrick (infinite range) Ising model (Sherrington and Kirkpatrick 1975). This model was first introduced as an approximation to a spin glass system dominated by the long range RKKY interaction. It was hoped that the infinite range interaction would lead to an exact solution, although the solution in the spin glass phase has turned out to be more complex than originally hoped and is still under scrutiny (Parisi 1983). Nevertheless, this is one of the more tractable spin glass Hamiltonians and one can in fact obtain an analytic result for P(h) in its paramagnetic phase. There are some distinctive features associated with the small h behavior of P(h) and these will be elaborated on in Chapters 7 and 8.

Finally, in Chapter 9 further studies of Ising systems are suggested as is the possibility of extending the P(h) formalism to non-Ising systems.

2. Transverse Susceptibility in One Dimensional Chains

The one dimensional Ising model is attractive in that many exact results for the system may be obtained through straightforward calculations. While this model does not exhibit any phase transitions for $T>0$, there are systems, such as $CoCl_2 \cdot 2NC_5H_5$, which behave at least approximately like one dimensional Ising chains (Takeda et. al. 1971). In this chapter, a generalized method will be developed for calculating the transverse susceptibility of Ising chains by using modified transfer matrices.

First, some background on the transfer matrix technique, developed by Kramers and Wannier (1941), must be introduced. One starts with a Hamiltonian of the form

$$H_N = -J \sum_{i=1}^{N} S_i^z S_{i+1}^z - \tfrac{1}{2}\mu h^z \sum_{i=1}^{N} (S_i^z + S_{i+1}^z) \quad , \tag{1}$$

describing a one dimensional spin S Ising chain in the presence of an external parallel field, $\vec{H} = h^z \hat{z}$. Defining $S_{N+1}^z = S_1^z$ ensures periodic boundary conditions.

The partition function Q_N is given by

$$Q_N = Tr[\exp(-\beta H_N)] \tag{2}$$

$$= \sum_{S_1^z} \sum_{S_2^z} \ldots \sum_{S_N^z} \exp\{\beta[J \sum_{i=1}^{N} S_i^z S_{i+1}^z + \tfrac{1}{2}\mu h^z \sum_{i=1}^{N} (S_i^z + S_{i+1}^z)]\} \quad . \tag{3}$$

The notation $\sum_{S_i^z}$ implies a sum over all $(2S+1)$ possible values of S_i^z and β is as usual $1/k_B T$. The $(2S+1) \times (2S+1)$ transfer matrix,

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T, is defined by its entries

$$T_{S_i^z S_{i+1}^z} = \exp\{\beta[JS_i^z S_{i+1}^z + \tfrac{1}{2}\mu h^z(S_i^z + S_{i+1}^z)]\} \quad . \tag{4}$$

In terms of this matrix,

$$Q_N = \sum_{S_1^z} \sum_{S_2^z} \cdots \sum_{S_N^z} T_{S_1^z S_2^z} T_{S_2^z S_3^z} \cdots T_{S_{N-1}^z S_N^z} T_{S_N^z S_1^z} \quad . \tag{5}$$

In going from equation (4) to (5), explicit use was made of the fact that all the operators in the Hamiltonian commute with each other.

The operation in equation (5) is now recognized as matrix multiplication, so that

$$Q_N = \sum_{S_1^z} (T^N)_{S_1^z S_1^z} \tag{6}$$

$$= \text{Tr}[T^N] \tag{7}$$

$$= \sum_{j=1}^{2S+1} \lambda_j^N \quad , \tag{8}$$

where λ_j is the jth eigenvalue of T. In the limit of infinite N, the maximum eigenvalue, λ_M, dominates:

$$Q_N = (\lambda_M)^N \qquad (N \to \infty) \quad . \tag{9}$$

Thermodynamic quantities may be obtained by the usual differentiation of $\ln Q_N$.

In the absence of an external field, for spin $\tfrac{1}{2}$,

$$T = \begin{pmatrix} \exp(\beta J/4) & \exp(-\beta J/4) \\ \exp(-\beta J/4) & \exp(\beta J/4) \end{pmatrix} \tag{10}$$

with

$$\lambda_1 = 2 \cosh(\beta J/4)$$

$$\lambda_2 = 2 \sinh(\beta J/4) \tag{11}$$

so that for large N one recovers the result (Kramers and Wannier 1941),

$$\ln Q_N = N\ln[2 \cosh(\beta J/4)] \quad . \tag{12}$$

For spin 1,

$$T = \begin{pmatrix} \exp(\beta J) & 1 & \exp(-\beta J) \\ 1 & 1 & 1 \\ \exp(-\beta J) & 1 & \exp(\beta J) \end{pmatrix} \tag{13}$$

giving

$$\lambda_1 = \cosh \beta J + \tfrac{1}{2} + \tfrac{1}{2}q$$

$$\lambda_2 = \cosh \beta J + \tfrac{1}{2} - \tfrac{1}{2}q \tag{14}$$

$$\lambda_3 = 2 \sinh \beta J$$

where

$$q = [(2 \cosh \beta J - 1)^2 + 8]^{\tfrac{1}{2}} \quad . \tag{15}$$

For large N,

$$\ln Q_N = N\ln[\cosh \beta J + \tfrac{1}{2} + \tfrac{1}{2}q] \quad . \tag{16}$$

With this background, it is now possible to proceed with the calculation of the transverse susceptibility of an infinite, pure Ising chain.

LETTER TO THE EDITOR

Transverse susceptibility in spin S Ising chains†

M F Thorpe and M Thomsen‡

Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48824, USA

Abstract. It is shown that the transverse susceptibility of a one-dimensional spin S Ising system can be calculated by combining linear response theory with the transfer matrix technique. Closed form expressions for infinite chains are obtained for $S = \frac{1}{2}$ and $S = 1$, and numerical results are displayed for $S = \frac{1}{2}$ to $S = \frac{5}{2}$.

The perpendicular susceptibility of a spin $\frac{1}{2}$ Ising chain has been calculated by several methods (e.g. Fisher 1963, Katsura 1962, and Grest and Rajagopal 1974). However, it would appear that these methods have not yet been generalised to higher spin. The free energy and *parallel* susceptibility have been found for higher spins using transfer matrix techniques (Suzuki *et al* 1967). In this paper the spin dependence of the *perpendicular* susceptibility will be studied. We use standard linear response theory (see for example Grest and Rajagopal 1974) and apply it with transfer matrices to obtain exact closed form expressions for the zero field *perpendicular* susceptibility for spin $\frac{1}{2}$ and spin 1 as well as numerical results for spin $\frac{3}{2}$, 2 and $\frac{5}{2}$.

Our Hamiltonian has the general form

$$H = H_0 + H_1 \tag{1}$$

and we wish to find the expectation value of an operator A to first order in H_1, where H_0, H_1 and A do not necessarily commute. It can be shown that if

$$\mathrm{Tr}[\exp(-\beta H_0)A] = 0 \tag{2}$$

then

$$\langle A \rangle = \frac{-\mathrm{Tr}\left[\int_0^\beta \exp[-(\beta - \tau)H_0]H_1 \exp(-\tau H_0)\, d\tau\, A\right]}{\mathrm{Tr}[\exp(-\beta H_0)]} \tag{3}$$

to first order in H_1.

In the Ising model for a closed cyclic chain we have

$$H_0 = -J \sum_{i=1}^{N} S_i^z S_{i-1}^z \tag{4}$$

$$H_1 = -\mu h \sum_{i=1}^{N} S_i^x \tag{5}$$

C8 — C

where the S_i are quantum spins ot magnitude S and site $N + 1$ is equivaient to site 1.

From equation (3) we find

$$\langle S_j^x \rangle = \text{Tr}\left[\int_0^\beta \exp[-(\beta - \tau) H_0]\mu h \sum_{i=1}^N S_i^x \exp(-\tau H_0)\, \mathrm{d}\tau\, S_j^x \right] \Big/ \text{Tr}[\exp(-\beta H_0)]. \quad (6)$$

The tracing operation ensures that only the $i = j$ term in the sum contributes. Furthermore, we note that all but two terms of H_0 (which are $-JS_{j-1}^z S_j^z - JS_j^z S_{j-1}^z$) commute with S_j^x so that equation (6) can be rewritten as

$$\langle S_j^x \rangle = \sum_{S_1^z} \sum_{S_2^z} \cdots \sum_{S_{j-1}^z} \sum_{S_{j-1}^z} \cdots \sum_{S_N^z} T_{S_1^z S_2^z}\, T_{S_2^z S_3^z}$$

$$\cdots T_{S_{j-2}^z S_{j-1}^z}\, T'_{S_{j-1}^z S_{j-1}^z}\, T_{S_{j-1}^z S_{j-2}^z} \cdots T_{S_N^z S_1^z} / \text{Tr}[\exp(-\beta H_0)] \quad (7)$$

where $\sum_{S_j^z}$ stands for the sum over the $2S + 1$ possible values of S_j^z. We have defined the standard transfer matrix (Suzuki *et al* 1967)

$$T_{S_j^z S_{j-1}^z} = \exp(\beta J S_j^z S_{j-1}^z) \quad (8)$$

and have defined a new transfer matrix

$$T'_{S_{j-1}^z S_{j-1}^z} = \mu h \sum_{S_j^x} \int_0^\beta \exp[J(\beta - \tau)(S_{j-1}^z S_j^z + S_j^z S_{j-1}^z)]$$

$$\times S_j^x \exp[J\tau(S_{j-1}^z S_j^z + S_j^z S_{j-1}^z)]\, \mathrm{d}\tau\, S_j^x. \quad (9)$$

Interpreting the sums in equation (7) as a trace and cyclically permuting, we obtain

$$\langle S_j^x \rangle = \text{Tr}[T^{N-2} T^x]/\text{Tr}[T^N]. \quad (10)$$

We now define the maximum eigenvalue of T and the corresponding eigenvector to be λ_m and $|m\rangle$ respectively, so that in the limit of $N \to \infty$,

$$\langle S_j^x \rangle = \langle m| T^x |m\rangle / \lambda_m^2. \quad (11)$$

Thus the zero field perpendicular susceptibility is

$$\chi_\perp = N \frac{\mu}{h} \frac{\langle m| T^x |m\rangle}{\lambda_m^2}. \quad (12)$$

The $(2S - 1)^2$ elements of T^x may be determined analyticaily from equation (9) by examining the $(2S + 1)^3$ states involved. However. since $T'_{S_{j-1}^z S_{j-1}^z}$ is a function oniy ot $|S_{j-1}^z + S_{j+1}^z|$, it can be shown that there are just $2S + 1$ independent elements of T^x and hence only $(2S + 1)^2$ states need be examined. A short computer algorithm was developed to evaluate equation (9) analytically for larger spins. For $S = \frac{1}{2}$, we find

$$T^x = \begin{pmatrix} \dfrac{h}{J} \sinh \dfrac{\beta J}{2} & \dfrac{\beta h}{2} \\[3mm] \dfrac{\beta h}{2} & \dfrac{h}{J} \sinh \dfrac{\beta J}{2} \end{pmatrix} \quad (13)$$

while when $S = 1$

$$T^x = \begin{pmatrix} \dfrac{h \sinh 2\beta J}{J} & \dfrac{2h \sinh \beta J}{J} & 2\beta h \\[2ex] \dfrac{2h \sinh \beta J}{J} & 2\beta h & \dfrac{2h \sinh \beta J}{J} \\[2ex] 2\beta h & \dfrac{2h \sinh \beta J}{J} & \dfrac{h \sinh 2\beta J}{J} \end{pmatrix}. \tag{14}$$

Combining well known transfer matrix results with (12) and (13), Fisher's (1963) result for $S = \frac{1}{2}$ is recovered:

$$\frac{\chi_-}{N\mu^2} = \frac{1}{2}\left[\frac{1}{4}\beta \operatorname{sech}^2 \frac{\beta J}{4} + \frac{\tanh (\beta J/4)}{J} \right] \tag{15}$$

while for $S = 1$ we obtain

$$\frac{\chi_-}{N\mu^2} = \frac{(\cosh \beta J - \frac{1}{2} + \frac{1}{2}q) \sinh 2\beta J - 8\sinh \beta J + 2\beta J q}{Jq(\cosh \beta J + \frac{1}{2} + \frac{1}{2}q)^2} \tag{16}$$

where

$$q = [(2 \cosh \beta J - 1)^2 + 3]^{1/2}. \tag{17}$$

With T and T^x both known analytically, equation (11) may be evaluated numerically for larger spins. The results for $S = \frac{1}{2}$ through $S = \frac{5}{2}$ are displayed in figure 1. By evaluating equation (6) considering the two low lying states, all spins pointing up and all spins pointing up with the exception that $S_j^z = S - 1$, it can be shown that[+]

$$\frac{J\chi_-(T = 0)}{N\mu^2} = \frac{1}{2} \tag{18}$$

independent of S, as is shown in figure 1.
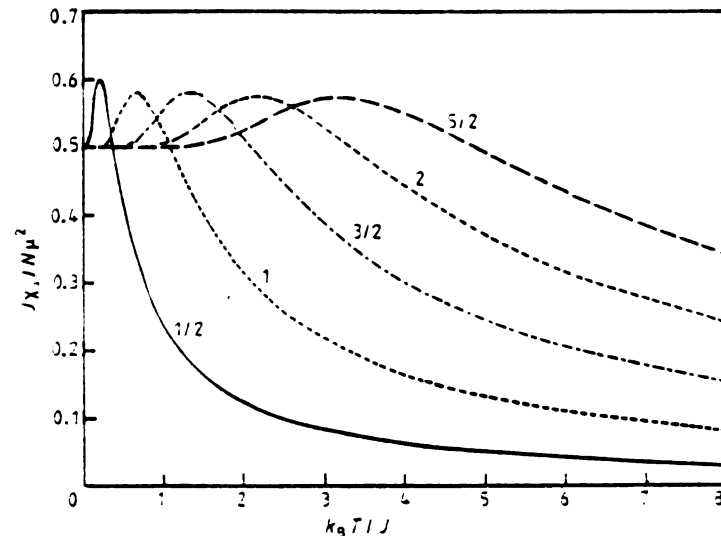
Figure 1. The perpendicular susceptibility $(J\chi_-/N\mu^2)$ plotted against reduced temperature $(k_B T/J)$ for $S = \frac{1}{2}, 1, \frac{3}{2}, 2$ and $\frac{5}{2}$.

[+] This result can be seen most easily by using ordinary second-order perturbation theory at $T = 0$ to give $\Delta E = N(\mu h/2)^2 [(\sqrt{2S})^2/2JS] = \frac{1}{2}\chi_- h^2$.
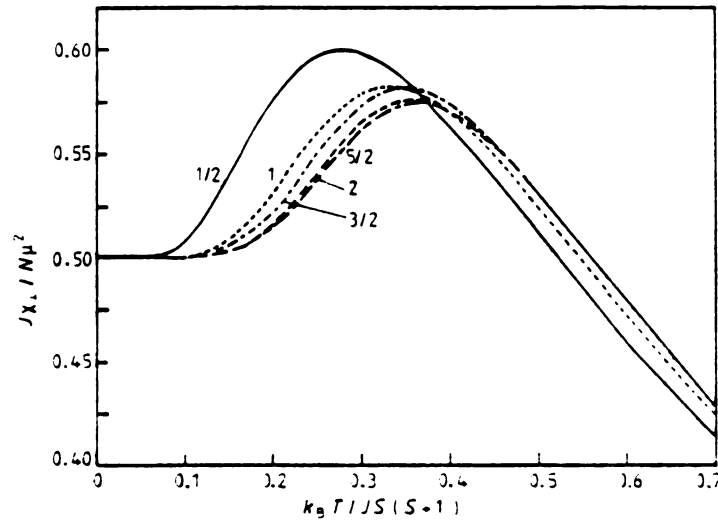
Figure 2. The perpendicular susceptibility $(J\chi_\perp \cdot N\mu^2)$ plotted against the reduced temperature $(k_\text{B}T/[JS(S - 1)])$. This is the same as figure 1 except for the rescaling of the temperature axes. Note that the vertical scale does not begin at zero. Values of S are shown for each curve.

The high-temperature limit

$$\frac{\chi_-}{N\mu^2} = \beta \frac{S(S + 1)}{3}$$ (19)

suggests rescaling the temperature. The plot in figure 2 of χ_- against $k_\text{B}T/S(S - 1)$ indicates that in addition the location of the peak scales roughly with $S(S - 1)$ for $S \geq 1$.

The perpendicular susceptibility for an infinite spin $\frac{1}{2}$ chain in the presence of a non-zero *parallel* field has already been calculated exactly by Grest and Rajagopal (1974). By including parallel field terms in the exponents in equations (8) and (9). similar results may be obtained numerically for larger spins. Finally, we note that some modifications after equation (7) will yield the perpendicular susceptibility for finite open Ising chains and hence for dilute Ising chains (Thomsen and Thorpe 1983).

We are indebted to Dr S D Mahanti for several useful discussions.

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Dilute Ising chains with spin S†

M Thomsen‡ and M F Thorpe

Department of Physics and Astronomy. Michigan State University. East Lansing, MI
48824, USA

Abstract. Randomly diluted one-dimensional Ising chains of spin S are studied by breaking
the systems down into non-interacting finite segments. Exact closed-form expressions are
obtained for the specific heat and *perpendicular* susceptibility of $S = \frac{1}{2}$ chains and numerically
exact results are given for spins up to $\frac{5}{2}$.

1. Introduction

The problem of a dilute one-dimensional spin system with nearest-neighbour interactions is tractable because it can be reduced to a collection of non-interacting finite segments. Matsubara and Katsura (1973) and Thorpe and Miyazima (1981) have exploited this fact to calculate thermodynamic properties for dilute XY quantum chains. Matsubara *et al* (1973) have investigated the specific heat and parallel susceptibility of dilute spin-$\frac{1}{2}$ Ising chains whilst Matsubara and Yoshimura (1973) have investigated the same quantities for $S > \frac{1}{2}$.

In this paper we use this technique to calculate the transverse susceptibility for spin-S dilute chains for the first time. This is an extension of previous work on pure spin-S chains by Thorpe and Thomsen (1983). The main problem to overcome is that the transverse field term in the Hamiltonian does not commute with the exchange part of the Hamiltonian. This can be handled as shown previously (Thorpe and Thomsen 1983) by introducing a new transfer matrix T^x. In addition we have to introduce another transfer matrix T^x in the dilute case to handle the situation when the field is on a spin at the *end* of a segment. Details of this calculation and results for $S = \frac{1}{2}$, $\frac{3}{2}$ and $\frac{5}{2}$ for concentrations $c = 0$, $\frac{1}{4}$, $\frac{1}{2}$, $\frac{3}{4}$ and 1 are given in § 3.

In § 2 we calculate the specific heat using the transfer matrix method. This serves to introduce much of the notation although results have previously been obtained for the specific heat and parallel susceptibility for $S > \frac{1}{2}$ by Matsubara and Yoshimura (1973). In neither of these calculations does one have to worry about non-commuting variables.

For $S = \frac{1}{2}$ it is well known that the specific heat per *bond* is independent of c. This is because each bond acts independently. We show that the specific heat per bond is weakly dependent on concentration for $S \geq 1$.

2. Specific heat

The transfer matrix technique was introduced by Kramers and Wannier (1941) to solve infinite and finite closed chains in the Ising model. One starts with an Ising Hamiltonian with a field in the z direction:

$$H = -J \sum_{i=1}^{r} S_i^z S_{i-1}^z - \mu h \sum_{i=1}^{r} S_i^z \tag{1}$$

where if $S_{r+1} = S$ the chain is closed. The partition function is

$$Q_r^c = \mathrm{Tr}[e^{-\beta H}] = \mathrm{Tr}\left(\prod_{i=1}^{r} \exp\{\beta[JS_i^z S_{i-1}^z - \tfrac{1}{2}\mu h(S_i^z - S_{i-1}^z)]\}\right). \tag{2}$$

If one defines a $(2S + 1) \times (2S + 1)$ transfer matrix T by

$$T_{S_i^z S_{i-1}^z} = \exp\{\beta[JS_i^z S_{i-1}^z + \tfrac{1}{2}\mu h(S_i^z + S_{i-1}^z)]\} \tag{3}$$

where the S_i^z refer to eigenvalues. not operators. then (2) becomes

$$Q_r^c = \sum_{S_1^z} \sum_{S_2^z} \dots \sum_{S_N^z} \langle S_1^z | T | S_2^z \rangle \langle S_2^z | T | S_3^z \rangle \dots \langle S_N^z | T | S_1^z \rangle \tag{4}$$

$$= \mathrm{Tr}[T^r]. \tag{5}$$

Taking λ_j to be the jth eigenvalue of T,

$$Q_r^c = \sum_{j=1}^{2S+1} \lambda_j^r. \tag{6}$$

To modify this for an open chain. we note that we need only set the bond energy of the $S_r^z S_1^z$ pair to zero. In analogy to the derivation of (5) we find for the open chain

$$Q_r^0 = \mathrm{Tr}[T'^{r-1} T'] \tag{7}$$

with

$$T'_{S_i^z S_i^z} = T_{S_i^z S_i^z}(J = 0) = \exp[\tfrac{1}{2}\beta \mu h(S_i^z - S_1^z)]. \tag{8}$$

The partition function (7) is generally evaluated by rotating T and T' into the representation which diagonalises T.

In this section we wish to find the *zero field* specific heat of a finite open segment. Noting that in zero field, $T'_{S_i^z S_i^z} = 1$ for all S_i^z and S_1^z, and defining $\mathbf{M}$ as the matrix that diagonalises T. it is easy to show that

$$Q_r^0 = \sum_{i=1}^{2S+1} \lambda_i^{r-1} \left|\sum_{j=1}^{2S+1} M_{ij}\right|^2. \tag{9}$$

For $S = \frac{1}{2}$, this yields

$$Q_r^0 = 2(2 \cosh \tfrac{1}{4}\beta J)^{r-1}. \tag{10}$$

while for $S = 1$ we find

$$Q_r^0 = \frac{3 - \lambda^-}{\lambda^- - \lambda^-}(\lambda^-)^r - \frac{\lambda^- - 3}{\lambda^- - \lambda^-}(\lambda^-)^r \tag{11}$$

where

$$\lambda^{\pm} = \cosh \beta J + \tfrac{1}{2} \pm [(\cosh \beta J - \tfrac{1}{2})^2 + 2]^{1/2}. \tag{12}$$

Using

$$\frac{1}{k_B} C_r = \frac{\partial}{\partial T}\left(T^2 \frac{\partial}{\partial T} \ln Q_r\right) \tag{13}$$

it follows that in the $S = \tfrac{1}{2}$ case

$$C_r/k_B = (r - 1)(\beta J/4)^2 \operatorname{sech}^2(\beta J/4) \tag{14}$$

(see also Stanley (1971)), while application of (13) to (11) yields an expression too complex to be of much use analytically. For general spin, the matrix calculations involved in (9) are performed by computer at three points close to each other so that the differentiation in (13) can be done numerically.
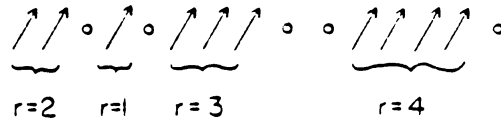
Figure 1. A dilute spin-S chain with segments of length $r = 1, 2, 3$ *and* 4.

In a dilute chain of length N $(N \to \infty)$ and concentration c, the number of segments containing exactly r consecutive spins (as shown in figure 1) is

$$P_r = N(1 - c)^2 c^r. \tag{15}$$

Since

$$C = \sum_r P_r C_r, \tag{16}$$

we find that the specific heat per bond in the spin-$\tfrac{1}{2}$ case is

$$C/N k_B c^2 = (\beta J/4) \operatorname{sech}^2(\beta J/4), \tag{17}$$

which agrees with Matsubara *et al* (1973).

We note that the specific heat per bond is independent of the concentration c because the spin-$\tfrac{1}{2}$ Ising chain can be mapped onto an equivalent system of independent bonds. This is done by defining a new variable $\tau_i = S_i S_{i-1}$. Because of the absence of loops the τ_i can take on values $\tau_i = \pm \tfrac{1}{4}$ and so in the absence of a field h, the Hamiltonian (1) splits up into non-interacting Hamiltonians each associated with a bond with a spin at each end.

For $S > \tfrac{1}{2}$, the specific heat per bond is *not* independent of c, as can be seen in figure 2. However, the specific heat *per bond* depends only weakly on the concentration and this dependence does not become greater as S increases.

A useful check is provided by noting that

$$\int_{\delta}^{\infty} \frac{C}{T} dT = S(\infty) - S(\delta) \tag{18}$$

where $S(\infty)$ is the entropy of the system at infinite temperature and $S(\delta)$ is the entropy
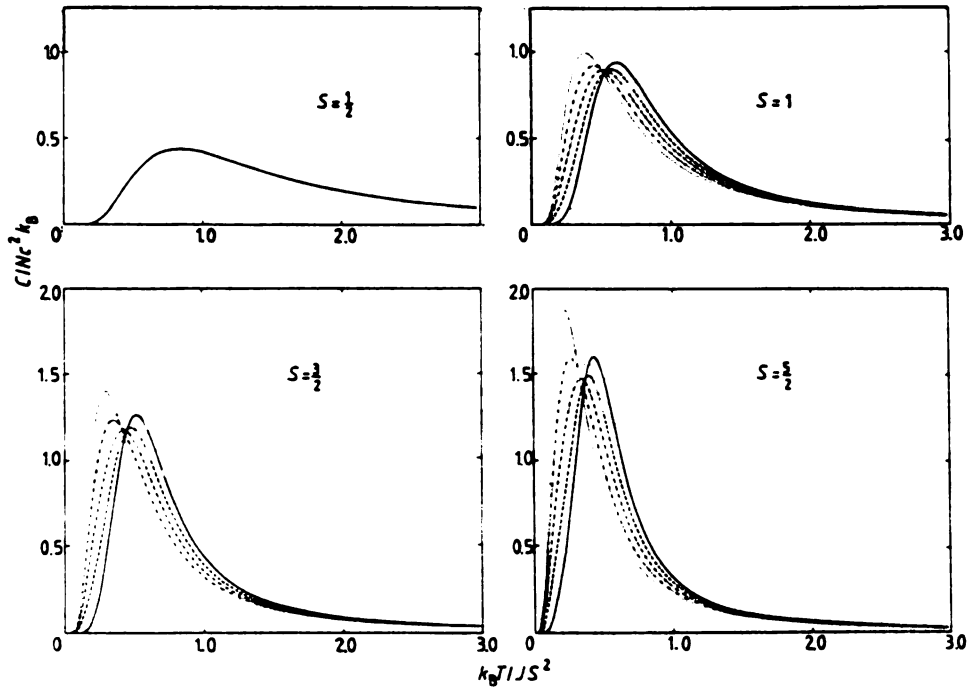
Figure 2. The specific heat per bond (C/Nc^2k_B) as a function of reduced temperature (k_BT/JS^2) for various values of spin S as indicated and concentration $c = 0$ ($\cdots\cdots$), $\frac{1}{4}$ ($\cdots-\cdots$), $\frac{1}{2}$ ($-\cdot-$), $\frac{3}{4}$ ($---$), 1 (———). For $S = \frac{1}{2}$ the specific heat per bond is independent of c as shown. The $c = 0$ limit corresponds to two spins joined by one bond and otherwise isolated.

at a small positive temperature δ. Since the total number of states is

$$(2S + 1)^{\text{number of spins}} = (2S + 1)^{Nc}$$

$$S(\infty) = Nk_Bc \ln(2S + 1). \tag{19}$$

On the other hand, the degeneracy of the ground state (in zero field) is $2^{N_2}(2S + 1)^{N_1}$ where N_1 is the number of isolated spins and N_2 is the number of segments of length greater than one. This gives

$$S(\delta) = Nk_B(1 - c)c^2 \ln 2 + Nk_B(1 - c)^2c \ln(2S + 1) \tag{20}$$

and hence

$$\int_\delta^\infty \frac{C}{T} dT = Nk_Bc^2[(2 - c) \ln(2S + 1) - (1 - c) \ln 2]. \tag{21}$$

The low-temperature behaviour of the specific heat is dominated by the lowest excited states. For $S = \frac{1}{2}$, this corresponds to flipping all the spins simultaneously in any part of that segment, provided that part includes an end spin, as shown in figure 3. For $S \geqslant 1$, the low-lying excitations come only from reducing by one unit the z component of an end spin which is also shown in figure 3†. It can thus be shown that at low

† For spin 1, additional degeneracy arises for the lowest excited states in segments of length 2. However, it is still true that all the lowest-lying excitations are governed by end segment spins for $S = 1$.

temperatures.

$$C/Nk_Bc^2 \approx (\beta JS)^2 \, e^{-\beta JS} \qquad\qquad S = \tfrac{1}{2} \qquad\qquad (22a)$$

$$C/Nk_Bc^2 \approx [\tfrac{3}{2} - \tfrac{1}{2}c](1 - c)(\beta JS)^2 \, e^{-\beta JS} \qquad S = 1 \qquad\qquad (22b)$$

$$C/Nk_Bc^2 \approx 2(1 - c)(\beta JS)^2 \, e^{-\beta JS} \qquad S \geq \tfrac{3}{2}. \qquad (22c)$$
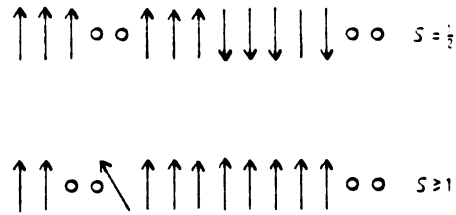
Figure 3. The lowest excitations for $S = \tfrac{1}{2}$ and $S \geq 1$ dilute chains as described in the text.

When $c \to 1$, the right-hand sides of equations $(22b)$ and $(22c)$ vanish since end-of-segment spin excitations are no longer possible, which can be seen in figure 2 where the $c = 1$ specific heats go to zero much more rapidly as $T \to 0$ for $S \geq 1$. This is because there is an extra factor 2 in the exponent of the next terms in $(22b)$ and $(22c)$ reflecting the fact that every spin has two neighbours rather than one.

We conclude this section by noting that when one evaluates the high-temperature expansion of $Q = \text{Tr}[e^{-\beta H}]$ in powers of β, it is found that

$$C/Nk_Bc^2 \approx [\tfrac{1}{3}S(S + 1)\beta J]^2 \qquad\qquad (23)$$

which is independent of c for all S.

3. Perpendicular susceptibility

Calculation of the perpendicular susceptibility is complicated by the fact that parts of the Hamiltonian do not commute with each other. In the absence of any parallel field

$$H = -J \sum_{i=1}^{r-1} S_i^z S_{i-1}^z - \mu h^x \sum_{i=1}^{r} S_i^x = H_0 - H_1 \qquad (24)$$

for an open segment of length r.

Using linear response theory, Grest and Rajagopal (1974) calculated the perpendicular susceptibility for a closed spin-$\tfrac{1}{2}$ chain. With transfer matrices, this was generalised to higher spins (Thorpe and Thomsen 1983). It was shown that the contribution of each spin to the magnetisation is

$$\langle S_i^x \rangle = \sum_{S_1^z} \sum_{S_2^z} \cdots \sum_{S_{i-1}^z} \sum_{S_{i-1}^z} \cdots \sum_{S_r^z} T_{S_1^z S_2^z} T_{S_2^z S_3^z} \cdots$$

$$\times T_{S_{i-2}^z S_{i-1}^z} T^x_{S_{i-1}^z S_{i-1}^z} T_{S_{i-1}^z S_{i-2}^z} \cdots T_{S_r^z S_1^z} / \text{Tr}[e^{-\beta H_0}] \qquad (25)$$

where $T_{S_i^z S_{i+1}^z}$ is as defined in (3) and

$$T^x{}_{S_{i-1}^z S_{i+1}^z} = \mu h^x \sum_{S_i^z} \int_0^\beta \exp[J(\beta - \tau)(S_{i-1}^z S_i^z + S_i^z S_{i+1}^z)]S_i^x$$

$$\times \exp[J\tau(S_{i-1}^z S_i^z + S_i^z S_{i+1}^z)] \, d\tau \, S_i^x. \tag{26}$$

Using $S_i^x = \frac{1}{2}(S_i^+ + S_i^-)$, the matrix T^x can be evaluated analytically for any S. In particular, when $S = \frac{1}{2}$

$$T^x = \begin{pmatrix} (\mu h^x/J) \sinh \frac{1}{4}\beta J & \frac{1}{2}\beta \mu h^x \\ \frac{1}{2}\beta \mu h^x & (\mu h^x/J)\sinh \frac{1}{4}\beta J \end{pmatrix}. \tag{27}$$

We now open the chain by setting $J = 0$ for the $S_i^z S_i^z$ term. If S_i is not at the end of a segment, then (25) becomes

$$\langle S_i^x \rangle = \sum_{S_1^z} \sum_{S_2^z} \cdots \sum_{S_{i-1}^z} \sum_{S_{i+1}^z} \cdots \sum_{S_i^z} T_{S_1^z S_2^z} T_{S_2^z S_3^z} \cdots$$

$$\times T_{S_{i-2}^z S_{i-1}^z} T^x{}_{S_{i-1}^z S_{i+1}^z} T_{S_{i+1}^z S_{i+2}^z} \cdots T_{S_{i-1}^z S_i^z} T'{}_{S_i^z S_i^z} / \text{Tr}[e^{-\beta H_0}] \tag{28}$$

where $T'_{S_i^z S_i^z}$ is defined in equation (8). In the case of an *end* spin,

$$\langle S_1^x \rangle = \langle S_r^x \rangle = \sum_{S_1^z} \sum_{S_2^z} \cdots \sum_{S_{i-1}^z} T_{S_1^z S_2^z} T_{S_2^z S_3^z} \cdots T_{S_{i-2}^z S_{i-1}^z} T^{x'}{}_{S_{i-1}^z S_i^z} / \text{Tr}[e^{-\beta H_0}] \tag{29}$$

with the new transfer matrix $T^{x'}$ defined as

$$T^{x'}{}_{S_{r-1}^z S_i^z} = \sum_{S_i^z} \mu h^x \int_0^\beta \exp[(\beta - \tau)J S_{r-1}^z S_r^z] S_r^x \exp[\tau J \, S_{r-1}^z S_r^z] \, d\tau \, S_r^x. \tag{30}$$

We note that the subscript S_i^z appears for formal reasons only—$T^x{}_{S_{i-1}^z S_i^z}$ is independent of S_i^z. For $S = \frac{1}{2}$, we obtain

$$T^{x'} = \begin{pmatrix} (2\mu h^x/J) \sinh \frac{1}{4}\beta J & (2\mu h^x/J) \sinh \frac{1}{4}\beta J \\ (2\mu h^x/J)\sinh \frac{1}{4}\beta J & (2\mu h^x/J)\sinh \frac{1}{4}\beta J \end{pmatrix}. \tag{31}$$

Using the above equations, we find the zero-field perpendicular susceptibility of a finite open Ising chain to be

$$\chi_{\perp r} = \frac{\mu}{h^x} \left[\left(\sum_{j=2}^{r-1} \text{Tr}[T^{j-2} T^x T^{r-j-1} T'] \right) + 2 \, \text{Tr}[T^{r-2} T^{x'}] \right] \Big/ \text{Tr}[T^{r-1} T']. \tag{32}$$

This expression is valid for $r \geqslant 2$. For $r = 1$, one uses the free-spin Curie susceptibility.

With all four matrices in equation (32) known analytically, it can be shown that for $S = \frac{1}{2}$

$$\chi_{\perp r} = [(r - 2)/2](\beta/4) \, \text{sech}^2 \tfrac{1}{4}\beta J + [(r + 2)/2J] \tanh \tfrac{1}{4}\beta J. \tag{33}$$

Performing a sum similar to equation (16), but singling out the special case of $r = 1$, we find that for a dilute spin-$\frac{1}{2}$ Ising chain

$$J\chi_\perp/Nc\mu^2 = (1 - c)^2 \tfrac{1}{4}\beta J + \tfrac{1}{4}\beta J \, c^2 \, \text{sech}^2 \tfrac{1}{4}\beta J + \tfrac{1}{4}(4c - 3c^2) \tanh \tfrac{1}{4}\beta J. \tag{34}$$

Setting $c = 1$ reproduces Fisher's (1963) result for a spin-$\frac{1}{2}$ pure Ising chain

$$J\chi_\perp/N\mu^2 = \tfrac{1}{4}\beta J \, \text{sech}^2 \tfrac{1}{4}\beta J + \tfrac{1}{2} \tanh \tfrac{1}{4}\beta J. \tag{35}$$

As c approaches 0 only the first term in equation (34) survives so that

$$J\chi_{-}/N\mu^2 c \approx \tfrac{1}{4}\beta J$$

as expected for Nc free spins.

All four matrices in equation (32) are known analytically for larger S, but the final evaluation of that expression must in general be performed numerically. The results are displayed in figure 4 where we have plotted the inverse susceptibility per spin as a
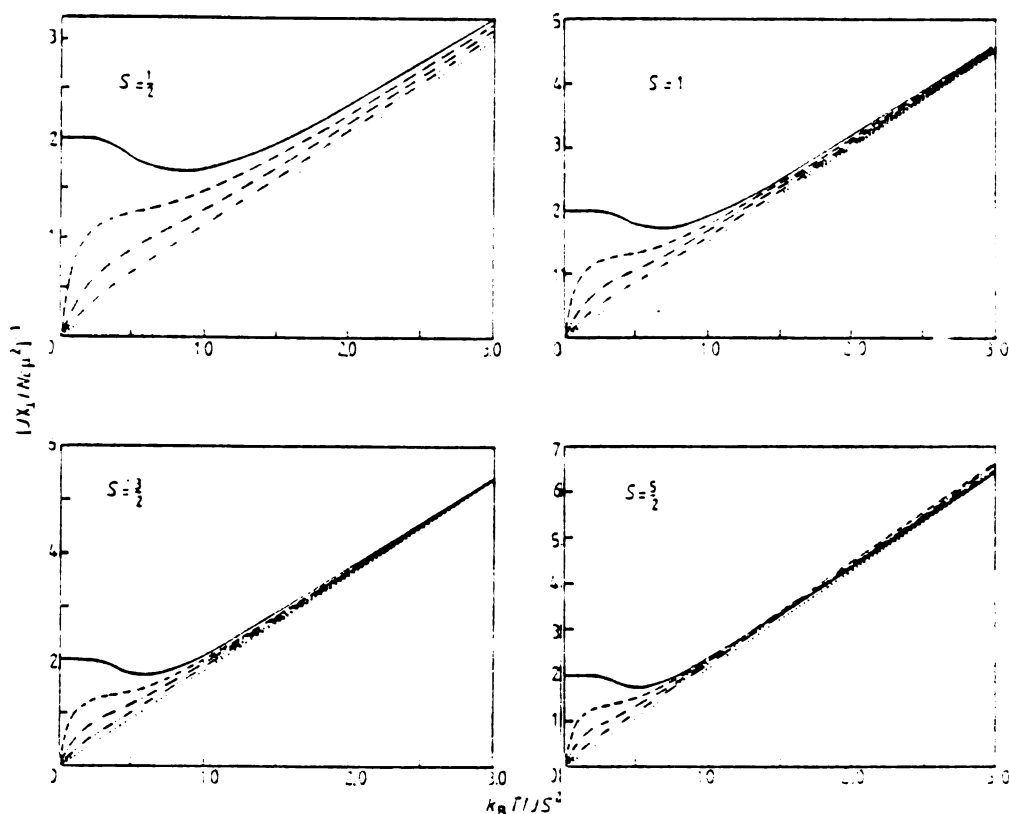
Figure 4. The inverse perpendicular susceptibility per spin $[J\chi_{-}Nc\mu^2]^{-1}$ as a function of reduced temperature $[k_B T/JS^2]$ for various values of spin S as indicated and concentration $c = 0\ (\cdots),\ \tfrac{1}{4}\ (\cdots\! -\!\cdots),\ \tfrac{1}{2}\ (\cdot\! -\! \cdot\! -),\ \tfrac{3}{4}\ (---),\ 1\ (———)$. The $c = 0$ limit corresponds to a single isolated spin.

function of temperature for four different spins: $S = \tfrac{1}{2},\ 1,\ \tfrac{3}{2},\ \tfrac{5}{2}$. We note that χ_{-}^{-1} approaches zero linearly for $c < 1$, reflecting the effect of $Nc(1 - c)^2$ isolated spins $[\chi_{-} = \tfrac{1}{3}N\mu^2 c(1 - c)^2 S(S + 1)/k_B T]$. For $c = 1$, we recover the result for the pure chain that $\chi_{-} = \tfrac{1}{4}N\mu^2/J$. At high temperatures we obtain the Curie susceptibility of Nc isolated spins $[\chi_{-} = \tfrac{1}{3}N\mu^2 cS(S + 1)/k_B T]$ so that $[J\chi_{-}/Nc\mu^2]^{-1}$ becomes independent of c.

4. Conclusion

The perpendicular susceptibility per spin and the specific heat per bond do not change dramatically upon dilution over much of the temperature range studied. The leading

term in the high-temperature expansion of each of these quantities is independent of concentration. For the special case of spin $\frac{1}{2}$, the specific heat per bond is independent of concentration for *all* temperatures. The most noticeable effect of diluting an Ising chain is in the way these thermodynamic quantities behave in the zero-temperature limit. The specific heat per bond differs in the nature of its exponential approach to zero upon dilution (for $S \geqslant 1$). Most striking is the divergence of χ_- at $T = 0$ when the chain is diluted, owing to the finite probability of finding isolated free spins.

We note that the results for both the specific heat and the perpendicular susceptibility depend only on $|J|$ and so are identical for an antiferromagnetic Ising chain. This is most easily seen by performing a rotation of 180° about the x axis.

One can expand on this study by turning on a weak interaction between segments, particularly those separated by just one non-magnetic site. However, the independent-segment assumption and hence equation (16) are not valid in this model and the problem becomes significantly more complex.

Acknowledgment

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Much of the preceding analysis can be carried out in the presence of an external parallel field, h^z. For instance, using equation (4) the standard transfer matrix for spin S is determined in a parallel field. From this one can obtain the partition function, although for $S > \frac{1}{2}$, the transfer matrix is not easily diagonalized analytically.

Similarly, one can write down the elements of the T^x transfer matrices, introduced in the $\chi_\perp$ calculation, in the presence of a parallel field:

$$T^x_{\substack{S^z_{i-1} \, S^z_{i+1}}} = h^x \sum_{S^z_i} \int_0^\beta \exp[(\beta-\tau)\Gamma_1] \, S^x_i \, \exp(\tau\Gamma_1) \, S^x_i \, d\tau \qquad (17)$$

$$T^{x'}_{\substack{S^z_{r-1} \, S^z_1}} = h^x \sum_{S^z_r} \int_0^\beta \exp[(\beta-\tau)\Gamma_2] \, S^x_r \, \exp(\tau\Gamma_2) \, S^x_r \, d\tau \qquad (18)$$

where

$$\Gamma_1 = JS^z_i(S^z_{i-1} + S^z_{i+1}) + h^z[(S^z_{i-1} + S^z_{i+1})/2 + S^z_i] \qquad (19)$$

$$\Gamma_2 = JS^z_{r-1}S^z_r + h^z[(S^z_{r-1} + S^z_1)/2 + S^z_r] \qquad . \qquad (20)$$

For instance, for $S=\frac{1}{2}$,

$$\frac{1}{h^z} T^x = \begin{pmatrix} \dfrac{\exp(\beta h^z/2)\sinh[\frac{1}{2}\beta(h^z+J)]}{J+h^z} & \dfrac{\sinh(\beta h^z/2)}{h^z} \\[3ex] \dfrac{\sinh(\beta h^z/2)}{h^z} & \dfrac{\exp(-\beta h^z/2)\sinh[\beta(J-h^z)/2]}{J-h^z} \end{pmatrix} \qquad (21)$$

and

$$\frac{1}{h^z} T^{x'} = \begin{pmatrix} \dfrac{2\exp(\beta h^z/2)\sinh[\beta(\frac{1}{4}J+\frac{1}{2}h^z)]}{J+2h^z} & \dfrac{2\sinh[\beta(\frac{1}{4}J+\frac{1}{2}h^z)]}{J+2h^z} \\[3ex] \dfrac{2\sinh[\beta(\frac{1}{4}J+\frac{1}{2}h^z)]}{J+2h^z} & \dfrac{2\exp(-\beta h^z/2)\sinh[\beta(\frac{1}{4}J-\frac{1}{2}h^z)]}{J-2h^z} \end{pmatrix} \qquad (22)$$

To calculate the transverse susceptibility for a pure chain, one needs to calculate the maximum eigenvalue, λ_m, and corresponding eigenvector $|m>$ of T^x. Then by equation (12) of the preceding letter, "Transverse susceptibility in spin S Ising chains," one can obtain

$$\frac{\chi_\perp}{N\mu_\perp^2} = \left(\frac{\exp(\beta h^z/2)\sinh[\beta(J+h^z)/2]}{2(J+h^z)} + \frac{\exp(-\beta h^z/2)\sinh[\beta(J-h^z)/2]}{2(J-h^z)} \right.$$

$$+ \frac{\exp(\beta J/4)\sinh(\beta h^z/2)}{2q_1} \left\{ \frac{\exp(\beta h^z/2)\sinh[\beta(J+h^z)/2]}{J+h^z} \right.$$

$$\left. \left. - \frac{\exp(-\beta h^z/2)\sinh[\beta(J-h^z)/2]}{J-h^z} + \frac{2\exp(-\beta J/2)}{h^z} \right\} \right)$$

$$\times [\exp(\beta J/4)\cosh(\beta h^z/2) + q_1]^{-2} \tag{23}$$

where

$$q_1 = [\exp(\beta J/2)\cosh^2(\beta h^z/2) - 2\sinh(\beta J/2)]^{\frac{1}{2}} . \tag{24}$$

This result was obtained earlier by Grest and Rajagopal (1974).

The modified transfer matrix, T^x, can be obtained straightforwardly for higher spins in a parallel field, but analytic calculation of $\chi_\perp$ is no longer tractable. Nevertheless, numerical results may be obtained easily.

Inspection of equation (23) reveals that for $h^z=\pm J$, there is the possibility of a divergence due to vanishing denominators. In fact, an antiferromagnetic chain in this field will have a divergent zero temperature transverse susceptibility, as noted by Grest and Rajagopal (1974). This can be seen for general spin by considering the Hamiltonian associated with a single bond:

$$H_{12} = J_o S_1^z S_2^z - h^z (S_1^z + S_2^z)/2 \qquad (25)$$

with

$$J_o \equiv -J > 0 \qquad . \qquad (26)$$

Taking $h^z = 2J_o S$,

$$H_{12} = (J_o S_2^z - J_o S)S_1^z - J_o S S_2^z \qquad . \qquad (27)$$

H_{12} can be minimized with respect to S_1^z by setting $S_1^z = S$, yielding a ground state energy

$$E_{12} = -J_o S^2 \qquad , \qquad (28)$$

independent of S_2^z.

As long as one spin in every bond is parallel to the field, the system is in a ground state. This state leaves a large number of spins free to point in any direction, which can be seen by noting that E_{12} is independent of S_2^z. These free spins are then able to line up in the direction of an infinitessimal transverse field, hence creating the divergence.

In particular, from equation (23), one can show that at $H = \pm J$ and as $T \to 0$,

$$\chi_\perp / N\mu_\perp^2 \simeq \beta(1+\sqrt{5})/(10+6\sqrt{5}) \qquad . \qquad (29)$$

The <u>dilute</u> chain transverse susceptibility in the presence of a parallel field may also be obtained using the formalism developed in the preceding paper. It should be noted that now the contribution of each spin in an open segment is a function of its location in the segment. This is a direct consequence of the fact that T and T' are not simultaneously diagonalizable in the presence of a field. Thus for dilute chains, analytic work stops at the writing

down of the four matrices T, T', T^x, $T^{x'}$, and the matrix multiplication and diagonalization is performed numerically.

It was seen earlier that the isolated spins contributed a divergence at $T=0$ to $\chi_\perp$. Application of a finite parallel field destroys this divergence. However, for the same reasons outlined for the pure chains, an antiferromagnetic chain will have another $T=0$ divergence in $\chi_\perp$ when $h^z=\pm 2JS$. A third divergence occurs at $h^z=\pm JS$ due to the spins at the end of open segments. Figure 1 illustrates one of these divergences, at $h^z=JS$, with a plot of $\chi_\perp^{-1}$ versus temperature. Since the divergence is proportional to β, $\chi_\perp^{-1}$ approaches zero linearly, as shown.

One limitation of this formalism that has been developed for the calculation of $\chi_\perp$ is that it is based on linear response theory and hence is valid only for infinitessimal h^x. However, in exchange for this restriction, one has gained the ability to calculate $\chi_\perp$ for a variety of models that are not tractable by other methods.

$$\left[\frac{|J|X_\perp}{Nc\mu^2}\right]^{-1}$$
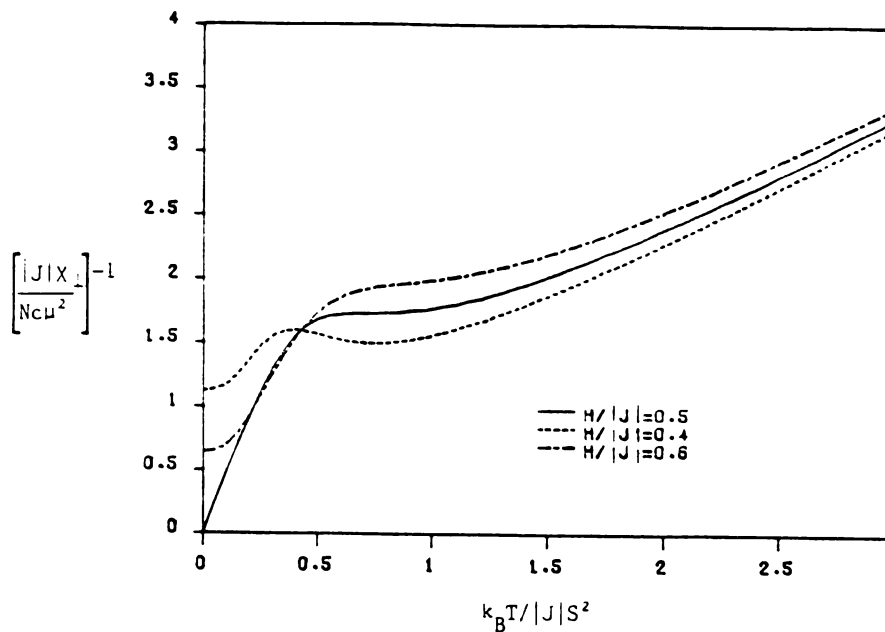
Figure 1. The inverse of the transverse susceptibility per spin of a dilute (c=0.25) Ising chain in the presence of three different parallel fields.

3. P(h): The Local Field Probability Distribution Function

The local field probability distribution function, P(h), has been studied at zero temperature for a variety of spin glass models (see, e.g., Palmer and Pond 1979 or Walker and Walstedt 1980). One of the distinctive features of P(h) these studies bring out is a dip at h=0. The nature of P(h), measuring the distribution of effective fields acting on a single spin, suggests that it be relegated to mean field theory or to low temperature studies. It is probably for this reason that the temperature dependence of the distribution has not been studied much before this. It turns out, however, that for Ising systems one may obtain exact thermodynamic relations using P(h).

This chapter is devoted to a formal discussion of the properties of P(h). While Appendix A contains details for a very broad class of Ising systems, for simplicity a more restrictive Hamiltonian is used here:

$$H = -\tfrac{1}{2} \sum_{i,j} J_{ij}\sigma_i\sigma_j \qquad (1)$$

where the σ_i's ($=\pm 1$) are spin $\tfrac{1}{2}$ Ising variables. The matrix defined by the J_{ij}'s is symmetric with vanishing diagonal elements but is otherwise arbitrary.

One begins by defining a local field operator, h_i:

$$h_i = \sum_j J_{ij}\sigma_j \qquad (2)$$

The missing factor of $\tfrac{1}{2}$ in equation (2) ensures that $h_i\sigma_i$ contains

<u>all</u> the σ_i terms in the original Hamiltonian. The local field probability distribution function at site i is defined by

$$P_i(h) = <\delta(h-h_i)> \quad . \tag{3}$$

The notation <...> refers to a thermal average. The site averaged distribution for a system of N spins is

$$P(h) = \frac{1}{N} \sum_i P_i(h) \quad . \tag{4}$$

This function is of course normalized:

$$\int P(h) \, dh \doteq 1 \quad . \tag{5}$$

Associated with P(h) are the following three <u>exact</u> results:

$$M = N \int \tanh(\beta h) \, P(h) \, dh \tag{6}$$

$$E = \frac{-N}{2} \int h \, \tanh(\beta h) \, P(h) \, dh \tag{7}$$

$$S(k,\omega) = \frac{N}{2}[P(\omega/2) + P(-\omega/2)]/[1 + \exp(-\beta\omega)] \quad . \tag{8}$$

These last three equations have simple physical interpretations. The magnetization of an isolated spin in a field h is $\tanh(\beta h)$. Equation (6) performs a weighted average with respect to h. Since $\tanh(\beta h)$ is odd, M couples to the antisymmetric part of P(h): $P_a(h)$. The second equation has a similar interpretation with an additional factor of $\frac{1}{2}$ present to correct for double counting of bonds. E couples to $P_s(h)$, the symmetric part of P(h). Finally, a beam of neutrons polarized in a direction perpendicular to the z axis interacts with the system by flipping individual spins at an energy cost proportional to the local field. Since these neutrons cannot distinguish between +z and −z, they couple to $P_s(h)$.

The statement these equations make is significant. Without any explicit knowledge of the J_{ij}'s, one can obtain the thermodynamics

of a system directly from $P(h)$. Furthermore, one can measure $P_s(h)$ directly, and that is sufficient to determine E.

Detailed proofs of equations (6) – (8) appear in Appendix A. However, to give the reader a flavor for the proofs, the energy equation, (7), is derived here. One begins with the energy of an isolated spin in a field h:

$$\varepsilon(h) = -h\ \tanh(\beta h)\ \ . \tag{9}$$

In its more primitive form, this is

$$\varepsilon(h) = \ Tr^0[\exp(-\beta H_0(h))\ H_0(h)]/Tr^0[\exp(-\beta H_0(h))] \tag{10}$$

where

$$H_0(h) = -h\sigma_0$$

and Tr^0 means trace over $\sigma_0 = \pm 1$. Denoting the energy of all the bonds terminating at site i by $2E_i$ (E_i is then the energy associated with site i), it needs to be shown that

$$\int \varepsilon(h)\ P(h)\ dh = 2E_i\ \ . \tag{11}$$

The following definitions need to be introduced:

$$Tr^i = \text{trace over } \sigma_i = \pm 1$$

$$Tr' = \text{trace over all spins } \underline{\text{except}}\ \sigma_i$$

$$H_i = -h_i\sigma_i$$

$$H' = H - H_i, \text{ which is independent of } \sigma_i$$

$$Z = Tr[\exp(-\beta H)]\ \ .$$

Then,

$$\int P(h)\ \varepsilon(h)\ dh$$

$$= \int dh\ \frac{Tr[\exp(-\beta H)\delta(h-h_i)]Tr^0[\exp(-\beta H_0(h))\ H_0(h)]}{Z\ Tr^0[\exp(-\beta H_0(h))]} \tag{12}$$

$$= \frac{1}{Z} \text{Tr} \left[\frac{\exp(-\beta H) \ \text{Tr}^0[\exp(-\beta H_0(h_i)) \ H_0(h_i)]}{\text{Tr}^0[\exp(-\beta H_0(h_i))]} \right] \qquad (13)$$

$$= \frac{1}{Z} \text{Tr}' \left[\frac{\exp(-\beta H') \ \text{Tr}^i[\exp(-\beta H_i)] \ \text{Tr}^0[\exp(-\beta H_0(h_i))H_0(h_i)]}{\text{Tr}^0[\exp(-\beta H_0(h_i))]} \right] \qquad (14)$$

In the last step, it is crucial that $[H', H_i] = 0$ so that the exponential can be split up. Since

$$\text{Tr}^i[\exp(-\beta H_i)] = \text{Tr}^0[\exp(-\beta H_0(h_i))] \qquad , \qquad (15)$$

one can cancel a term from the denominator and the numerator. Now σ_0 can be relabelled σ_i and the traces can be regrouped, giving

$$\int P(h) \ \varepsilon(h) \ dh = \frac{1}{Z} \text{Tr}[\exp(-\beta H) \ H_i] \qquad (16)$$

$$= 2E_i \qquad , \qquad (17)$$

which was to be shown.

P(h) is fundamentally a <u>local</u> quantity coupling to local properties such as E_i and M_i. The specific heat and other quantities which involve long range correlations require differentiation of P(h). The free energy, meanwhile, is obtained by integration of E in equation (7). Thus P(h) contains not only all the information found in the free energy, but it also contains additional information such as $S(k, \omega)$.

This formalism does not of course provide short cuts to solving for the thermodynamics of a system. The price one pays for the additional information in P(h) is that it in general is harder to calculate than the free energy. The remainder of this chapter will be devoted to methods for calculating P(h).

This part of the discussion will be limited to ferromagnetic systems with nearest neighbor interactions (although some of the techniques will be generalizable). Setting the interaction parameter $J = 1$, the Hamiltonian becomes

$$H = - \sum_{<ij>} \sigma_i \sigma_j \qquad (18)$$

where $\sum_{<ij>}$ indicates a sum over nearest neighbor pairs and the spins are assumed to lie on a lattice. One of the advantages of this simplification is that $P_i(h) = P(h)$.

The first approach to calculating the distribution is a formal one starting from the definition,

$$P_i(h) = <\delta(h-h_i)> \qquad . \qquad (19)$$

An integral representation of the δ function is used, and a little algebra yields the form

$$P_i(h) = \sum_{s=-z}^{z} w_s \, \delta(h-s) \qquad . \qquad (20)$$

z is the lattice coordination and the sum is over the allowed values of the local field, $-z$, $-z+2$, ..., $z-2$, z. Details of this approach are in Appendix A. It is shown there that the weights w_s involve numerical factors, which depend only on coordination number (not on the lattice itself), and all possible correlations among the nearest neighbors of site i. Hence the real work involved with this calculation becomes the determination of those correlation functions. This method will be demonstrated in Chapter 5.

For a system of coordination of two or three the correlations on the nearest neighbor shell can be eliminated in favor of the

nearest neighbor correlation, $\langle\sigma_0\sigma_1\rangle$ and the magnetization, $\langle\sigma_0\rangle$. If, for example, $z=3$, then the possible field values are ±3 and ±1 and so four equations are needed to determine the four weights, w_s. These equations are obtained by using the normalization requirement, (5), the energy and magnetization relations, (7) and (6), and the fact that $\langle h\rangle = 3\langle\sigma_0\rangle$. One then obtains

$$(w_3 + w_{-3}) + (w_1 + w_{-1}) = 1 \tag{21}$$

$$(w_3 + w_{-3})3\tanh(3\beta) + (w_1 + w_{-1})\tanh(\beta) = 3\langle\sigma_0\sigma_1\rangle \tag{22}$$

$$(w_3 - w_{-3})\tanh(3\beta) + (w_1 - w_{-1})\tanh(\beta) = \langle\sigma_0\rangle \tag{23}$$

$$3(w_3 - w_{-3}) + 1(w_1 - w_{-1}) = 3\langle\sigma_0\rangle \quad . \tag{24}$$

The first two equations yield $P_s(h)$ and the last two, $P_a(h)$. These equations can be solved explicitly to yield

$$w_{\pm1} = \frac{1}{2}\left[\frac{3(\tanh(3\beta) - \langle\sigma_0\sigma_1\rangle)}{3\tanh(3\beta) - \tanh(\beta)} \pm \frac{3\langle\sigma_0\rangle(\tanh(3\beta) - 1)}{\tanh(3\beta) - 3\tanh(\beta)}\right] \tag{25}$$

$$w_{\pm3} = \frac{1}{2}\left[\frac{3\langle\sigma_0\sigma_1\rangle - \tanh(\beta)}{3\tanh(3\beta) - \tanh(\beta)} \pm \frac{\langle\sigma_0\rangle(1-3\tanh(\beta))}{\tanh(3\beta) - 3\tanh(\beta)}\right] , \tag{26}$$

showing explicitly in this case that the w's depend only on $\langle\sigma_0\sigma_1\rangle$ and $\langle\sigma_0\rangle$. No reference is made here to the particular network other than it has coordination three and is compatible with a Hamiltonian of the form given in (18).

Finally, some systems lend themselves to calculation of the moments $\langle h^n\rangle$ by standard thermodynamic methods. If one knows all the moments up to $\langle h^z\rangle$, then the $z+1$ equations,

$$\langle h^n\rangle = \sum_s w_s s^n \tag{27}$$

can be inverted to find the w_s directly.

These methods may be generalized to <u>some</u> other systems, such as antiferromagnets, but their generalization to disordered systems is nontrivial. Different and specialized techniques must be developed for calculation of P(h) on these systems and so discussion of such techniques will be postponed until a specific disordered system is introduced (Chapter 7).

4. P(h) for Bethe Lattices

A simple system for which P(h) can be determined consists of S=½ Ising spins on a Bethe lattice with constant nearest neighbor ferromagnetic interactions. The Bethe "lattice" is really a pseudolattice (see Figure 2). It has the unfortunate property that, even in the thermodynamic limit, a finite fraction of its sites lie on the surface. On the other hand, it has the advantage that its coordination number, z, is easily varied. The z=2 case, a linear chain, will not be considered here since many of its properties are distinctly different from the z>2 Bethe lattices.

Because of the large surface area, calculations must be approached with caution. For instance, Eggarter (1973) pointed out that by assuming free boundaries, the Bethe lattice does not exhibit a phase transition. However, the more traditional Bethe-Peierls approach (Bethe 1935, Peierls 1936) which assumes boundary conditions determined by self-consistent fields, does find a phase transition. This latter approach will be used in this discussion.

The Bethe-Peierls method, leading to the self-consistent field equation (8) below, is described in Domb (1960) and is shown to be an exact solution for the system. An effective Hamiltonian is assumed for a cluster consisting of site 0 and its z nearest neighbors:

$$H_z = -J \sum_{j=1}^{z} \sigma_0 \sigma_j - H_0 \sigma_0 - H_1 \sum_{j=1}^{z} \sigma_j \quad . \qquad (1)$$
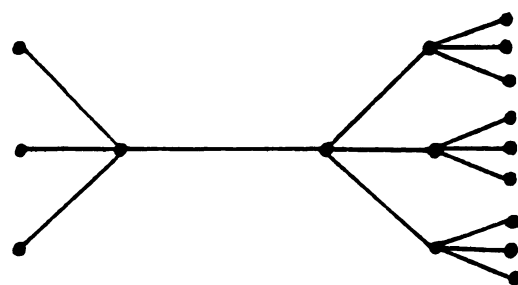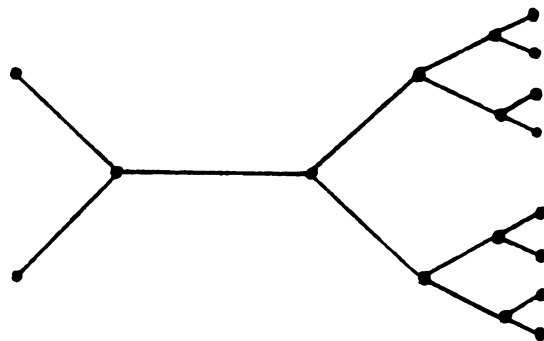
Figure 2. Section of a Bethe lattice for z=3(upper)
and z=4(lower).

H_0 is an external field acting on the system and will be set to zero later in the calculation. H_1 is an effective, temperature dependent field acting on the σ_j's accounting for both H_0 and the z-1 neighbors (other than σ_0) of σ_j. It can be shown that the partition function for H_z is

$$Q_z = \lambda_0^{-\frac{1}{2}} (\lambda_1^{-\frac{1}{2}}x^{-\frac{1}{2}} + \lambda_1^{\frac{1}{2}}x^{\frac{1}{2}})^z + \lambda_0^{\frac{1}{2}} (\lambda_1^{\frac{1}{2}}x^{-\frac{1}{2}} + \lambda_1^{-\frac{1}{2}}x^{\frac{1}{2}})^z \qquad (2)$$

where

$$\lambda_0 = \exp(-2H_0/k_BT) \qquad (3)$$

$$\lambda_1 = \exp(-2H_1/k_BT) \qquad (4)$$

$$x = \exp(-2J/k_BT) \qquad . \qquad (5)$$

To obtain H_1, one requires

$$\langle\sigma_0\rangle = \langle\sigma_j\rangle \qquad ,$$

or equivalently,

$$\lambda_0 \frac{\partial}{\partial\lambda_0} \ell nQ_z = \frac{\lambda_1}{z} \frac{\partial}{\partial\lambda_1} \ell nQ_z \qquad . \qquad (6)$$

Using equation (2), some algebra yields

$$\lambda_1/\lambda_0 = [(\lambda_1 + x)/(1 + \lambda_1 x)]^{z-1} \qquad . \qquad (7)$$

The external field H_0 will now be set to zero, having served its purpose. Some rearrangement gives

$$\frac{\tanh[H_1/(z-1)k_BT]}{\tanh(H_1/k_BT)} = \tanh(J/k_BT) \qquad , \qquad (8)$$

and this specifies H_1 as a function of temperature. An expansion for small H_1 gives a transition temperature defined by

$$\tanh(J/k_BT_c) = 1/(z-1) \qquad . \qquad (9)$$

Above T_c, $H_1 = 0$, and the effective partition function becomes

$$Q_z = 2[\cosh(J/k_BT)]^z \quad , \tag{10}$$

corresponding to z independent bonds. This result is typical for spin $\frac{1}{2}$ Ising systems with no loops, in the paramagnetic phase (see, e.g., Thorpe 1982). It should be noted that Q_z determines only local quantities such as the energy associated with σ_0 or the local magnetization $<\sigma_0>$. It is <u>not</u> true that the free energy F is given by $-\beta F = \ln Q_z$.

Below T_c, one needs to determine H_1. Introducing two new variables

$$Y = \lambda_1^{1/(z-1)} \tag{11}$$

$$t = \tanh(J/k_BT) \quad , \tag{12}$$

it is now possible to rewrite the self-consistent equation (8) as

$$\frac{1-Y}{1+Y} \cdot \frac{1+Y^{z-1}}{1-Y^{z-1}} = t \tag{13}$$

or

$$(1-t)Y^{z-1} - 2t \sum_{i=1}^{z-2} Y^i + (1-t) = 0 \quad . \tag{14}$$

By symmetry ($H_1 \leftrightarrow -H_1$), one expects that if Y_0 is a solution to this equation, Y_0^{-1} is also a solution. This fact can be exploited to reduce the degree of the polynomial by a factor of two. Since a fourth degree polynomial is solvable (Burington 1946), one can in principle obtain analytic expressions for H_1 up to $z = 10$. In practice, the complexity of these solutions makes some of the

larger z results not worth pursuing analytically.

For completeness sake, analytic expressions giving λ_1 ($=\exp(-2H_1/k_BT)$) as a function of x ($=\exp(-2J/k_BT)$) are shown below for z=3 up to z=6:

z=3 $\quad \lambda_1 = \frac{1}{2}[x^{-2} - 2x^{-1} - 1 + (x^{-2}-x^{-1})(1-2x-3x^2)^{\frac{1}{2}}]$ $\qquad$ (15)

z=4 $\quad \lambda_1 = \frac{1}{2}[x^{-3} - 3x^{-1} + (x^{-2}-1)(x^{-2}-4)^{\frac{1}{2}}]$ $\qquad$ (16)

z=5 $\quad$ Define $C = [1 - x + (5x^2+2x+1)^{\frac{1}{2}}]/2x$

$\qquad$ Then $\lambda_1 = \{[C + (C^2-4)^{\frac{1}{2}}]/2\}^4$ $\qquad$ (17)

z=6 $\quad$ Define $D = [x^{-1} + (x^{-2}+4)^{\frac{1}{2}}]/2$

$\qquad$ Then $\lambda_1 = \{[D + (D^2-4)^{\frac{1}{2}}]/2\}^5$ $\quad$. $\qquad$ (18)

A system with infinite range interactions produces a mean field result (Stanley 1971). On the Bethe lattice this corresponds to the $z \to \infty$ limit, which is readily accessible. In order to keep the energy finite, this limit must be taken holding Jz constant. Since H_1 should scale with Jz,

$$\lambda_1^{\pm\frac{1}{2}} x^{\pm\frac{1}{2}} \simeq \lambda_1^{\pm\frac{1}{2}} \qquad , \qquad (19)$$

reducing the partition function (2) to

$$Q_z = 2\cosh(H_0/k_BT)[2\cosh(H_1/k_BT)]^z \quad . \qquad (20)$$

The self-consistent field equation, (8), becomes

$$H_1/Jz = \tanh(H_1/k_BT) \qquad (21)$$

Which has a nontrivial solution if and only if $k_BT < Jz$. Hence

$$k_BT_c = Jz \quad . \qquad (22)$$

With the fundamental equations in place, it is now possible to calculate P(h) for Bethe lattices. This is most easily done

by calculating the moments of the distribution. Inspection of the Hamiltonian (1) reveals that these moments may be obtained by differentiation of Q_z. Taking

$$h/J = \sum_j \sigma_j \quad , \tag{23}$$

(assuming zero external field), one finds

$$\langle (h/J)^n \rangle = \frac{1}{Q_z} \left(-2\lambda_1 \frac{\partial}{\partial \lambda_1} \right)^n Q_z \quad . \tag{24}$$

As pointed out in the previous chapter, given the moments up to $\langle (h/J)^z \rangle$, one can solve for the weights in the $z+1$ δ functions associated with $P(h)$. This process, while straightforward, yields very complex analytic expressions which by themselves do not provide much insight. For this reason, they are omitted here in favor of the numerical results below.

The mean field result is easily derived. Starting from the partition function, (20), and applying a modified form of equation (24), one obtains for $H_0 = 0$,

$$\langle (h/J)^n \rangle = (2\cosh\beta H_1)^{-z} \left(\frac{\partial}{\partial \beta H_1} \right)^n (2\cosh\beta H_1)^z \tag{25}$$

$$= z(z-1)\ldots(z-n-1)\tanh^n\beta H_1 + O(z^{n-1}) \tag{26}$$

Thus

$$\langle (h/Jz)^n \rangle = \tanh^n\beta H_1 + O(1/z) \tag{27}$$

This implies the δ function distribution

$$P(h) = \delta(h - Jz\tanh\beta H_1) \quad . \tag{28}$$

Using equation (21), this can be rewritten

$$P(h) = \delta(h - H_1) \quad , \tag{29}$$

which is another way of saying that in the large z limit, mean field theory becomes exact.

In Figure 3, P(h) is plotted against h/z for z = 3, 4, 6, and infinity. It is symmetric for $T \geq T_c$, reflecting the fact that the magnetization is zero. At infinite temperature, the weights are determined by counting the number of ways to make a particular value of h. Since there are more ways to make h = 0, the distribution is peaked there. When $T = T_c$, the distribution is still peaked at small h, with more weight being at h = 0 as the mean field limit is approached. The symmetry is broken below T_c when spontaneous magnetization sets in. Again the approach to mean field theory is seen as the maximum in P(h) moves from h = Jz (z = 3) to h = Jzm for larger z.

It is apparent that there is strong dependence of P(h) on coordination number for Bethe lattices. While the number of δ functions is clearly determined by z, the profile of the distribution, particularly at T_c, is also sensitive to z. It is interesting to note that the nearest neighbor correlation at T_c is also strongly z dependent:

$$\langle \sigma_0 \sigma_j \rangle_{T=T_c} = 1/(z-1) \qquad . \qquad (30)$$

It will be argued later that this correlation plays an important role in the profile of P(h).

40
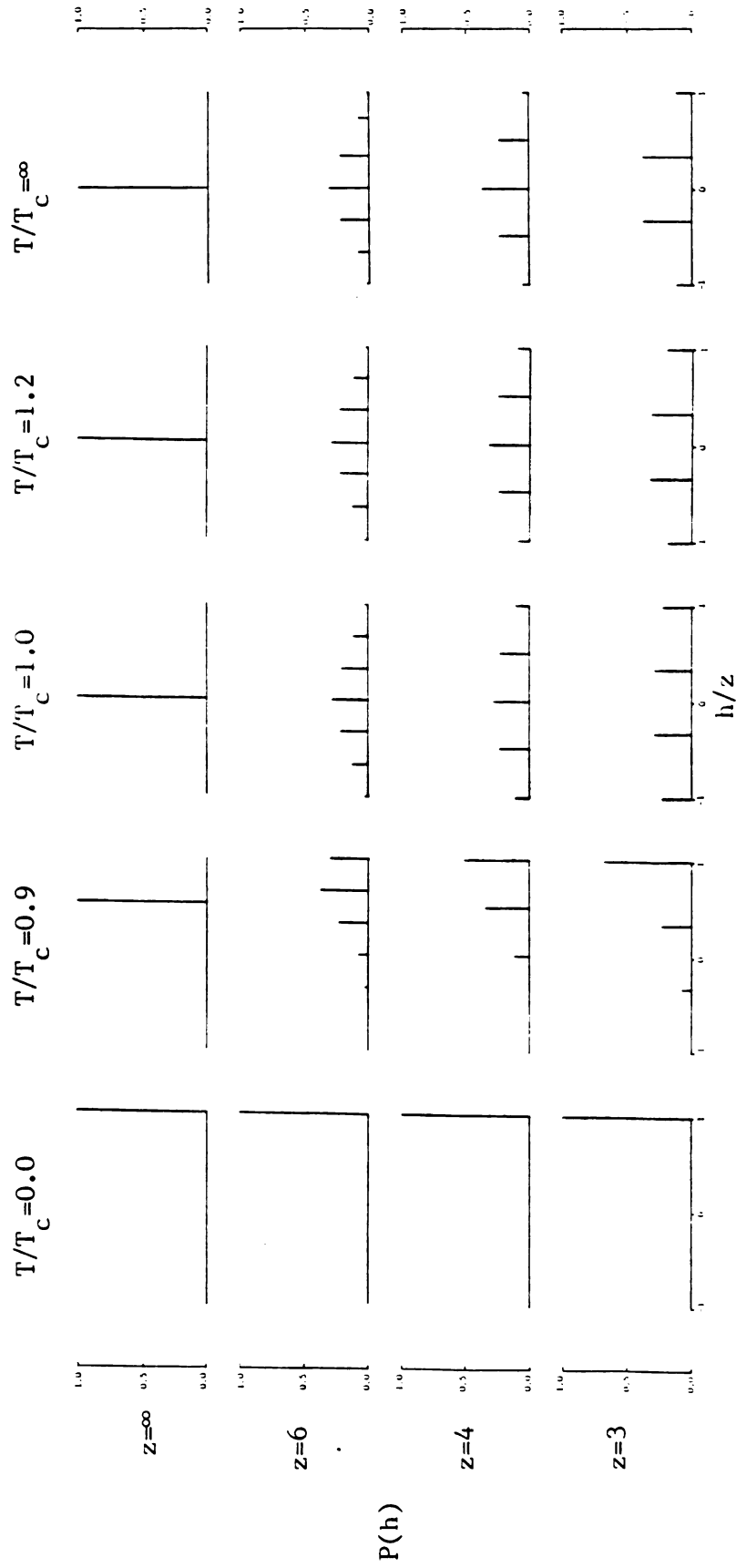
Figure 3. P(h) for Bethe lattices of coordination 3, 4, 6, and ∞.

5. P(h) for Two Dimensional Ferromagnets

There are several two dimensional Ising systems for which
P(h) can be calculated exactly. These analytic results can provide
useful insight into systems with phase transitions not dominated
by surface effects (in contrast to the Bethe lattice).

The first two dimensional Ising system to be solved was the
square net with uniform nearest neighbor interactions (Onsager
1944). Taking the ferromagnetic case and setting $J = 1$ yields
a Hamiltonian of the form

$$H = - \sum_{<ij>} \sigma_i \sigma_j \qquad . \qquad (1)$$

Since the square net has coordination four, the possible values
of h are ± 4, ± 2, and 0. The weights of the corresponding δ func-
tions in P(h) are easily expressed in terms of correlation functions
using equations (38) and (43) and Table 1 of Appendix A. The
nearest neighbors of an arbitrary site, 0, have been numbered
cyclically. One finds:

$$w_{\pm 4} = \frac{1}{16} \pm \frac{1}{4}<\sigma_1> + \frac{1}{4}<\sigma_1 \sigma_2> + \frac{1}{8}<\sigma_1 \sigma_3>$$
$$\pm \frac{1}{4}<\sigma_1 \sigma_2 \sigma_3> + \frac{1}{16}<\sigma_1 \sigma_2 \sigma_3 \sigma_4> \qquad (2)$$

$$w_{\pm 2} = \frac{1}{4} \pm \frac{1}{8}<\sigma_1> \mp \frac{1}{8}<\sigma_1 \sigma_2 \sigma_3> - \frac{1}{4}<\sigma_1 \sigma_2 \sigma_3 \sigma_4> \qquad . \qquad (3)$$

$$w_0 = \frac{3}{8} - \frac{1}{2}<\sigma_1 \sigma_2> - \frac{1}{4}<\sigma_1 \sigma_3> + \frac{3}{8}<\sigma_1 \sigma_2 \sigma_3 \sigma_4> \qquad . \qquad (4)$$

Apparently, $<\sigma_1 \sigma_2 \sigma_3>$ is not in the literature, nor is it easily
calculable. This problem is dealt with by using the magnetization

equation ((6) in Chapter 3) to eliminate $<\sigma_1\sigma_2\sigma_3>$ in favor of $<\sigma_0>$.

The even spin correlations can be reduced to elliptic integrals using the Pfaffian method described by Montroll, Potts and Ward (1963). While all of the two spin correlations needed appear explicitly in that paper, the four spin correlation does not. Details concerning the calculation of the latter in terms of elliptic integrals are given in Appendix B. The final step, evaluation of the integrals, must be performed numerically.

In Figure 4, excerpted from the preprint in Appendix A, P(h) is shown at five different temperatures. The infinite temperature distribution, as for the Bethe lattices, has roughly a Gaussian profile reflecting the fact that there are more h = 0 states than h = ±4 states. However, in contrast to the Bethe lattice, a pronounced dip has developed at T_c. This dip will be discussed in more detail later in this chapter. Below T_c, the asymmetry in P(h) develops very quickly, reflecting the rapid rise of the magnetization.

Results for the honeycomb lattice are more easily obtained. Since the lattice sites are threefold coordinated, equations (25) and (26) of Chapter 3 apply and one needs just the magnetization, $<\sigma_0>$, and the nearest neighbor correlation, $<\sigma_0\sigma_1>$. The former has been calculated by Naya (1954), while the latter may be obtained by differentiation of the partition function in Green and Hurst (1964). The expression for $<\sigma_0\sigma_1>$ thus obtained involves a double integral, making it somewhat awkward to evaluate numerically.
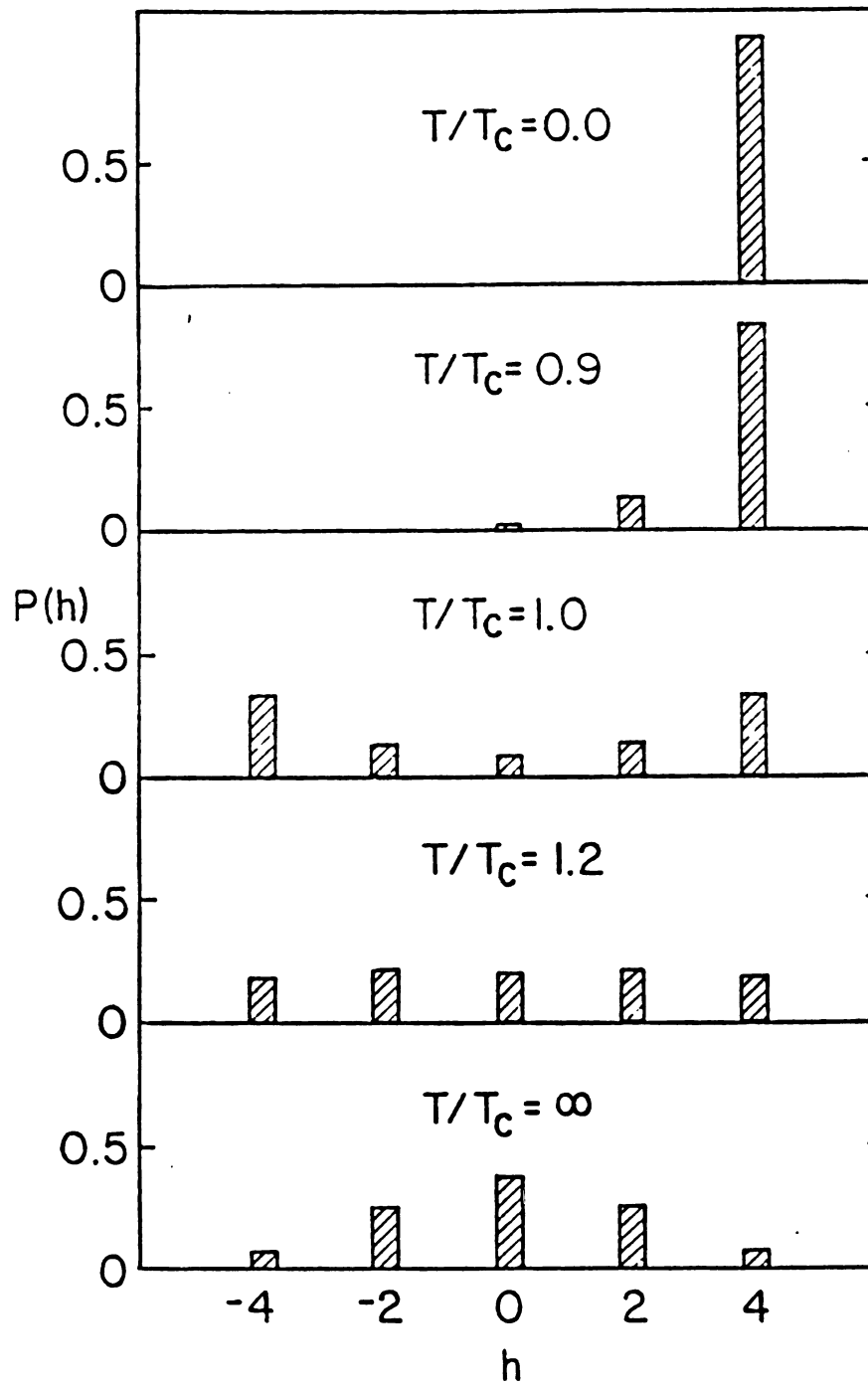
Figure 4. P(h) for the ferromagnetic square net.

Analytic work reduced this form to a single integral, details of which appear in Appendix B. A plot of P(h) for the honeycomb lattice in Figure 5, excerpted from Appendix A, reveals that it shares many of the features found in the square net, including having a dip at T_c.

One can also investigate P(h) for a triangular net. A problem arises however since for a sixfold coordinated lattice, many more correlations are needed. While the even spin correlations can be obtained (Choy 1984), not all of the odd spin correlations can be. Hence the results in Figure 6, also excerpted from Appendix A, are incomplete. Nevertheless, one can clearly see similarities between these results and the earlier two. In particular, there is once again a pronounced dip at T_c.

The existence of the h = 0 dip means that at T_c most spins find themselves in the presence of a nonzero local field. This suggests that perhaps small domains form in the system before long range order sets in. The existence of strong short range order is consistent with the value at T_c of $<\sigma_0\sigma_1>$, which for these lattices is 0.71±.06 (Domb 1974). One might expect that for systems which require short range order stronger than this before long range order sets in, the h = 0 dip should be even larger at T_c.

A lattice with a larger value of $<\sigma_0\sigma_1>$ at T_c can be formed following a procedure described by Syozi (1972). One starts by decorating the bonds of a honeycomb lattice with two sites and then one performs a star-triangle transformation, eliminating the original honeycomb sites (see Figure 7). This process can be carried out
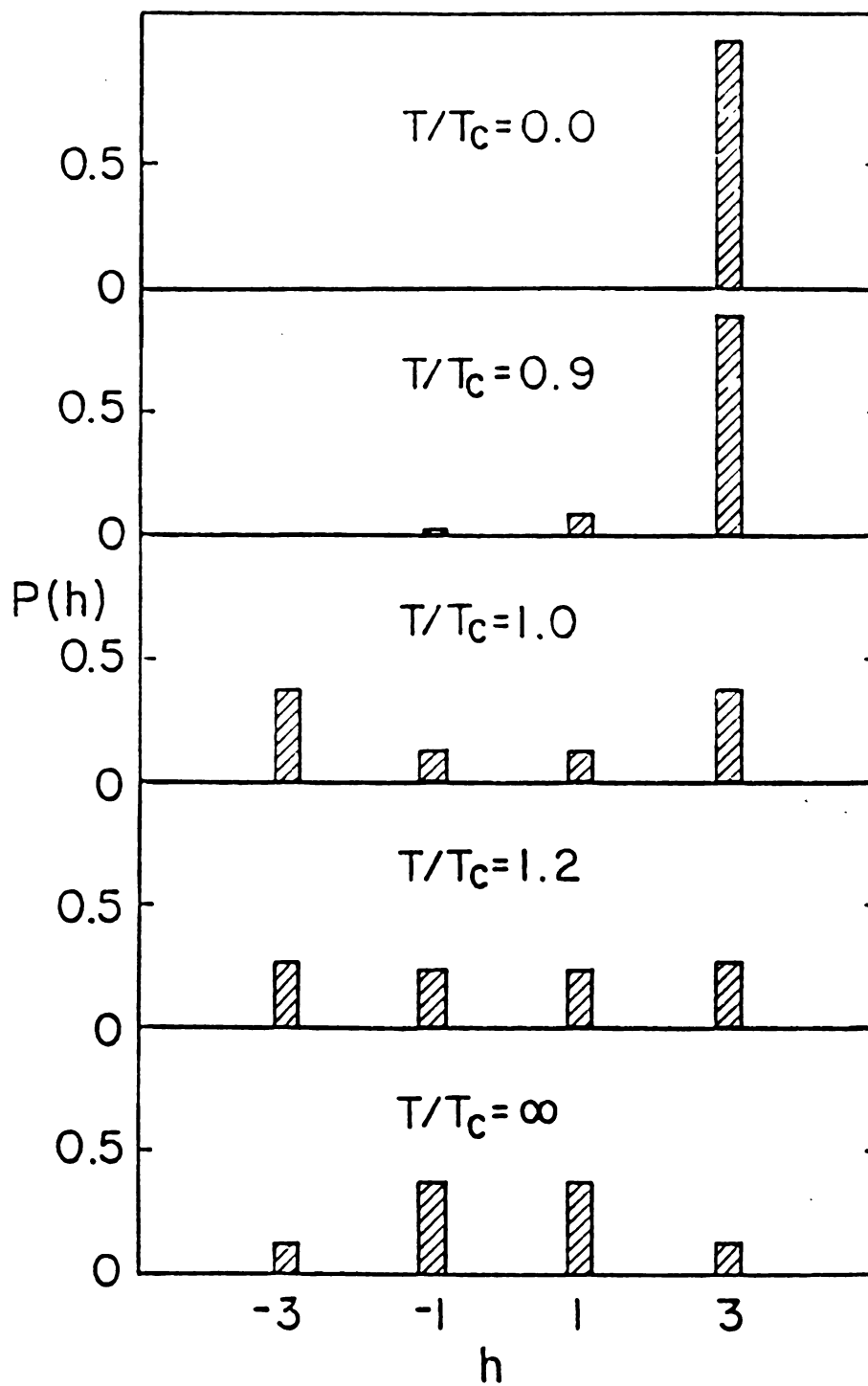
Figure 5. P(h) for the ferromagnetic honeycomb lattice.
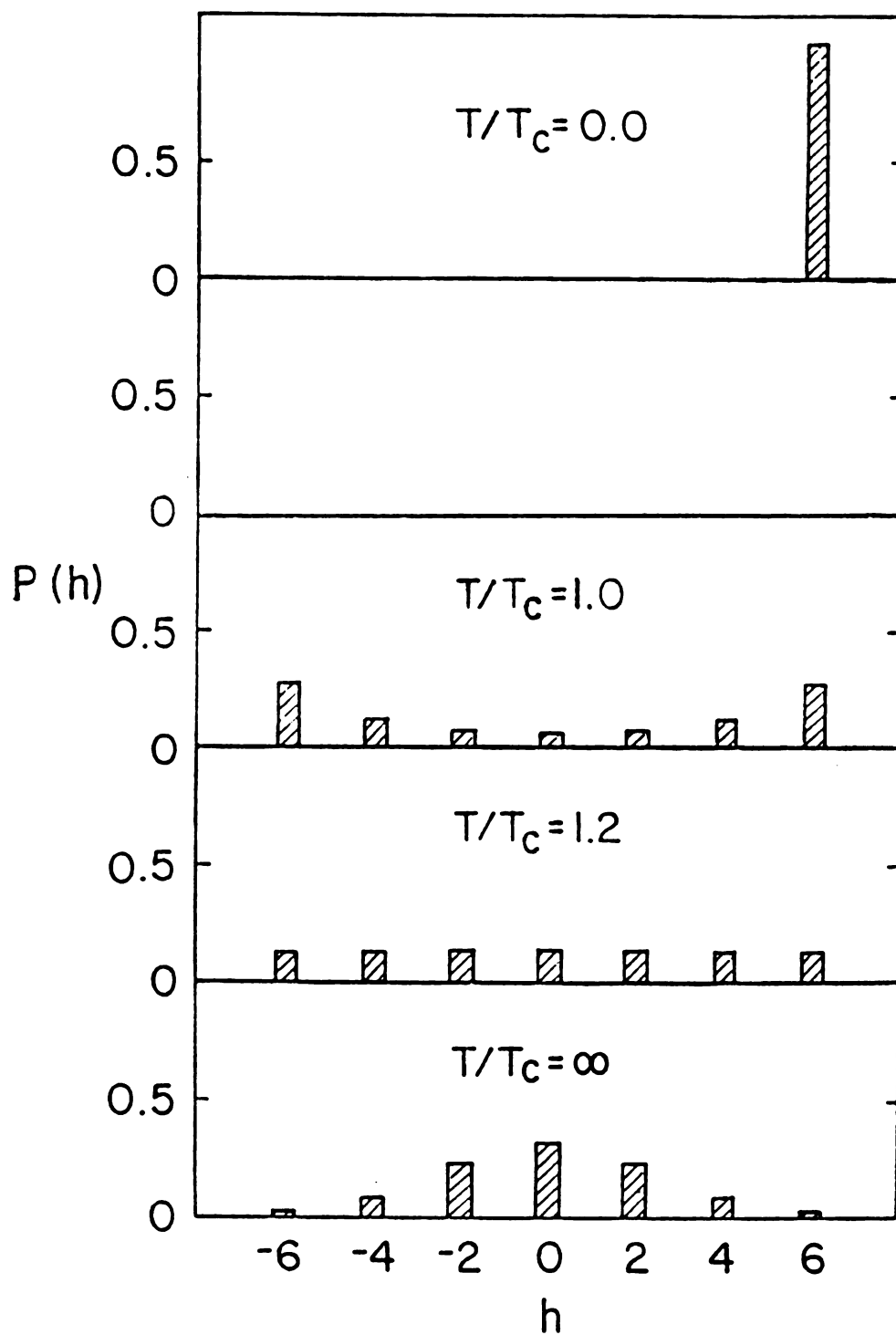
Figure 6. P(h) for the ferromagnetic triangular lattice.

—Decoration→

Star-Triangle
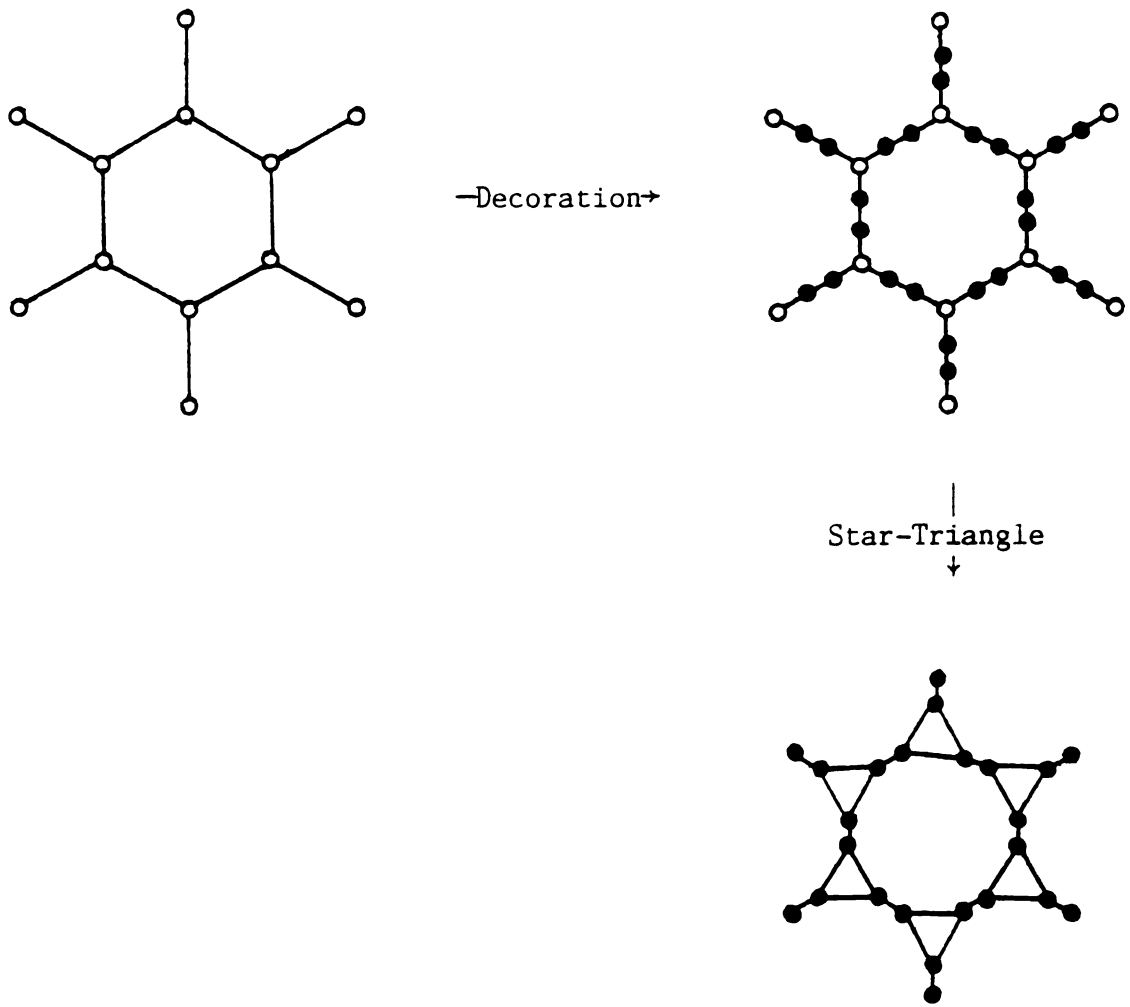
Figure 7. Generating the 3-12 lattice from the honeycomb lattice.

mathematically, generating exact results from analagous honeycomb results. The new lattice, called the 3-12 lattice, is more open than the previous one and hence requires more short range order, $<\sigma_0\sigma_1>_{T_c}$ = 0.8751, before long range order sets in. Note that for the honeycomb, $<\sigma_0\sigma_1>_{T_c}$ = 0.7698. A comparison of P(h) at T_c for these two lattices is made in Figure 8. As anticipated, the dip is bigger for the 3-12 lattice.

From the two dimensional lattices, one sees that the profile of P(h) above T_c reflects short range order in the system; there appears to be little effect due to coordination number. Below T_c, the rapid onset of the magnetization dominates. Finally, it should be noted that many of these calculations can easily be modified for antiferromagnets. For instance, a square net or honeycomb structure can be broken up into two sublattices so that at T = 0 the system can order by designating one sublattice as a spin up sublattice and the other as a spin down sublattice. The spin up sublattice will have a P(h) precisely as in Figure 4 (for a square net), while the down sublattice will have the same profile but with peaks on the -h side below T_c. The resultant P(h) for the entire system is symmetric, but below T_c,

$$P_i(h) \neq P(h) \quad . \tag{5}$$

The antiferromagnetic triangular net does not decompose into two sublattices and hence cannot order. Calculations by Choy (1984) indicate that P(h) for this system changes very little with temperature, which is consistent with its inability to order.
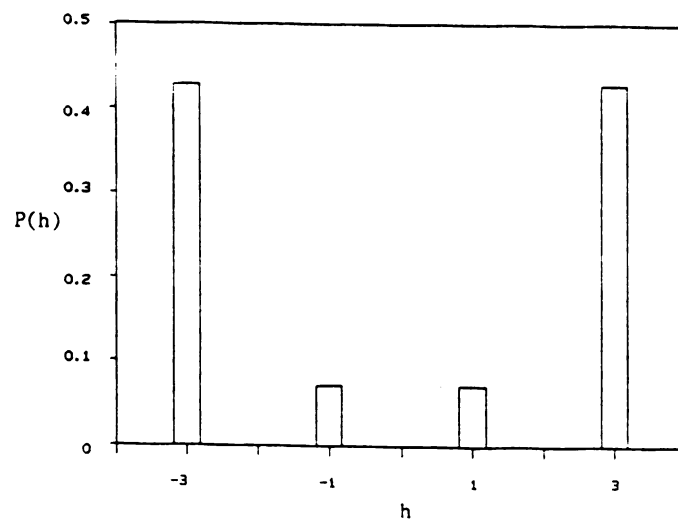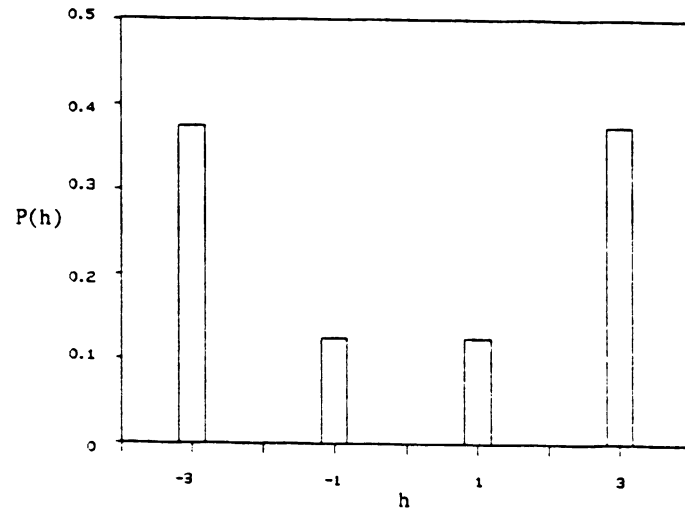
Figure 8. Showing P(h) at T_c for the honeycomb(upper) and 3-12 (lower) lattices.

6. P(h) for Ferromagnetic Systems of Higher Dimension

There are no exact solutions for Ising models on standard three or four dimensional lattices. However, it would still be interesting to obtain some information, if only approximate, on systems of dimension greater that two in order to gauge the effect lattice dimension has on P(h).

Frank et. al. (1982) developed an approximation method which effectively allowed them to estimate the moments of P(h) for a variety of three dimensional lattices at T_c. In principle, one can take their moments and recover the original distribution. In practice, the error bars associated with those moments were too large, so that negative weights appeared in the reconstructed distribution. Since it appeared that little progress would be made analytically, Monte Carlo simulations were developed.

The temperature scale for these simulations was set by the values for T_c based on high temperature series and reported elsewhere: $k_B T_c/J$ = 2.7044±.0001 (diamond), 4.5108±.0002 (simple cubic), 6.3533 ±.0010 (body centered cubic), and 9.7952±.0005 (face centered cubic) from Domb (1974), and $k_B T_c/J$ = 6.6817±.0015 (four dimensional simple cubic) from Gaunt et. al. (1979). No attempt was made to locate T_c precisely with these simulations since detailed information (such as critical exponents) was not sought.

Simulations generally have the most trouble converging when $T = T_c$. However, since it is known that P(h) is symmetric at T_c,

only $P_s(h)$ need be extracted at the critical temperature. This function couples to the energy, or equivalently to the nearest neighbor correlation $<\sigma_0\sigma_1>$, which is less sensitive to critical fluctuations than the magnetization and $P_a(h)$. The criterion for convergence at T_c was thus taken to be that $<\sigma_0\sigma_1>$ should equilibrate. This correlation can then be compared to estimates obtained from high temperature series.

The numerical simulations were performed on lattices of varying sizes and with periodic boundary conditions, employing the standard Metropolis algorithm (Metropolis et. al. 1953). Technical details associated with these studies appear in Appendix C. A given system would initially be brought into equilibrium and then be allowed to remain there while data was accumulated for thermal averages. Statistical errors quoted refer to the fluctuations in the thermal average during the second half of the averaging part of the simulation. The simulation was performed on three different lattice sizes (four at T_c), with the largest system containing roughly 30,000 spins. Then the data was plotted against the inverse of the number of spins in the system to allow extrapolation to infinite size. Figure 9 shows an example of an extrapolation of $<\sigma_0\sigma_1>$ for a simple cubic at T_c. The size of the data points is of the same order as the statistical error.

The results of these extrapolations can now be compared to high temperature series results (see Domb 1974 and Sykes 1979) to gauge the accuracy of the simulation. This comparison, reported in Table 1, shows reasonable agreement between the two results.
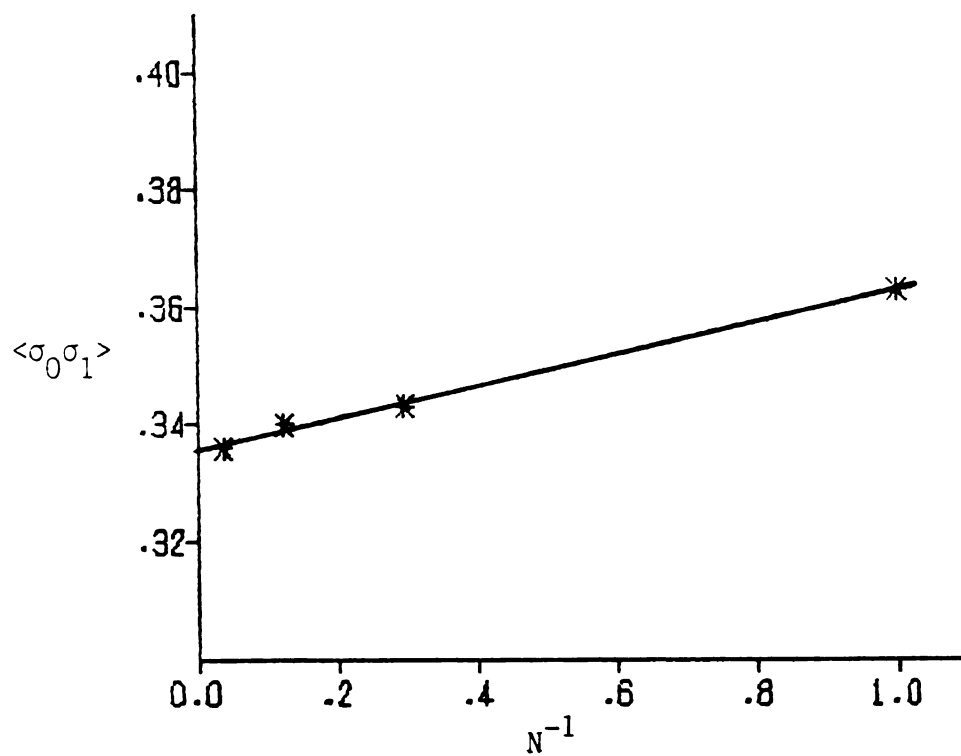
Figure 9. Extrapolation of $\langle \sigma_0 \sigma_1 \rangle$ to the infinite lattice
limit for a simple cubic at T_c.

Table 1. $\langle\sigma_0\sigma_1\rangle_{T_c}$ as obtained from Monte Carlo simulations and compared to high temperature series results.

Lattice	High T Series	Simulation
Diamond	.437 ± .003	.44 ± .01
SC	.3307 ± .0001	.34 ± .01
BCC	.2732 ± .0002	.28 ± .01
FCC	.2474 ± .0001	.26 ± .01
Hypercubic	.188 ± .003	.20 ± .01

Based on this, one would expect the data for P(h) to be accurate to within a few (3 or 4) percent, which is sufficient to determine the general nature of P(h).

Figure 10 displays P(h) for four different three dimensional lattices. All of these lattices show an extremely flat profile near T_c. Whether there is a slight dip or bump at h = 0 cannot be conclusively determined from this data, but it is clear that these profiles differ from those of the two dimensional lattices. It is also evident that in three dimensions as in two, coordination number plays very little role in the profile.

To see the dimensional dependence explicitly, it is constructive to look at the simple cubics in dimensions one through four (i.e., the linear chain, the square net, the simple cubic, and the hypercubic). These lattices all have coordination number equal to twice their dimension. The infinite dimension limit yields the mean field result discussed in Chapter 4, and will be included with this group too. These lattices have critical temperatures scaling roughly with coordination z, providing a consistent way to normalize all the temperatures at which P(h) was measured (either analytically or by simulation). More exactly, one finds

$$0 \leq T_c/z \leq 1 \tag{1}$$

where the lower limit corresponds to the linear chain and the upper limit to mean field theory.

The graphs in Figure 11 show P(h) for each of the five systems measured at each of the five (renormalized) transition temperatures. The profiles for any group of lattices above their transition
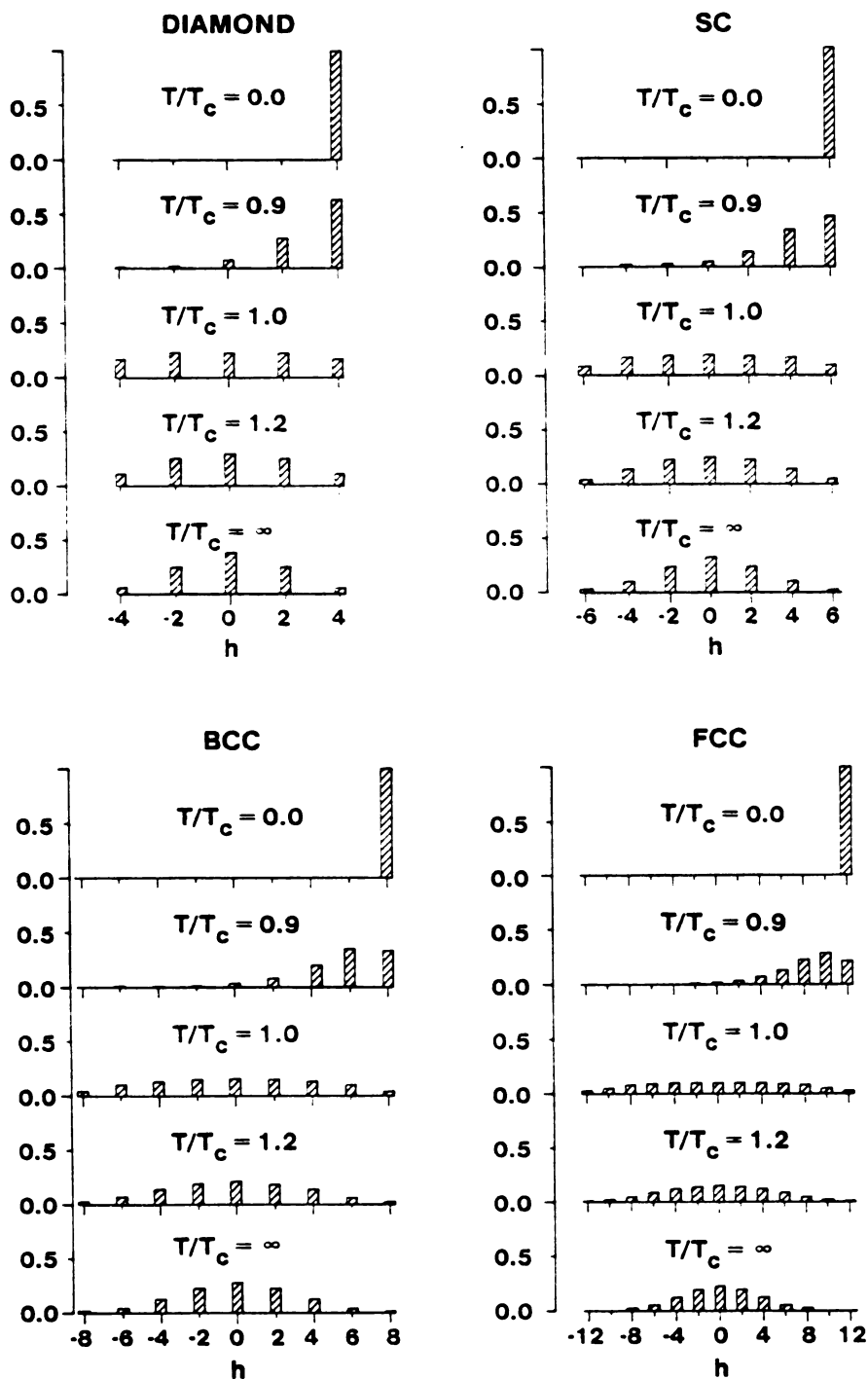
Figure 10. P(h) for four different three dimensional ferromagnets.
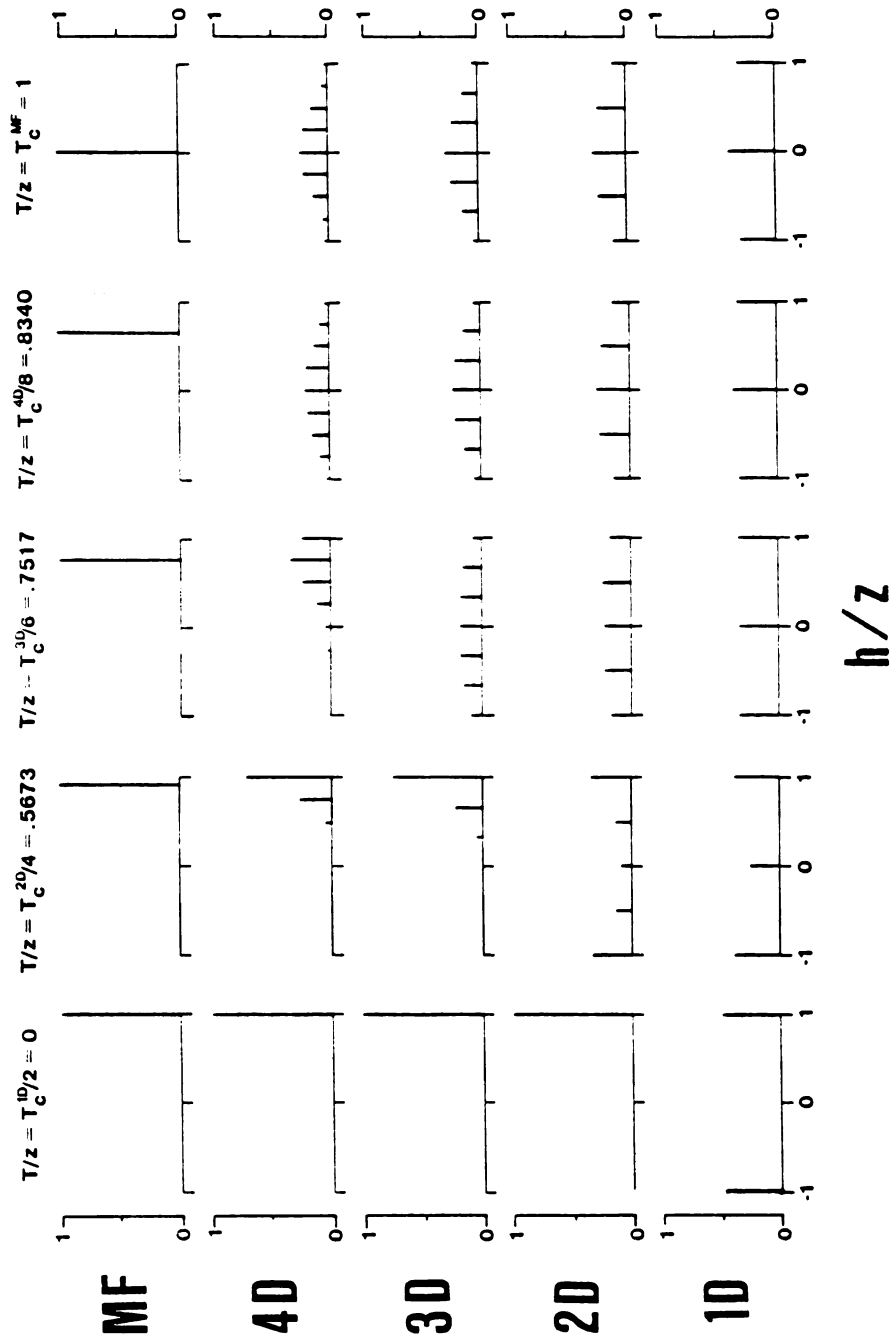
Figure 11. P(h) for simple cubics of dimensions one through four and for the mean field limit.

temperatures are very similar provided they are measured at the same renormalized temperature. The most dramatic example of this is seen by looking at the one, two, and three dimensional data at a temperature corresponding to T_c in three dimensions. All three profiles are extremely flat.

Below T_c, the symmetry is broken and the profiles lose much of their similarity. In the case of the four dimensional hyper-cubic, the approach to mean field theory can be seen by noting the development of a peak away from h = Jz.

Clearly the coordination of a lattice affects P(h) in that it determines the number of δ functions. It additionally helps set the temperature scale. Beyond that, the profile of P(h) is sensitive more to the dimension than to the coordination. At T_c, this dimension dependence comes chiefly through $\langle \sigma_0 \sigma_1 \rangle_{T_c}$, reflecting the amount of local order required before long range order can be established. Thus in four dimensions, P(h) at T_c is more nearly Gaussian than in one or two dimensions because less short range order is required in four dimensions for long range order to set in.

7. The Sherrington-Kirkpatrick Spin Glass Model

Having looked at P(h) for a wide variety of ordered systems,
it is now useful to turn to a disordered system, in particular, to
a spin glass model. The model used is based on the Edwards and
Anderson (1975) concept of a spin glass arising from some form of
random interactions among spins. In the spin glass phase, the spins
appear to be randomly oriented, but they are in fact frozen in. If
one defines a quantity q by

$$q = \lim_{t \to \infty} \langle S_i(0)S_i(t) \rangle \quad , \tag{1}$$

then it becomes nonzero in the spin glass phase. Edwards and Ander-
son argued that at least within mean field theory, this model is
capable of reproducing some of the characteristics of experimentally
observed spin glasses such as a cusp in the susceptibility which
is rounded by the application of a field. Whether or not the Edwards
and Anderson approach to spin glasses is an accurate description
of experimentally observed spin glasses is not the focus of this
investigation. Rather, as before, known results of a model will
be exploited to calculate P(h). This form of P(h) will look substan-
tially different from those found in the ferromagnets. Having ob-
tained P(h), one can then perform a neutron scattering experiment
on a disordered Ising system (preferably a spin glass) to link up
with experiment.

The spin glass model to be investigated is that introduced by

Sherrington and Kirkpatrick (1975). They assumed a Hamiltonian of

the form

$$H = -\tfrac{1}{2} \sum_{i,j} J_{ij}\sigma_i\sigma_j \tag{2}$$

with the matrix of J_{ij}'s symmetric and having vanishing diagonal

elements. The J_{ij}'s are otherwise independently distributed random

variables with mean J_o and variance J^2. Since this system has infi-

nite range interactions, one might hope some sort of mean field theory

would work. The infinite range interaction also means some variables

must be rescaled with the number of spins, N:

$$\tilde{J}^2 = J^2 N \tag{3}$$

$$\tilde{J}_o = J_o N \quad . \tag{4}$$

The energy scale is then set by $\tilde{J}$ or $\tilde{J}_o$.

When this model was introduced, Sherrington and Kirkpatrick

proposed a solution based on the replica method. Starting from the

identity

$$\ell n\ Z = \lim_{n\to o}(Z^n-1)/n \tag{5}$$

where

$$Z = Tr[exp(-\beta H)] \tag{6}$$

the calculation involves looking at Z^n for integral n. Some algebra

reduces this to n replicas of the original system with an effective

interaction between a spin in one system and the same spin in a rep-

lica. The new system, exactly solvable, depends on the integer n.

One then analytically continues Z^n to $n=0$, recovering the free energy

of the original system.

While there appear to be no problems with this approach in the

paramagnetic phase, it yields incorrect results in the spin glass phase (e.g., negative entropy). The analytic continuation of Z^n with respect to n and replica symmetry breaking are thought to be at the heart of the problem. The phase diagram obtained by the replica method is shown in Figure 12. Due to the problems with the calculation outside the paramagnetic phase, the spin glass-ferromagnetic phase boundary may not be correct. However, since most subsequent studies have been limited to $J_o=0$, this appears to be the most accurate phase diagram available.

Although Parisi (1980a) has devised a method for obtaining exact convergent series for various thermodynamic quantities in the spin glass phase, the less complete solution due to Thouless, Anderson and Palmer (1977), hereafter referred to as TAP, is more relevant to this study of P(h). Looking at the SK model for $J_o=0$, TAP compared it to a Bethe lattice with the coordination number, z, tending to infinity. The interactions on the Bethe lattice were taken to be nearest neighbor only and with a random distribution identical to that for the standard SK model. In the paramagnetic phase, TAP showed that the difference between the free energy per spin associated with such a Bethe lattice and the free energy per spin of the SK model with z spins, vanishes in the infinite z limit. They were also able to show this is true just below the transition temperature and for temperatures near zero.

The TAP equations reproduce the replica result in the paramagnetic phase,

$$E/N = -\tfrac{1}{2}\beta J^2 \quad . \tag{7}$$
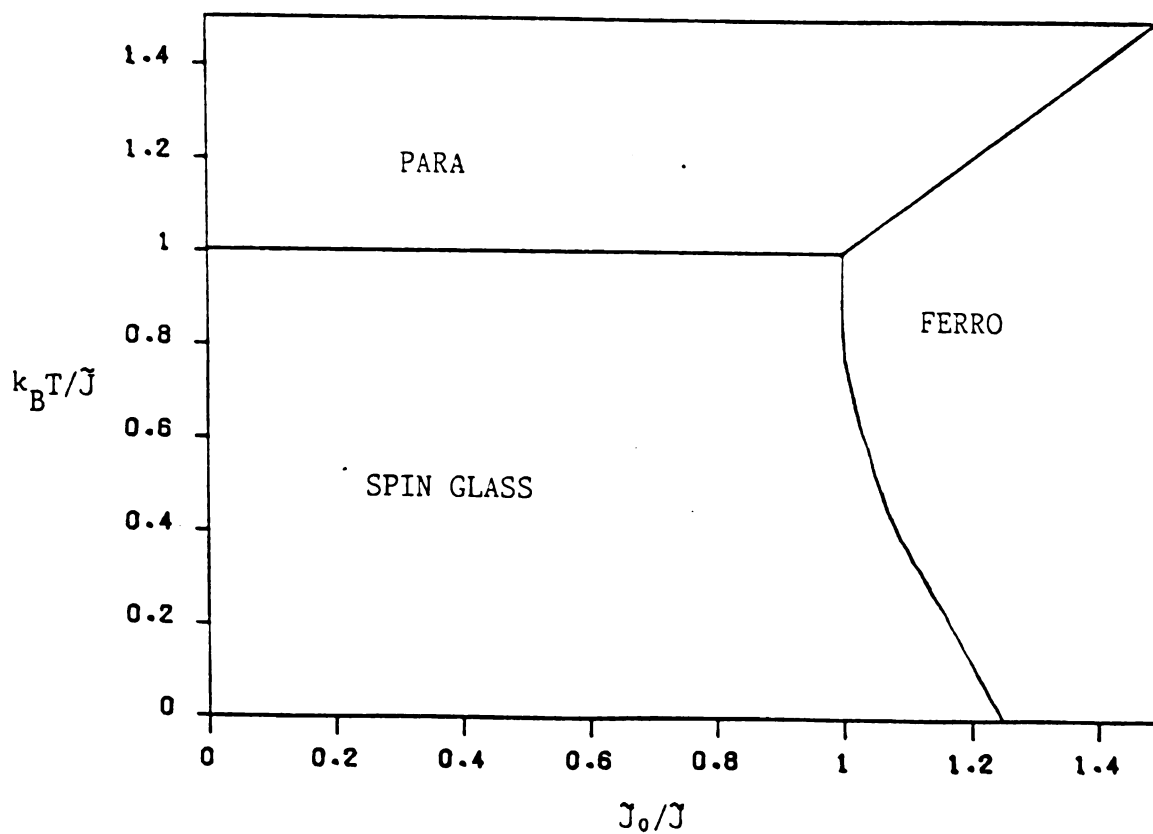
Figure 12. The phase diagram of the Sherrington-Kirkpatrick model (reproduced from Sherrington and Kirkpatrick 1975).

Unfortunately, their equations do not lead to exact, closed form solutions below T_{SG}. They do however yield some information about the zero temperature form of P(h) for small h.

First, a digression is required to a discussion which appeared in a paper by Palmer and Pond (1979). They assumed that

$$P(h,T=0) \propto h^t \qquad\qquad (8)$$

and tried to determine t. Starting with the system in a local minimum, the N sites are relabelled in order of increasing $|h_i|$. The spins at sites 1 through n are flipped, where

$$1 << n << N \quad . \qquad\qquad (9)$$

Before the spins were flipped, the energy associated with all the bonds comming into a given site was just $-|h_i|$. By flipping the spins, the energy has changed by an amount

$$\Delta E = 2 \sum_{i=1}^{n} |h_i| - 2 \sum_{i=1}^{n} \sum_{j=1}^{n} J_{ij}\sigma_i\sigma_j \quad . \qquad\qquad (10)$$

If the system was originally in a local minimum, then

$$\Delta E \geq 0 \quad . \qquad\qquad (11)$$

Consider $\left| \sum_{j=1}^{n} J_{ij}\sigma_j \right|$: one expects that the signs of J_{ij} and σ_j are not correlated so that the sum should yield

$$\left| \sum_{j=1}^{n} J_{ij}\sigma_j \right| \simeq n^{\frac{1}{2}}J = \mathcal{J}n^{\frac{1}{2}}/N^{\frac{1}{2}} \quad .$$

However, the signs of $\sum_{j=1}^{n} J_{ij}\sigma_j$ and σ_i are correlated in the ground state so that

$$\sum_{i=1}^{n} \sum_{j=1}^{n} J_{ij} \sigma_i \sigma_j \sim J n^{3/2}/N^{1/2} \quad . \tag{12}$$

Returning to the first term in (10), assume that for small h,

$$P(|h|) = Ah^t \quad . \tag{13}$$

Then,

$$\frac{n}{N} = \int_0^{h_m} Ah^t dh$$

$$= \frac{A}{t+1} h_m^{t+1} \quad , \tag{14}$$

where h_m is the largest field associated with the n flipped spins. Thus

$$h_m = \left(\frac{t+1}{A} \frac{n}{N}\right)^{1/(t+1)} \quad , \tag{15}$$

so that

$$\sum_{i=1}^{n} |h_i| = N \int_0^{h_m} Ah^{t+1} dh$$

$$= N \frac{A}{t+2} h_m^{t+2}$$

$$= \frac{NA}{t+2} \left(\frac{t+1}{A} \frac{n}{N}\right)^{(t+2)/(t+1)}$$

$$= \text{const} \times N \frac{n}{N} (n/N)^{1/(t+1)}$$

$$= \text{const} \times n (n/N)^{1/(t+1)} \quad . \tag{16}$$

If the constants are dropped, requiring that $\Delta E \geq 0$ yields

$$n(n/N)^{1/(t+1)} \geq n/(n/N)^{1/2}$$

or,

$$\frac{1}{t+1} \ln(n/N) \geq \frac{1}{2} \ln(n/N) \quad . \tag{17}$$

Since $\ln(n/N)<0$, this requires

$$\frac{1}{2} \geq \frac{1}{t+1}$$

or,

$$t \geq 1 \quad . \tag{18}$$

This is as far as Palmer and Pond took their analysis. It shows that it is <u>plausible</u> that

$$P(h,T=0) \propto h \quad .$$

In fact their simulations of the SK model at zero temperature as well as simulations by Kirkpatrick and Sherrington suggested that this was the case (Kirkpatrick and Sherrington 1978).

This evidence makes reasonable the assumption by TAP that for small h,

$$P(h,T=0) = h/H^2 \quad . \tag{19}$$

They were able to obtain some information about the slope, H^{-2}. It should be noted that their definition of $P(h)$,

$$P_{TAP}(h) = \frac{1}{N} \sum_i \delta(h-|<h_i>|) \quad , \tag{20}$$

is in general not equivalent to the definition used in equations (3) and (4) of Chapter 3,

$$P(h) = \frac{1}{N} \sum_i <\delta(h-h_i)> \quad .$$

However, at T=0 for a system that orders, that is, when $P_i(h)$ is of the form

$$P_i(h) = \delta(h-h_i^0) \quad , \tag{21}$$

these two definitions yield essentially the same result.

$P_{TAP}(h)$ has the advantage that at low temperatures, it appears

to be less temperature sensitive than P(h) so that TAP can neglect temperature dependence in their calculation. However, $P_{TAP}(h)$ is a mean field quantity and will not necessarily yield exact results.

Returning to their calculation, they first define

$$m_i = <\sigma_i> \quad .$$ (22)

Using the fact that the J_{ij}'s scale with $J = \mathcal{J}/\sqrt{z}$ and are all hence small, and using standard Bethe lattice techniques, they arrive at

$$\sum_j J_{ij} m_j - m_i \beta \sum_j J_{ij}^2 (1-m_j^2) = k_B T \tanh^{-1} m_i \quad .$$ (23)

This equation is simplified by approximating

$$\sum_j J_{ij}^2 (1-m_j^2) \simeq (1-\overline{m_j^2}) \sum_j J_{ij}^2$$

$$\equiv (1-q) \mathcal{J}^2$$ (24)

where q is the Edwards–Anderson order parameter. It will turn out to be consistent to take the low temperature behavior of q to have the form

$$q = 1 - \alpha(k_B T/\mathcal{J})^2 \quad .$$ (25)

To further simplify notation, define

$$h_i^* \equiv <h_i> = \sum_j J_{ij} m_j \quad .$$ (26)

Then equation (23) can be rewritten

$$h_i^* = \alpha k_B T m_i + T \tanh^{-1} m_i \quad .$$ (27)

While an exact expression for q is

$$q = \overline{m_i^2} = \frac{1}{N} \sum_i [\int P_i(h) \tanh \beta h \, dh]^2 \quad ,$$

it is plausible within the mean field limit to write

$$q = \int m^2(h^*) P_{TAP}(h^*) \, dh^* \quad ,$$ (28)

where m(h) is obtained by inverting (27). No attempt is made either here or in TAP to rigorously justify (28). Combining equations (28), (25), and (19) one arrives at

$$\alpha\left(\frac{k_BT}{J}\right)^2 = \int_0^\infty [1-m^2(h^*)] \frac{h^*}{H^2} dh^*$$

$$= \int_0^1 [1-m^2] \frac{h^*}{H^2} \frac{dh^*}{dm} dm \quad . \tag{29}$$

Equation (27) will provide $h^*(m)$ and its derivative so that

$$\alpha\left(\frac{k_BT}{J}\right)^2 = \left(\frac{k_BT}{H}\right)^2 \int_0^1 [1-m^2] [\alpha m + \tanh^{-1}m] [\alpha + \frac{1}{1-m^2}] dm \quad . \tag{30}$$

Integration and rearrangement yields

$$(H/J)^2 = \frac{\alpha}{4} + \frac{2\ell n2+1}{3} + \frac{\ell n2}{\alpha} \quad . \tag{31}$$

While this equation relates H^2 to α, it does not determine either of them. It is consistent with the results of Monte Carlo simulations reported in Palmer and Pond (1979) to take the minimum value of H^2 compatible with (31). This occurs when

$$\alpha = 2\sqrt{\ell n2} \tag{32}$$

giving

$$(H/J)^2 = \frac{2\ell n2+1}{3} + \sqrt{\ell n2} \quad . \tag{33}$$

Taking care of a factor of two discrepancy arising from the different definitions of P(h) used, one would then expect at T=0

$$P(h) = 0.307h \qquad \text{(small h)} , \tag{34}$$

where P(h) is as defined in Chapter 3.

Clearly, the approach used in TAP to calculate this slope has been mean field. Nevertheless, as reported in the next chapter, it meets with much success when compared to Monte Carlo simulations. Finally, because of TAP's definition of $P(h)$, there appears to be no straightforward way to use this argument to investigate the low temperature properties of the $P(h)$ defined in Chapter 3.

8. P(h) for the Sherrington-Kirkpatrick Model

As pointed out in the previous chapter, most of the attention paid to P(h) has been concentrated on the zero temperature problem. However, using the TAP trick of replacing the SK model with a Bethe lattice, it is possible to obtain P(h) in the entire paramagnetic regime of this model. To do this, one makes use of the fact that for a Bethe lattice in the paramagnetic phase, that is when boundary conditions are of no concern,

$$\langle \sigma_i \sigma_{i+2} \rangle = \langle \sigma_i \sigma_{i+1} \rangle \langle \sigma_{i+1} \sigma_{i+2} \rangle \tag{1}$$

$$= \tanh\beta J_{i,i+1} \ \tanh\beta J_{i+1,i+2} \quad . \tag{2}$$

This is valid when site i+1 is the only site crossed by the path from i to i+2 (see Chapter 4 or Thorpe 1982). In this model, the temperature scale is set by

$$k_B T \sim \mathcal{J} = J\sqrt{N} \tag{3}$$

so that

$$\beta J_{ij} \sim 1/\sqrt{N} \tag{4}$$

and one can approximate

$$\tanh\beta J_{ij} \simeq \beta J_{ij} \quad . \tag{5}$$

Starting from the integral representation of the δ function,

$$P_i(h) = \int d\theta \ \exp(-ih\theta) \ \langle \ \exp(ih_i \theta) \ \rangle \tag{6}$$

or

$$P_i(\theta) = \langle \exp(ih_i \theta) \rangle \quad , \tag{7}$$

and using

$$h_i = \sum_j J_{ij}\sigma_j \qquad (8)$$

(where the sum is over the z neighbors of site i), it follows that

$$\tilde{P}_i(\theta) = \langle \prod_j \exp(iJ_{ij}\sigma_j\theta) \rangle$$

$$= \langle \prod_j [\cos(J_{ij}\theta) + i\sigma_j\sin(J_{ij}\theta)] \rangle$$

$$= \langle \prod_j \cos(J_{ij}\theta)[1 + i\sigma_j\tan(J_{ij}\theta)] \rangle$$

$$\simeq \langle \prod_j \cos(J_{ij}\theta)[1 + i\sigma_j J_{ij}\theta] \rangle \qquad . \qquad (9)$$

$\tilde{P}(\theta)$ is obtained by averaging over all configurations of $\{J_{ij}\}$. That average will be denoted by an overbar. Thus

$$\tilde{P}(\theta) = \overline{\tilde{P}_i(\theta)}$$

$$= \overline{\langle \prod_j \cos(J_{ij}\theta)[1 + i\sigma_j J_{ij}\theta] \rangle}$$

$$= \overline{\cos(J_{ij}\theta)}^{\,z}\, [\, 1 + iz\overline{(J_{ij}\theta\langle\sigma_j\rangle)}$$

$$+ i^2 \frac{z(z-1)}{2!} \overline{J_{ij}J_{ik}\theta^2\langle\sigma_j\sigma_k\rangle}$$

$$+ i^3 \frac{z(z-1)(z-2)}{3!} \overline{J_{ij}J_{ik}J_{il}\theta^3\langle\sigma_j\sigma_k\sigma_l\rangle}$$

$$+ i^4 \frac{z(z-1)(z-2)(z-3)}{4!} \overline{J_{ij}J_{ik}J_{il}J_{im}\theta^4\langle\sigma_j\sigma_k\sigma_l\sigma_m\rangle}$$

$$+ \ldots] + O(1/z) \qquad . \qquad (10)$$

The order $1/z$ corrections, arising from averaging over all the $\cos(J_{ij}\theta)$ terms independently of the $J_{ij}\langle\ldots\sigma_j\ldots\rangle$ terms, are neglected.

In the paramagnetic phase, the thermal average of an odd number of spins is zero. Furthermore, using equations (2) and (5),

$$\langle\sigma_j\sigma_k\rangle \simeq \beta^2 J_{ij}J_{ik} \quad . \tag{11}$$

Thus, in the large z limit,

$$\tilde{P}(\theta) = \overline{\cos(J_{ij}\theta)}^{\,z}[1 - \frac{z^2}{2!}\beta^2\left(\overline{J_{ij}^2}\right)^2\theta^2 + \frac{z^4}{4!}\beta^4\left(\overline{J_{ij}^2}\right)^4\theta^4 - \ldots] \quad . \tag{12}$$

This last step has used

$$\overline{J_{ij}^2 J_{ik}^2} = \left(\overline{J_{ij}^2}\right)^2 \tag{13}$$

which holds since J_{ij} and J_{ik} are independent random variables.

The infinite sum in (12) is the Taylor expansion of cosine, so that

$$\tilde{P}(\theta) = \overline{\cos(J_{ij}\theta)}^{\,z}\,\cos(\beta z\overline{J_{ij}^2}\theta) \quad . \tag{14}$$

Using notation and scaling introduced earlier,

$$\overline{J_{ij}^2} = J^2 + J_o^2$$

$$= \mathfrak{J}^2/z + \mathfrak{J}_o^2/z^2 \quad . \tag{15}$$

For large z,

$$z\,\overline{J_{ij}^2} \simeq \mathfrak{J}^2 \quad . \tag{16}$$

Furthermore,

$$\overline{\cos(J_{ij}\theta)}^{\,z} = (1 - \tfrac{1}{2}\theta^2\overline{J_{ij}^2} + \ldots)^z$$

$$= [1 - \frac{\theta^2\mathfrak{J}^2}{2z} + O(1/z^2)]^z$$

$$= \exp(-\theta^2\mathfrak{J}^2/2) \tag{17}$$

and hence

$$P(\theta) = \exp(-\theta^2\mathfrak{J}^2/2)\,\cos(\beta\mathfrak{J}^2\theta) \quad . \tag{18}$$

Taking the inverse fourier transform, one obtains

$$P(h) = \frac{1}{\sqrt{2\pi}J} \exp(-\beta^2 J^2/2 - h^2/2J^2) \cosh(\beta h) \quad . \tag{19}$$

Equation (19) is valid throughout the entire paramagnetic phase

and interestingly contains no explicit J_o dependence.

Figure 13 shows a plot of $P(h)$ at three temperatures. It

was assumed that $J_o < J$ so that (19) would be valid at $k_B T = J$,

which is then the spin glass temperature. The infinite temperature

limit is, as expected, a Gaussian:

$$P(h, T=\infty) = \frac{1}{\sqrt{2\pi}J} \exp(-h^2/2J^2) \quad . \tag{20}$$

When the temperature is decreased, the Gaussian broadens and flat-

tens, a phenomenom made clearer by looking at the small h expansion,

$$P(h) = \frac{1}{\sqrt{2\pi}J} \exp(-\beta^2 J^2/2) \; [1 - \frac{h^2}{2J^2}(1 - \beta^2 J^2)$$

$$+ \frac{h^4}{J^4}(1/8 - \beta^2 J^2/4 + \beta^4 J^4/24) + \ldots] \quad . \tag{21}$$

The fact that the h^2 term vanishes precisely at T_{SG} indicates

how extremely flat this function becomes for small h.

This calculation of $P(h)$ cannot be repeated in an ordered

phase for several reasons, among which are

$$<\sigma_j> \neq 0$$

$$<\sigma_j \sigma_k> \neq <\sigma_j \sigma_i><\sigma_i \sigma_k> \quad .$$

Without being able to express higher order correlation functions in

terms of the nearest neighbor correlation functions, there appears

to be little hope for finding an analytic expression for $P(h)$ in
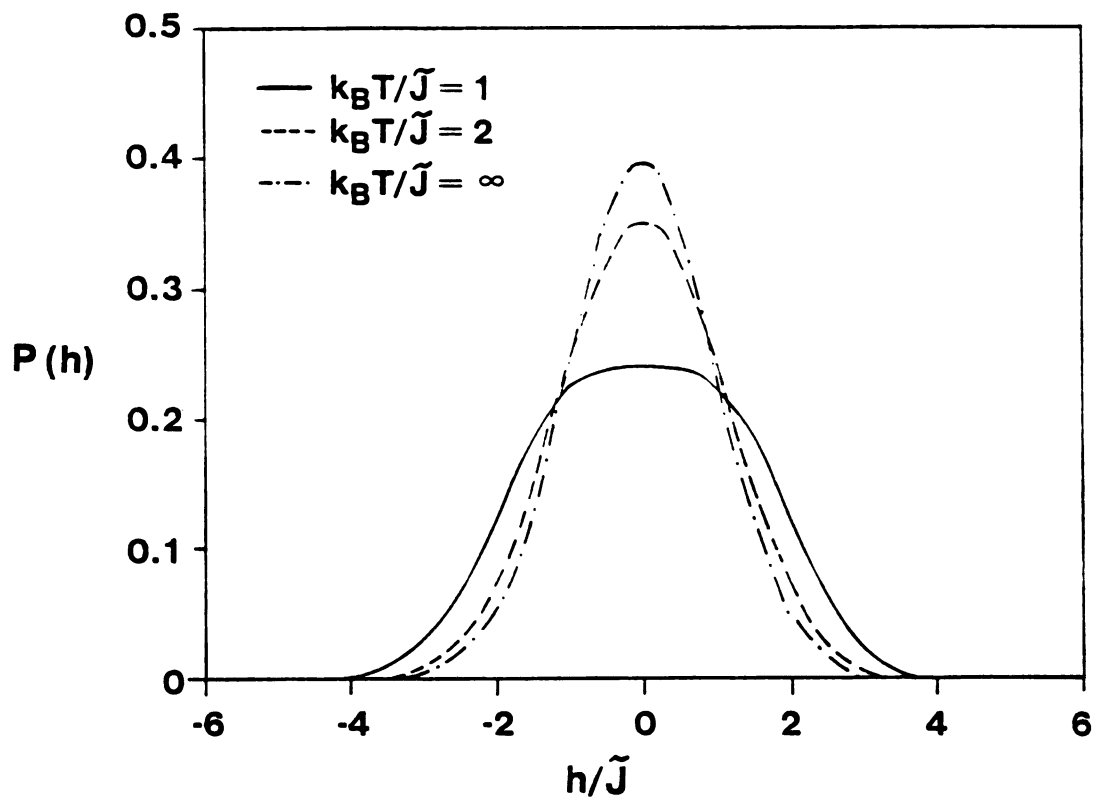
Figure 13. P(h) from the analytic result for the Sherrington-Kirkpatrick model in the paramagnetic phase ($\tilde{J}_o < \tilde{J}$).

the spin glass phase of the model. For this reason, a Monte Carlo simulation was employed to study an ordered phase, specifically, the spin glass regime.

The probability distribution for the J_{ij}'s was taken to be of the form

$$p(J_{ij}) = a\delta(J_{ij} - J) + (1 - a)\delta(J_{ij} + J) , \qquad (22)$$

where

$$a = \tfrac{1}{2}(1 + J_o/J) . \qquad (23)$$

This form ensures

$$\overline{J_{ij}} = J_o$$

and

$$\overline{J_{ij}^2} = J^2 .$$

Since it was explicitly seen in the paramagnetic phase that once J_o and J^2 have been fixed, the details of the J_{ij} distribution are irrelevant, it is clear that in this phase one is free to choose the particular form of $p(J_{ij})$ for convenience. The same statement cannot be proved in the spin glass phase but is believed to be true there owing to the infinite range of the interaction.

The advantage of the distribution defined in (22) is that now J_{ij} can be represented as a single binary digit. This fact was exploited to increase the effective memory available for the computer simulation and to increase the execution speed of the simulation. The details of this technique are provided in Appendix C. Unless otherwise noted, the data displayed in this chapter results from an average over four different 1020 spin systems.

In Figure 14 the results of a simulation for $J_o = 0$ at $T = 2T_{SG}$ are compared to the analytic calculation, and a similar comparison at $T = T_{SG}$ is made in Figure 15. While there is some noise in these simulations, it is clear that they are in essential agreement with the analytic result.

In Figure 16, P(h) as obtained from the simulation is plotted at four temperatures. In keeping with the trend established above T_{SG}, a dip at $h = 0$ has now developed below T_{SG}.

The data at $T = 0$ was accumulated by taking forty different $\{J_{ij}\}$ configurations and searching for one state in each that was stable against single spin flips. Kirkpatrick and Sherrington (1978) and Palmer and Pond (1979) have already studied the zero temperature problem in detail, so no attempt was made to be more careful in searching for local minima. Those authors, in fact, report lower values for P(h=0,T=0), and it is believed that for an infinite system, P(0,0) = 0. However, even using states stable against only single spin flips, the small h slope obtained from this simulation, $0.311/J^2$, is in excellent agreement with the TAP (1977) prediction of $0.307/J^2$ discussed in the previous chapter. Hence the slope appears to be less sensitive than the intercept to the particular local minimum one is in.

As the temperature is reduced from $T_{SG}/2$ to 0, most of the change in P(h) occurs for small h. The large h regions are relatively stable. This suggests that the formation of the h = 0 dip is an important characteristic of the spin glass phase.

To study P(0) in more detail, first note that above T_{SG},
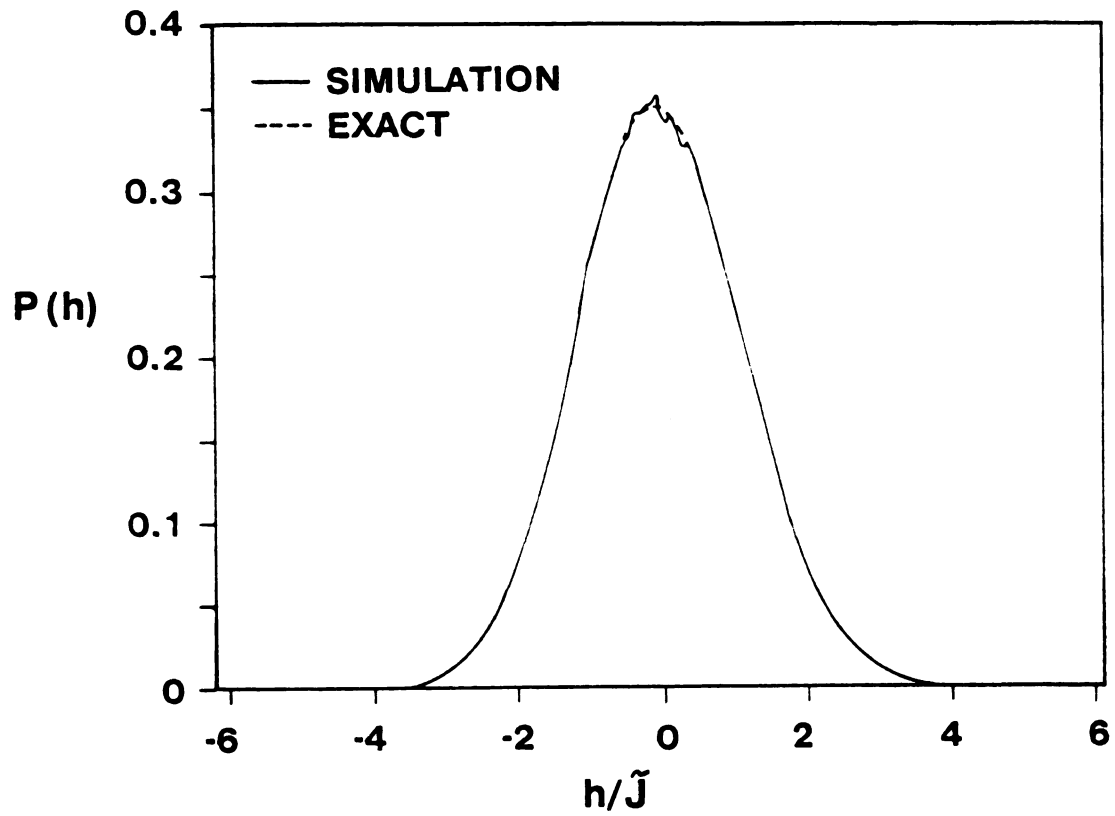
Figure 14. A comparison between the Monte Carlo simulation of the Sherrington-Kirkpatrick model and the analytic result: $T = 2T_{SG}$.
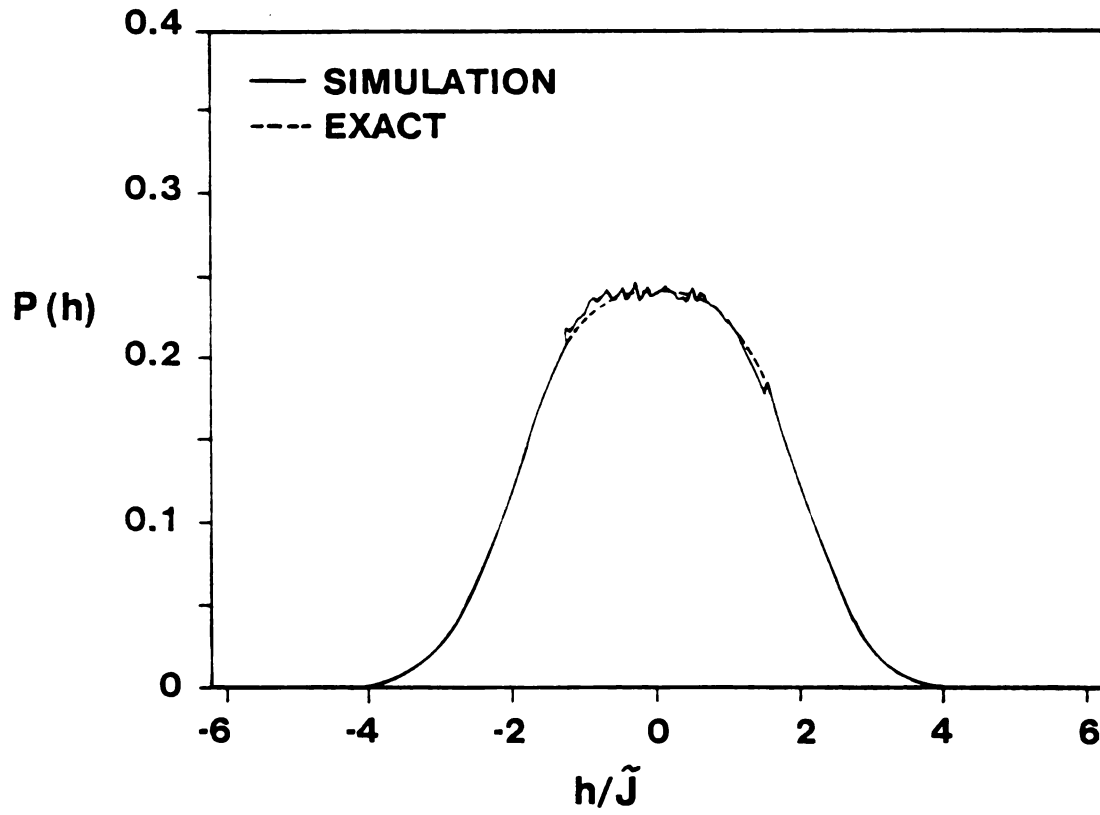
Figure 15. A comparison between the Monte Carlo simulation of the Sherrington-Kirkpatrick model and the analytic result: $T = T_{SG}$.
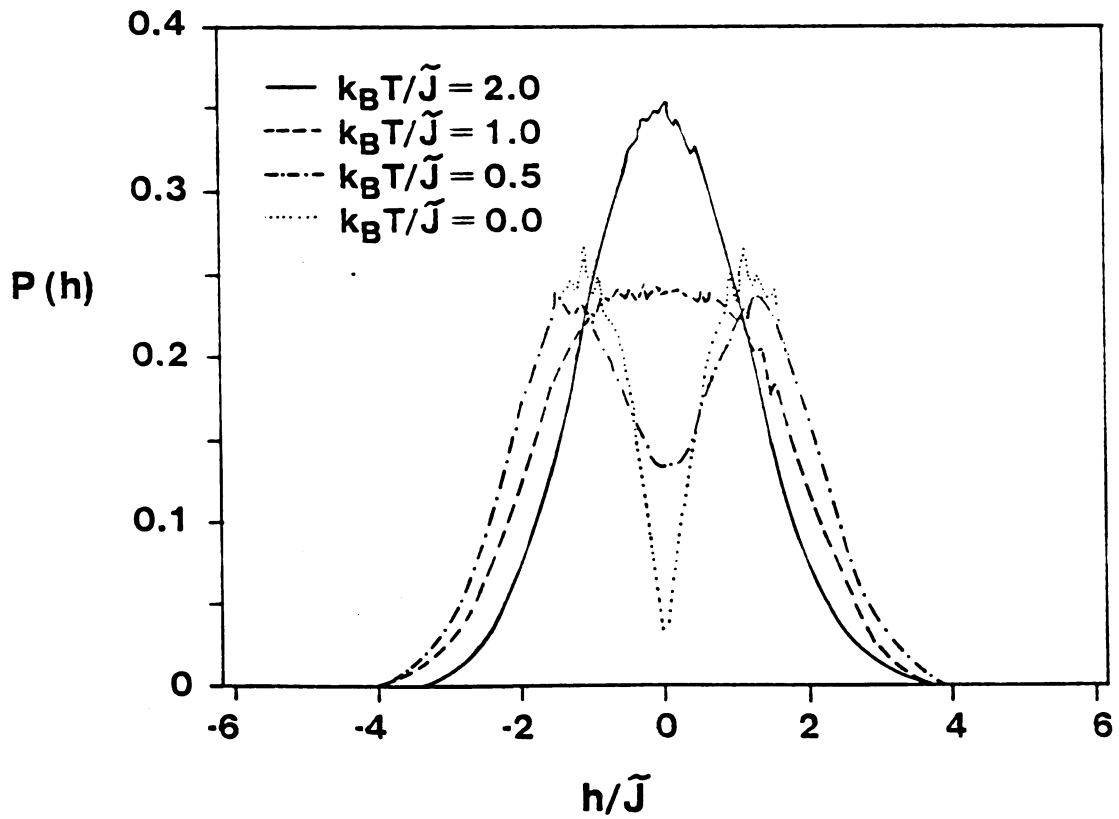
Figure 16. Results of the Monte Carlo simulations of the
Sherrington-Kirkpatrick model: P(h) at four dif-
ferent temperatures. The T=0 data has been
symmetrized.

$$P(h=0,T) = \frac{1}{\sqrt{2\pi}J} \exp(-\beta^2 J^2/2) \qquad (24)$$

so that at $T_{SG} = J/k_B$,

$$P(h=0,T_{SG}) = \frac{1}{\sqrt{2\pi}J} e^{-\frac{1}{2}} \qquad . \qquad (25)$$

It is also easily shown that

$$\frac{\partial P(h=0,T)}{\partial(k_B T)} \bigg|_{T_{SG}} = \frac{1}{\sqrt{2\pi}J^2} e^{-\frac{1}{2}} \qquad . \qquad (26)$$

Since it is believed that the specific heat and energy are

continuous at T_{SG} for this model, these values hold for just under

T_{SG} also. If one adds to this the assumption that

$$P(0,0) = 0 \qquad , \qquad (27)$$

there are three constriants on $P(h=0,T)$ for $0 \leq T \leq T_{SG}$. One solution,

but certainly not the only solution, is to try the linear form

$$P(h=0,T<T_{SG}) = \frac{1}{\sqrt{2\pi}J} e^{-\frac{1}{2}} \frac{k_B}{J} T \qquad . \qquad (28)$$

Figure 17 compares this function to the data from Monte Carlo simu-

lations. The deviation at $T = 0$ is probably, as discussed before,

a finite size effect. Attempts to study the size dependence in

the rest of the regime were not conclusive. It is clear, however,

that even if (28) is not exact, it is at least a good approximation.

It was noted in Chapter 5 that for the antiferromagnetic square

net below T_c, $P(h)$ is symmetric while $P_i(h)$ is not. That is, when

the phase transition occurs, a symmetry is broken so that there are

two distinct sublattices, one with a positively biased $P_i(h)$ and

the other with a negatively biased $P_i(h)$. One might expect a similar

symmetry breaking for this model. While an extensive study was not
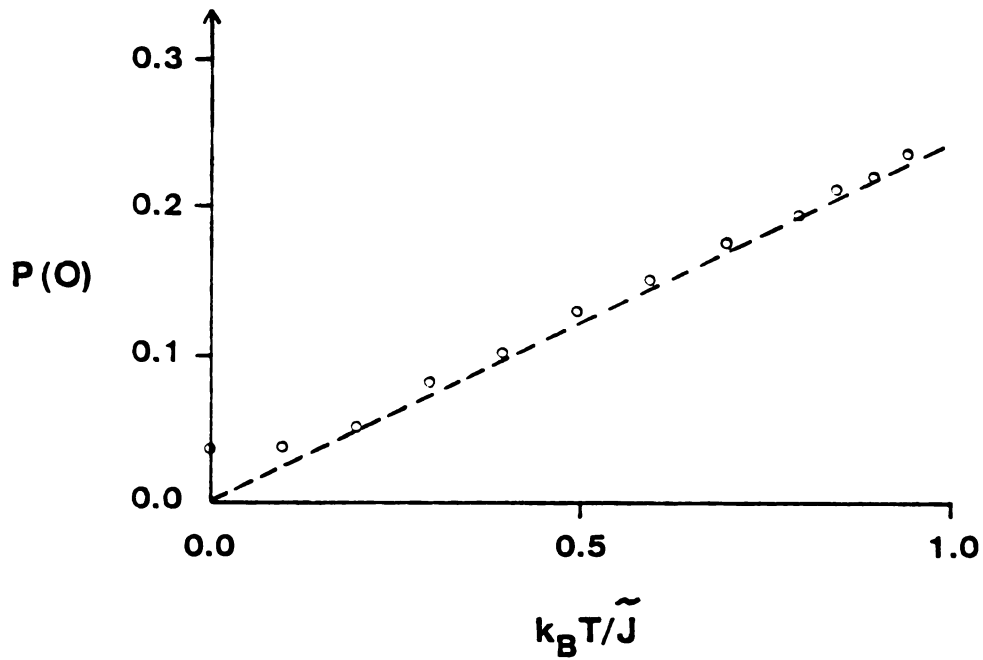
Figure 17. P(0) as a function of temperature in the spin
glass phase of the Sherrington-Kirkpatrick model.
Open circles indicate simulation results. The
dashed line represents the linear hypothesis.

made, a few simulations of a 540 spin system ($J_o = 0$) yield the tentative conclusion that

$$P_i(h) = P(h) \qquad T > T_{SG} \qquad (29)$$

$$P_i(h) \neq P(h) \qquad T < T_{SG} \qquad . \qquad (30)$$

The detailed nature of this broken symmetry is not as of yet clear, although one can say that it is substantially more complicated than the two sublattice state of the antiferromagnet.

Following the temperature development of P(h) has allowed the tracking of its development from a Gaussian function to a function with a hole in the center. It has been seen that the dip develops precisely at T_{SG} and the system very quickly establishes the large h states. Below about $T_{SG}/2$, most of the action in P(h) occurs in the small h region.

There has been some recent work (Mézard et. al. 1984) suggesting that the relevant order parameter in this system is not q (the Edwards-Anderson order parameter), nor is it q(x), a generalized probability function introduced by Parisi (1980a). Rather it has been suggested that the system is best described by a probability distribution governing the distribution q(x). That is, by performing a configurational average to calculate q(x), one is throwing away valuable information in the spin glass state. One might be concerned then that the Monte Carlo simulations performed configurational averages and that what should have been measured was the probability distribution of the distribution, P(h). However, it has been noted

earlier that one cannot calculate q directly from P(h); one needs
to know P_i(h) at all sites. Thus q is not expected to couple strongly
to P(h). It is not unreasonable that even though q and q(x) may
not be well defined thermodynamic variables, P(h) may nevertheless
be well defined for this model.

9. Future Work

While the nature of disorder in Ising systems has been examined here, the major development has been that of a new tool, $P(h)$, to study Ising systems at all temperatures. This function leads to exact thermodynamic results as well as having a measurable symmetric component.

An understanding of this function for a wide variety of Ising ferromagnets is in hand. However, only one disordered system, the Sherrington-Kirkpatrick spin glass model, has been studied. While some useful conclusions were drawn, it was not possible to determine which general characteristics of $P(h)$ were common to Ising spin glasses in general and which were peculiar to infinite range spin glasses. Therefore, it would be useful to look at an Ising spin glass model with short range interactions. It is reasonable to expect that a system that orders will have a dip at $h = 0$, but beyond that it is difficult to generalize on the basis of the Sherrington-Kirkpatrick model.

One can extend the definition of $P(h)$ for Ising systems to a $P(\vec{h})$ for classical XY and Heisenberg systems. While the relationship between this function and the inelastic neutron scattering law is not clear, inspection of the proof in Chapter 2 reveals that a similar relation between the energy and $P(\vec{h})$ should hold. It was crucial in that proof that all parts of the Hamiltonian commute with each other, and this is the case for these classical systems.

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Extension to these systems would allow for the simulation of a Heisenberg spin glass. One possibility would be the $Eu_xSr_{1-x}S$ system. Eu^{2+} ions have spin 7/2 and lie on an FCC lattice. They have ferromagnetic nearest neighbor interactions and antiferromagnetic next nearest neighbor interactions. EuS acts as a ferromagnet, but dilution with the nonmagnetic Sr^{2+} ions enhances the competition between the nearest and next nearest neighbor interactions, creating a spin glass at appropriate concentration and temperature. This system has been well studied both experimentally and by simulation (see, e.g., Krey 1981). To the extent that spin 7/2 can be approximated as classical, $Eu_xSr_{1-x}S$ then provides a prime candidate for studying the temperature dependence of $P(\vec{h})$ in a well characterized system. A connection between $S(\vec{k},\omega)$ and $P(\vec{h})$ could be extremely useful in comparing simulation results to experiment.

Another system worth investigating consists of classical XY spins on a triangular lattice with nearest neighbor antiferromagnetic interactions. A study by Lee et. al. (1984) indicates a very rich phase diagram in the H-T plane. With this single system it would be possible to sample several different phases.

It may also be possible to extend the definition of $P(\vec{h})$ to the spherical model (Berlin and Kac 1952). This would provide access to the well studied spherical infinite range spin glass model (Kosterlitz et. al. 1976).

A more difficult extension of this formalism is to quantum Heisenberg or XY models. Problems arise early on since the local field operator,

$$\vec{h}_i = \sum_j J_{ij} \vec{S}_j \qquad (1)$$

is not diagonalizable. Hence,

$$P_i(\vec{h}) = \langle \delta(\vec{h} - \vec{h}_i) \rangle \qquad (2)$$

is not well defined. Preliminary efforts to relate the Ising P(h) to $P(|\vec{h}|)$ or to $P(h_z)$ for quantum systems have not yielded a useful formalism. It could be that there exists a relation between the energy and some generalization of the Ising P(h) that is more complicated than a simple integral. Any such hypothesized relationship can be checked against the known results for the infinite quantum XY chain (see, e.g., Lieb et. al. 1961) or for finite length quantum Heisenberg systems (Bonner and Fisher 1964). An extension of the P(h) formalism to quantum systems, while difficult, has the potential for providing new insight into these models.

Appendix A.

Local Magnetic Field Distributions I.

Two-Dimensional Ising Models

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Two-Dimensional Ising Models

M. Thomsen[†]

Department of Physics and Astronomy

Michigan State University

East Lansing, MI 48824 U.S.A.

M. F. Thorpe[††]

Cavendish Laboratory, Madingley Road

Cambridge CB3 OHE, U.K.

T. C. Choy and D. Sherrington

Physics Department, Imperial College

London SW7 2BZ, U.K.

[†]Exxon Fellow

[††]Permanent address: Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48824, U.S.A.

Abstract

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 like 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.[1-5] Despite the fact that P(h) has a simple physical interpretation, it has <u>not</u> 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 <u>not</u> 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 around in the literature of the early 1960's[1-4] and are summarized by Southern.[5] 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 <u>symmetric</u> 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 <u>symmetric</u> part of P(h), if all the $H_i = 0$. Other thermodynamic quantities of interest, like 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 and <u>no other information about the system</u>. In the case where the $H_i \neq 0$, the energy, 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 net 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 to be 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 competing interactions in their ground or low-lying metastable states.[5] A similar minimum has been found in simulations of amorphous antiferromagnets.[7,3] Because of the interesting new results found for simple Ising models, we have deferred a discussion of more complex spin systems with competing interactions until a subsequent paper.[9]

II. GENERAL FORMALISM

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

$$H = -\frac{1}{2} \sum_{ij} J_{ij} \sigma_i \sigma_j - \sum_i H_i \sigma_i \tag{1}$$

where the J_{ij}, 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 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

$$H = - \sum_i h_i \sigma_i \tag{2}$$

where

$$h_i = \frac{1}{2} \sum_j J_{ij} \sigma_j + H_i \quad . \tag{3}$$

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

$$H = - h_i \sigma_i + H' \tag{4}$$

where

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

The first term in Eq. (4) contains <u>all</u> terms involving σ_i and other terms are lumped together in H'. Notice that h_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 <u>energy</u> of the system later in this section.

We consider the thermal average $< O \sigma_i >$ where O is any <u>operator</u> not involving site i;

$$< 0\sigma_i > = < \mathop{\mathrm{Tr}}_i \left[0\sigma_i \exp(\beta h_i \sigma_i) \right] / \mathop{\mathrm{Tr}}_i \left[\exp(\beta h_i \sigma_i) \right] >$$

$$= < 0 \tanh \beta h_i > . \tag{6}$$

Putting 0 equal to the unit operator we find that[2,3]

$$< \sigma_i > = < \tanh \beta h_i > = < \tanh \beta \left(\sum_j J_{ij} \sigma_j + H_i \right) > . \tag{7}$$

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.[2] Putting 0 equal to h_i in (6) leads to

$$< h_i \sigma_i > = < \sum_j J_{ij} \sigma_i \sigma_j + H_i \sigma_i >$$

$$= < h_i \tanh \beta h_i > \tag{8}$$

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

$$E_i = - < h_i \tanh \beta h_i >$$

$$= - \frac{1}{2} < (h_i + H_i) \tanh \beta h_i > . \tag{9}$$

The magnetization M and the energy E are given by

$$M = \sum_i < \sigma_i >$$

$$E = \sum_i E_i$$

(10)

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

$$P_i(h) = < \delta(h - h_i) >$$

(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 $P_i'(h)$ with only the internal field contribution counted;

$$P_i'(h) = < \delta(h - \sum_j J_{ij} \sigma_j) > = P_i(h - H_i) \quad .$$

(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)

$$< (\sum_j J_{ij} \sigma_i + H_i)^n > = \int h^n P_i(h) \, dh \quad ,$$

(14)

and, from (7) and (9),

$$< \sigma_i > = \int \tanh \beta h \, P_i(h) \, dh$$

(15)

$$E_i = - \frac{1}{2} \int h \tanh \beta h \, P_i(h) \, dh - \frac{1}{2} H_i < \sigma_i > \quad .$$

(16)

The distribution function $P(h)$ for the whole 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 βh, only the **antisymmetric** part $P_a(h)$ of $P(h)$ contributes to M;

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

(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)

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

(21)

and E can be calculated directly from $P(h)$ without any knowledge of the J_{ij}.

Because (h tanh βh) is an even function of h, only the symmetric part P_s(h) of

P(h) contributes to E ;

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

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

In this case the free energy F is given by

$$\beta F = -N \ln 2 + \int_{\beta_0}^{\beta} E \, d\beta .$$ (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

$$E = - \frac{N}{2} \int (h + H) \tanh \beta h \, P(h) \, dh$$ (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 like 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 play a special
role when the statistical mechanics is done via P(h). This point appears not to
have been appreciated by Klein and Brout[4] who attempted to write the free energy
as an integral over P(h) [see their equation (2.5)].

The function $P(h)$ contains more than just thermodynamic information; it is directly related to the inelastic neutron scattering cross section,[10]

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

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[11],

$$S(\vec{k},\omega) = \frac{1}{3\pi} \int_{-\infty}^{+\infty} e^{-i\omega t} \, dt \sum_i \langle \sigma_i^{\,+}\sigma_i^{\,-}(t) + \sigma_i^{\,-}\sigma_i^{\,+}(t) \rangle \; . \tag{27}$$

The time dependence of these operators is given by

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

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

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

Using equation (6), this can be rewritten as

$$S(\vec{k},\omega) = \frac{1}{2\pi} \int\limits_{-\infty}^{+\infty} e^{-i\omega t} \, dt \, \sum_i \langle \cos 2th_i + i \tanh \beta h_i \sin 2th_i \rangle$$

$$= \frac{1}{2\pi} \int\limits_{-\infty}^{+\infty} e^{-i\omega t} \, dt \, \sum_i (\cos 2th + i \tanh \beta h \sin 2th) \, P_i(h)dh$$

$$= \frac{N}{2} \left[P(\omega/2) + P(-\omega/2) \right] / \left[1 + \exp(-\beta\omega) \right] \quad , \tag{29}$$

which shows that the neutron scattering law provides a direct measurement of the __symmetric__ part $P_s(h)$ of $P(h)$;

$$S(\vec{k},\omega) = N \, P_s(\omega/2) / \left[1 + \exp(-\beta\omega) \right] \tag{30}$$

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

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

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

and if all the $H_i = 0$

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

Both (31) and (32) hold for arbitrary J_{ij}. The 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.[12] This is straightforward but does serve to illustrate some of the points made in the previous 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 ;

$$H = -\frac{1}{2} \sum_{ij} \sigma_i \sigma_j \tag{33}$$

where the sum goes over nearest neighbor pairs only and the factor ½ is to prevent double counting. In what follows we use a slightly modified form of the notation of Choy and Sherrington.[13] As all sites are equivalent we can ignore the distinction between $P_i(h)$ and $P(h)$. Therefore

$$P(h) = < \delta(h - \sum_{j=1}^{z} \sigma_j) > \tag{34}$$

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

$$P(h) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp(-ih\theta) \, d\theta < \exp(i \theta \sum_{j=1}^{z} \sigma_j) >$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp(-ih\theta) \, d\theta < \prod_{j=1}^{z} (1 + i \sigma_j \tan \theta) > \cos^z \theta \tag{35}$$

where we have used the an integral representation of the Dirac delta function with the usual convergence factors implied at $\pm\infty$.

Multiplying out the brackets in the product, this becomes

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

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

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

with

$$w_s = \frac{1}{2^z} \sum_{r=0}^{z} a_{rs}^z c_r \tag{38}$$

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

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} \exp(-ih\theta) \, d\theta \, \cos^{z-r} \theta \, \sin^r \theta \, i^r$$

$$= \frac{1}{2^z} \sum_{s=-z}^{z} a_{rs}^z \delta(h - s) \quad . \tag{39}$$

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 1. The c_r are correlation functions[13] defined by

$$c_r = \sum_{(ij\ldots\ell)} \langle \sigma_i \sigma_j \ldots \sigma_\ell \rangle \tag{40}$$

where the round brackets denote that only the <u>distinct</u> products of r operators among the z nearest neighbors are to be taken. If we label the z nearest neighbors of an atom <u>cyclically</u> from 1 to z, then for the linear chain

$$
\left.
\begin{aligned}
c_0 &= 1 \\[2ex]
c_1 &= \sum_{(i)} \langle \sigma_i \rangle = 2 \langle \sigma_1 \rangle \\[2ex]
c_2 &= \sum_{(ij)} \langle \sigma_i \sigma_j \rangle = \langle \sigma_1 \sigma_2 \rangle
\end{aligned}
\right\} \qquad (41)
$$

.

For the honeycomb lattice $(z = 3)$

$$
\left.
\begin{aligned}
c_0 &= 1 \\[2ex]
c_1 &= \sum_{(i)} \langle \sigma_i \rangle = 3 \langle \sigma_1 \rangle \\[2ex]
c_2 &= \sum_{(ij)} \langle \sigma_i \sigma_j \rangle = 3 \langle \sigma_1 \sigma_2 \rangle \\[2ex]
c_3 &= \sum_{(ijk)} \langle \sigma_i \sigma_j \sigma_k \rangle = \langle \sigma_1 \sigma_2 \sigma_3 \rangle
\end{aligned}
\right\} \qquad (42)
$$

.

For the square net ($z = 4$)

$$c_o = 1$$

$$c_1 = \sum_{(i)} \langle \sigma_i \rangle = 4 \langle \sigma_1 \rangle$$

$$c_2 = \sum_{(ij)} \langle \sigma_i \sigma_j \rangle = 4 \langle \sigma_1 \sigma_2 \rangle + 2 \langle \sigma_1 \sigma_3 \rangle$$

$$c_3 = \sum_{(ijk)} \langle \sigma_i \sigma_j \sigma_k \rangle = 4 \langle \sigma_1 \sigma_2 \sigma_3 \rangle$$

$$c_4 = \sum_{(ijk\ell)} \langle \sigma_i \sigma_j \sigma_k \sigma_\ell \rangle = \langle \sigma_1 \sigma_2 \sigma_3 \sigma_4 \rangle$$

$$\left. \right\rbrace \quad (43)$$

and for the triangular net ($z = 6$)

$$c_o = 1$$

$$c_1 = \sum_{(i)} \langle \sigma_i \rangle = 6 \langle \sigma_1 \rangle$$

$$c_2 = \sum_{(ij)} \langle \sigma_i \sigma_j \rangle = 6 \langle \sigma_1 \sigma_2 \rangle + 6 \langle \sigma_1 \sigma_3 \rangle + 3 \langle \sigma_1 \sigma_4 \rangle$$

$$c_3 = \sum_{(ijk)} \langle \sigma_i \sigma_j \sigma_k \rangle = 6 \langle \sigma_1 \sigma_2 \sigma_3 \rangle + 12 \langle \sigma_1 \sigma_2 \sigma_4 \rangle + 2 \langle \sigma_1 \sigma_3 \sigma_5 \rangle$$

$$c_4 = \sum_{(ijk\ell)} \langle \sigma_i \sigma_j \sigma_k \sigma_\ell \rangle = 6 \langle \sigma_1 \sigma_2 \sigma_3 \sigma_4 \rangle + 6 \langle \sigma_1 \sigma_2 \sigma_3 \sigma_5 \rangle$$
$$+ 3 \langle \sigma_1 \sigma_2 \sigma_4 \sigma_5 \rangle$$

$$c_5 = \sum_{(ijk\ell m)} \langle \sigma_i \sigma_j \sigma_k \sigma_\ell \sigma_m \rangle = 6 \langle \sigma_1 \sigma_2 \sigma_3 \sigma_4 \sigma_5 \rangle$$

$$c_6 = \sum_{(ijk\ell mn)} \langle \sigma_i \sigma_j \sigma_k \sigma_\ell \sigma_m \sigma_n \rangle = \langle \sigma_1 \sigma_2 \sigma_3 \sigma_4 \sigma_5 \sigma_6 \rangle$$

$$\left. \right\rbrace \quad (44)$$

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 $K = 2J$, where J has previously been set equal to one.

For the linear chain[14]

$$\left.\begin{array}{l} c_0 = 1 \\[10pt] c_1 = 0 \\[10pt] c_2 = \tanh^2 K \end{array}\right\} \tag{45}$$

so that from (38) we have

$$\left.\begin{array}{l} w_0 = \frac{1}{2}(1 - \tanh^2 K) \\[14pt] w_2 = w_{-2} = \frac{1}{4}(1 + \tanh^2 K) \end{array}\right\} \tag{46}$$

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

For the honeycomb lattice all the c_r can be expressed in terms of the reduced energy ε and the reduced magnetization m

$$\left.\begin{array}{l} \varepsilon = \langle \sigma_0 \sigma_1 \rangle \\[14pt] m = \langle \sigma_0 \rangle \end{array}\right\} \tag{47}$$

where σ_o is the spin at the site of interest. This is achieved by rewriting (6) as [15-18]

$$< 0 \; \sigma_o > \; = \; A < 0(\sigma_1 + \sigma_2 + \sigma_3) > \; + \; B < 0 \; \sigma_1 \; \sigma_2 \; \sigma_3 > \qquad (48)$$

where

$$\left. \begin{array}{l} A = \dfrac{1}{4} \left[\tanh 3K + \tanh K \right] \\[2ex] B = \dfrac{1}{4} \left[\tanh 3K - 3 \tanh K \right] \end{array} \right\} \qquad . \qquad (49)$$

Putting $0 = 1$ yields

$$< \sigma_1 \; \sigma_2 \; \sigma_3 > \; = \; m(1 - 3A) \; / \; 3 \qquad (50)$$

and putting $0 = \sigma_1$ yields

$$< \sigma_1 \; \sigma_2 > \; = \; (\varepsilon - A) \; / \; (2A + 3) \qquad . \qquad (51)$$

Combining all these results we find that[19]

$$\left. \begin{array}{l} h_{\pm 1} = \dfrac{1}{2} \left[\dfrac{3(\tanh 3K - \varepsilon)}{3 \tanh 3K - \tanh K} \quad \pm \quad \dfrac{3m(\tanh 3K - 1)}{\tanh 3K - 3 \tanh K} \right] \\[4ex] h_{\pm 3} = \dfrac{1}{2} \left[\dfrac{3\varepsilon - \tanh K}{3 \tanh 3K - \tanh K} \quad \pm \quad \dfrac{m(1 - 3 \tanh K)}{\tanh 3K - 3 \tanh K} \right] \end{array} \right\} \qquad (52)$$

The reduced energy ε can be written as an elliptic integral [12,13] and the reduced magnetization m is a known function[20] 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 $^{z}C_{\frac{1}{2}(z + h)} / 2^{z}$ so that at infinite temperature

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

As z gets large this 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 honeycomb lattice as shown in Fig. 1. At T_{c}, the values of w_{s} can be obtained by putting $\varepsilon_{c} = 4\sqrt{3}/9$, $m_{c} = 0$ 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 $(T_{c} - T)^{3}$ with $\beta = 1/8$. 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 α (through ε) and β (through m) in Eqs. (52). All the critical exponents of interest can be obtained from these two.[21]

As the coordination increases, so does the number of correlation functions that must be known. For the <u>square net</u>, the three spin correlation function is still proportional to the reduced magnetization via a relationship similar to (50).[15-18] However, it is necessary to compute two other independent even spin correlation functions as they <u>cannot</u> all be reduced to just ε via relations like (48) and (49). These involve evaluating elliptic integrals. For the <u>triangular net</u> 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[22]. The details are complicated and are given elsewhere[23]. While the magnetization is given by Potts[24], the remain-

ing odd spin correlations can be found using the methods of Barry, Múnera and Tanaka[25]. 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. 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[13] by two of us for the <u>antiferro-magnetic</u> 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 their ferromagnetic counterparts as they are both bichromatic. Using 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 so $P(h)$ for the whole 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 get the staggered magnetization it would be necessary to know $P_i(h)$ at the up and down sites <u>separately</u> 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 $w_o = 0$ 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

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

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

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

and is shown in Fig. 4 for <u>ferromagnetic</u> interactions in the honeycomb, square net and triangular net. At high temperatures $v \to 1$ 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 <u>antiferromagnetic</u> interactions, the quantity v keeps going up as the temperature is lowered. For two sublattice antiferromagnets, like 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 monotonically from 1 at high temperatures to z at zero temperature. For the triangular net antiferromagnet v increases from 1 at high temperatures to 1.097809 at zero temperature.[13]

Finally in this section, we consider the neutron scattering law (26) and (30). The scattering only takes place at discrete energies. In Table 2 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 $\omega = 8$.[10] This corresponds to flipping a spin where all its nearest neighbors are parallel. As the temperature is raised, other peaks have nonzero weights.

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 3 nearest neighbors are up and 1 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 $\frac{1}{2}$ (additional to (31) and (32)) which shows that the total integrated intensity is independent of temperature, as is clear from Table 2;

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

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.

ACKNOWLEDGMENTS

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

$$H = -\frac{1}{2} \sum_{ij} J_{ij} S_i^z S_j^z - \sum_i H_i S_i^z \quad . \tag{A1}$$

Note that this J_{ij} differs from the J_{ij} in the main text by a factor 4 in the limit when the spin becomes ½. This is because we found it more convenient to use Pauli operators in the main text. In a similar way there is a factor 2 different in the definition of H_i. Rather than redefine these quantities we prefer to start from (A1). 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 (A1) is

$$H = -\sum_i h_i S_i^z \tag{A2}$$

where

$$h_i = \frac{1}{2} \sum_j J_{ij} S_j^z + H_i \tag{A3}$$

but the most useful for our purposes is

$$H = -h_i S_i^z + H' \tag{A4}$$

where

$$h_i = \sum_j J_{ij} S_j^z + H_i \quad . \tag{A5}$$

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

The thermal average $< 0 \; S_i^z >$ where 0 is <u>any operator</u> not involving site i is given by

$$< 0 \; S_i^z > = < \text{Tr} \, [0 \; S_i^z \exp(\beta h_i S_i^z)] \, / \, \text{Tr} \, [\exp(\beta h S_i^z)] > \atop i \qquad\qquad\qquad\qquad i$$

$$= < 0 \; B_{S_i}(\beta h_i) > \quad , \tag{A6}$$

where the <u>modified Brillouin function</u>[26] is defined by

$$B_S(x) = (S + \tfrac{1}{2}) \coth \left[(S + \tfrac{1}{2}) x \right] - \tfrac{1}{2} \coth (x/2) \quad ,$$

and hence

$$B_{\frac{1}{2}}(x) = \tfrac{1}{2} \tanh x/2.$$

Putting 0 equal to the unit operator in (A6) we find that

$$< S_i^z > = < B_{S_i}(\beta h_i) > \quad ; \tag{A7}$$

putting 0 equal to h_i leads to

$$< h_i S_i^z > = < \sum_j J_{ij} S_i^z S_j^z + H_i S_i^z >$$

$$= < h_i B_{S_i}(\beta h_i) > \quad . \tag{A8}$$

There is the same problem with the factor ½ in obtaining the energy as before and we have

$$E_i = - < h_i B_{S_i} (\beta h_i) >$$

$$= - \frac{1}{2} < (h_i + H_i) B_{S_i} (\beta h_i) > \quad . \tag{A9}$$

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

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

$$P(h) = [\sum_i B_{S_i} (\beta h) P_i(h)] / [\sum_i B_{S_i} (\beta h)] \tag{A11}$$

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

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

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 $B(\beta h)$.

From (7) and (9) we have

$$< s_i^z > = \int B_{S_i} (\beta h) P_i(h) dh \tag{A15}$$

and

$$E_i = - \frac{1}{2} \int h B_{S_i} (\beta h) P_i(h) dh - \frac{1}{2} H_i < s_i^z > \quad . \tag{A16}$$

The magnetization M is given by

$$M = N \int B (\beta h) P(h) dh \tag{A18}$$

and, as before, it is <u>not</u> 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 zero, then from (10) and (A16)

$$E = - \frac{N}{2} \int h \, \beta \, (\beta h) \, P(h) \, dh \quad , \tag{A21}$$

the free energy F is given by

$$\beta F = - \sum_i \ln(2S_i + 1) - \int_0^\beta E \, d\beta \quad , \tag{A24}$$

and equation (21) generalizes in the obvious way with $\tanh \beta h \to \beta(\beta h)$.

The inelastic neutron scattering cross section is given by

$$S(\vec{k},\omega) = \frac{2}{\tau} \int_{-\infty}^{+\infty} e^{-i\omega t} \, dt \sum_{ij} \exp\left[i \, \vec{k} \cdot (\vec{R}_i - \vec{R}_j)\right] < S_i^x \, S_j^x(t) > \tag{A26}$$

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

$$S(\vec{k},\omega) = \frac{1}{2\pi} \int_{-\infty}^{-\infty} e^{-i\omega t} \, dt \sum_i < S_i^+ \, S_i^- \, (t) + S_i^- \, S_i^+ \, (t) >$$

$$= 2 \sum_i \left[P_i(\omega) + P_i(-\omega) \right] \, \beta_{S_i}(\beta\omega) \, / \, \left[1 - \exp(-\beta\omega) \right]$$

$$= 2N \left[P(\omega) + P(-\omega) \right] \, \beta(\beta\omega) \, / \, \left[1 - \exp(-\beta\omega) \right] \tag{A29}$$

or

$$S(\vec{k},\omega) = 4NP_s(\omega) \, \beta(\beta\omega) \, / \, [\, 1 - \exp(-\beta\omega) \,] \quad . \tag{A30}$$

These lead to the sum rules

$$\frac{1}{2N} \int S(\vec{k},\omega) \quad \frac{1 - \exp(-\beta\omega)}{2 \, \beta(\beta\omega)} \quad d\omega = 1 \tag{A31}$$

and if all the $H_i = 0$

$$\frac{1}{3} \int S(\vec{k},\omega) \, [\, 1 - \exp(-\beta\omega) \,] \quad \omega \, d\omega = -E \quad . \tag{A32}$$

These sum rules are very general and can be proved without introducing $P(h)$. The second one is particularly easy to establish as the magnitude of the spin does not enter explicitly.
Using the identity[27]

$$< A(0) \, B(t) > = < B(t - i\beta) \, A(0) >$$

for any operators A,B; we see that

$$S(\vec{k},\omega) \, [\, 1 - \exp(-\beta\omega) \,]$$

$$= \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{-i\omega t} \, dt \sum_{ij} \exp\left[i \, \vec{k} \cdot (\vec{R}_i - \vec{R}_j) \right] < S_i^+ S_j^-(t) + S_i^- S_j^+(t)$$

$$- S_j^-(t) S_i^+ - S_j^+(t) S_i^- >$$

Only the diagonal terms contribute for Ising models so that

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

$$\left. + \left[S_i^-, S_i^+(t) \right] \right> .$$

Therefore

$$\int S(\vec{k},\omega) \left[1 - \exp(-\beta\omega) \right] \omega d\omega$$

$$= -i \sum_i \left< \left[S_i^+, \frac{\partial S_i^-}{\partial t} \right] + \left[S_i^-, \frac{\partial S_i^+}{\partial t} \right] \right>$$

$$= \sum_i \left< \left[S_i^+, h_i S_i^- \right] - \left[S_i^-, h_i S_i^+ \right] \right>$$

$$= 4 \sum_i \left< h_i S_i^z \right>$$

$$= -\beta E$$

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$$\int P(h) \, dh = 1 \quad , \quad \int h \tanh \beta h \, P(h) \, dh = 3\epsilon \quad ;$$

$$\int h \, P(h) \, dh = 3m \text{ and } \int \tanh \beta h \, P(h) \, dh = m \quad .$$

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

by including a prefactor of S, and a factor S in both arguments so that $B_s(x) = S \cdot B_s(Sx)$. This saves having to write a lot of factors S_i in subsequent formulae.

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Table Captions

Table 1

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

Table 2

The 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 $2w_3/[1 + \exp(-\beta\omega)]$ of the five delta functions.

Table 1

z = 2

s\r	0	1	2
2	1	1	1
0	2	0	-2
-2	1	-1	1

z = 3

s\r	0	1	2	3
3	1	1	1	1
1	3	1	-1	-3
-1	3	-1	-1	3
-3	1	-1	1	-1

z = 4

s\r	0	1	2	3	4
4	1	1	1	1	1
2	4	2	0	-2	-4
0	6	0	-2	0	6
-2	4	-2	0	2	-4
-4	1	-1	1	-1	1

z = 6

s\r	0	1	2	3	4	5	6
6	1	1	1	1	1	1	1
4	6	4	2	0	-2	-4	-6
2	15	5	-1	-3	-1	5	15
0	20	0	-4	0	4	0	-20
-2	15	-5	-1	3	-1	-5	15
-4	6	-4	2	0	-2	4	-6
-6	1	-1	1	-1	1	-1	1

Table 2

ω\T	T = 0	T = T_c	T = ∞
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

Figure Captions

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.

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.

Fig. 4   The fluctuation v in the local field as a function of reduced

temperature T/T_c for ferromagnetic interactions in the honeycomb,
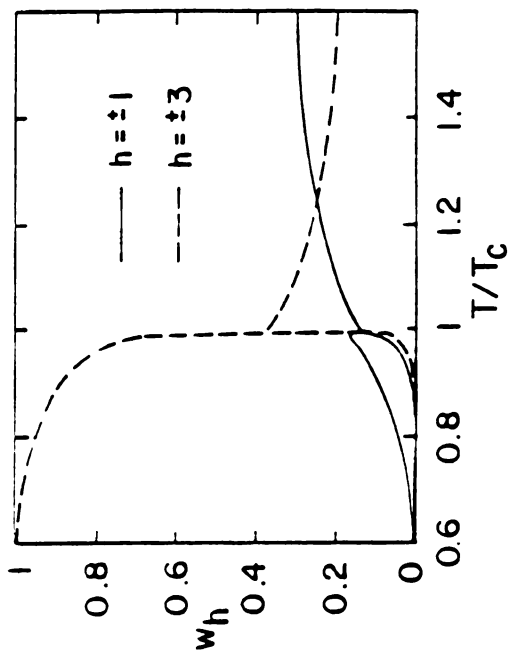
square net and triangular net.

Figure 1

	T=0	T=T_c	T=∞
w_4	1	$3x/2 = 0.325483$	$1/16 = 0.0625$
w_2	0	$1-4x = 0.132045$	$1/4 = 0.25$
w_0	0	$5x-1 = 0.084943$	$3/8 = 0.375$
w_{-2}	0	$1-4x = 0.132045$	$1/4 = 0.25$
w_{-4}	0	$3x/2 = 0.325483$	$1/16 = 0.0625$

Figure 2

Legend:
- h=0
- h=±2
- h=±4
- h=±6

w_h vs T/T_c: axis values 0.6, 0.8, 1, 1.2, 1.4; vertical 0.2, 0.4, 0.6, 0.8
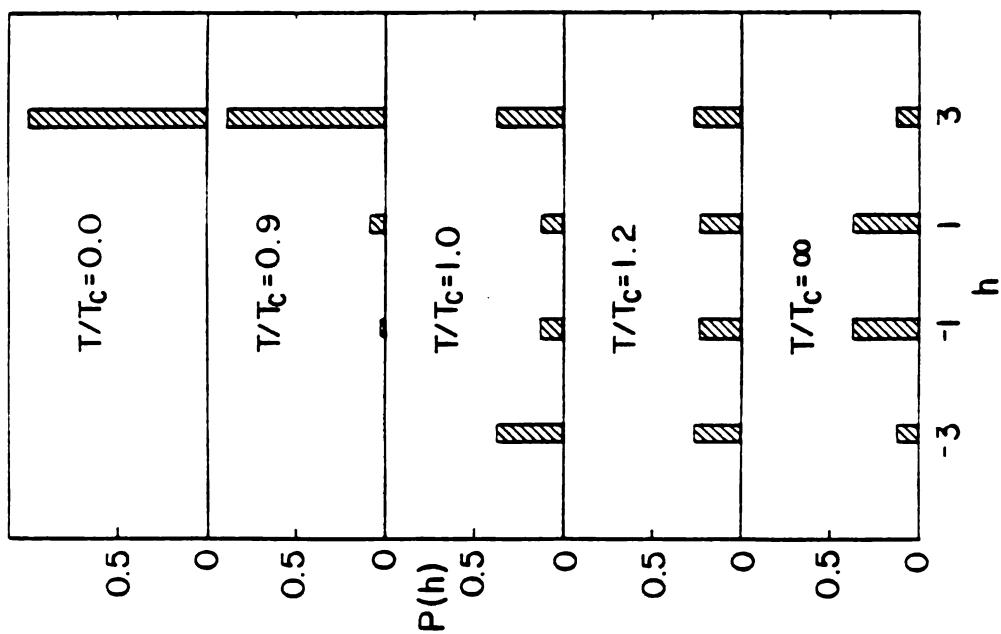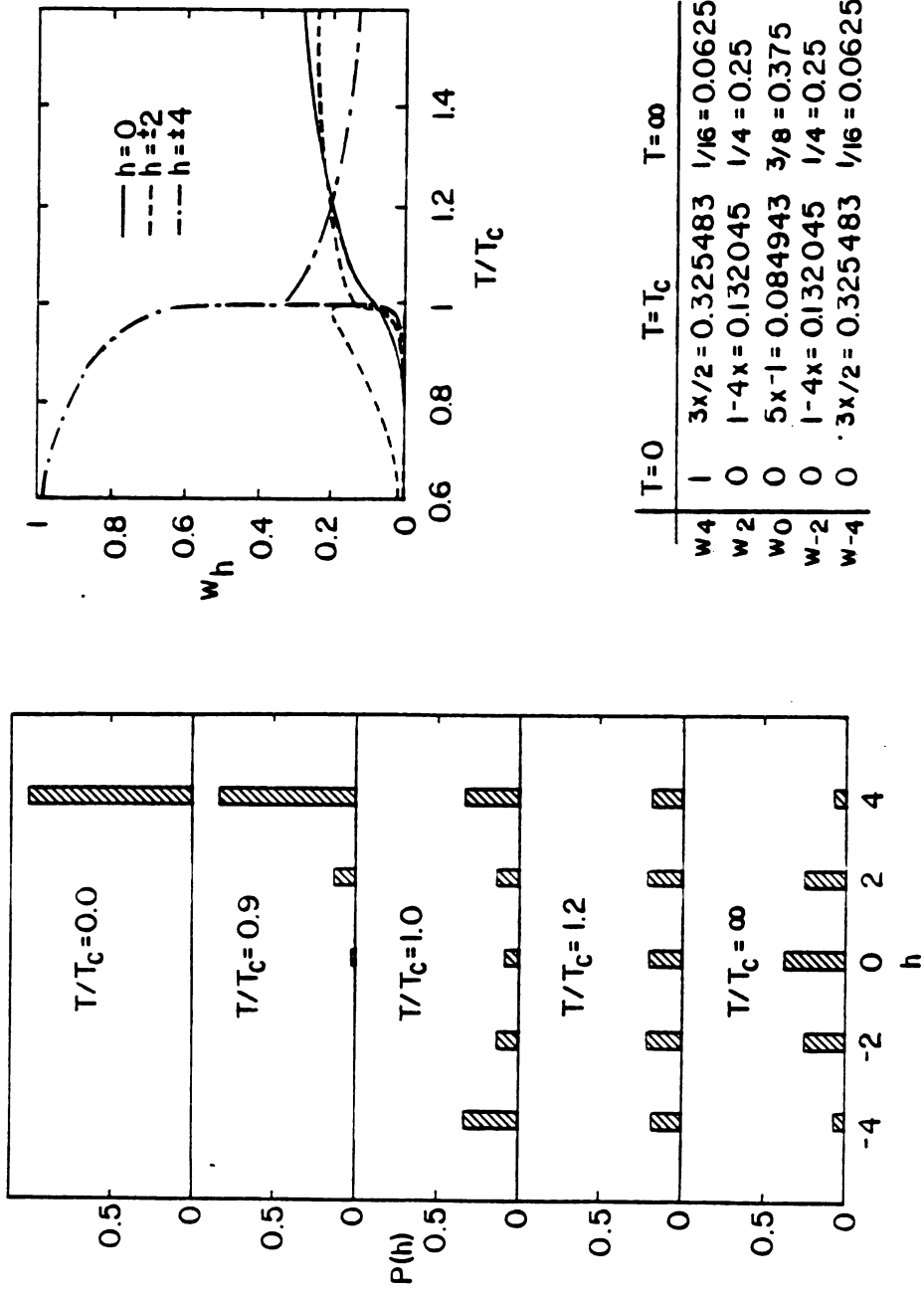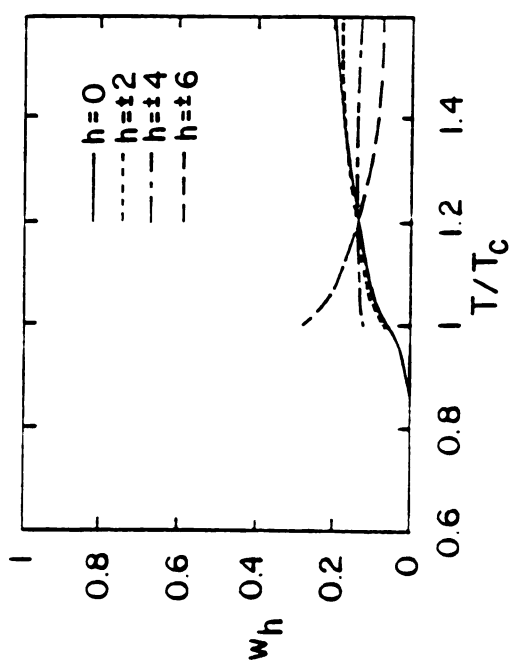
	T=0	T=T_c	T=∞
w_6	1	0.275842	$1/64 = 0.015625$
w_4	0	0.122099	$3/32 = 0.09375$
w_2	0	0.072446	$15/64 = 0.234375$
w_0	0	0.059225	$5/16 = 0.3125$
w_{-2}	0	0.072446	$15/64 = 0.234375$
w_{-4}	0	0.122099	$3/32 = 0.09375$
w_{-6}	0	0.275842	$1/64 = 0.015625$

$p(h)$ vs h for $T/T_c = 0.0$, $T/T_c = 1.0$, $T/T_c = 1.2$, $T/T_c = \infty$; h axis: -6, -4, -2, 0, 2, 4, 6; vertical 0, 0.5
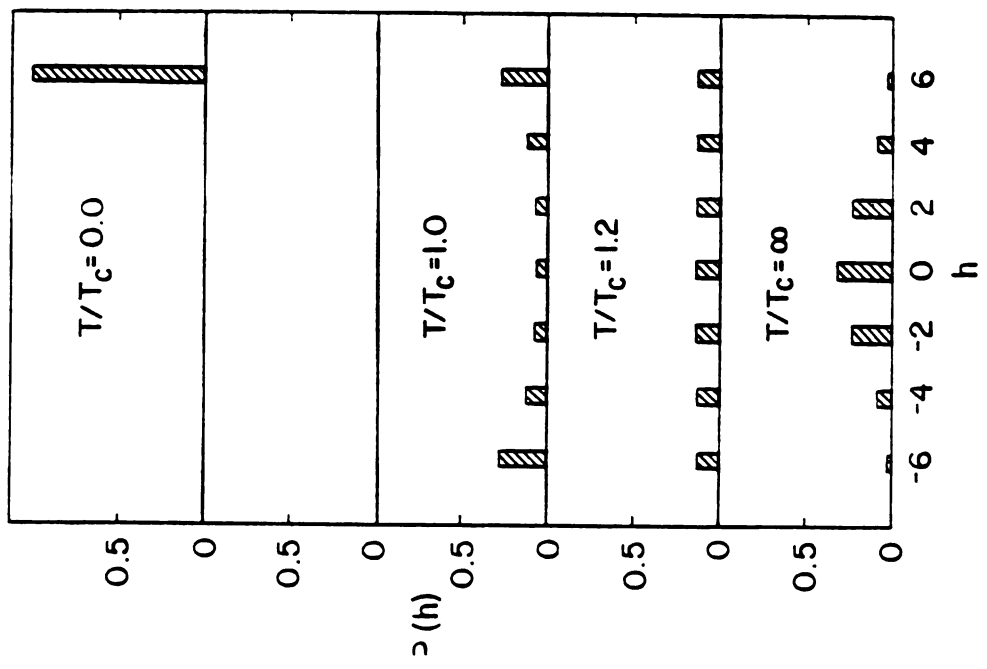
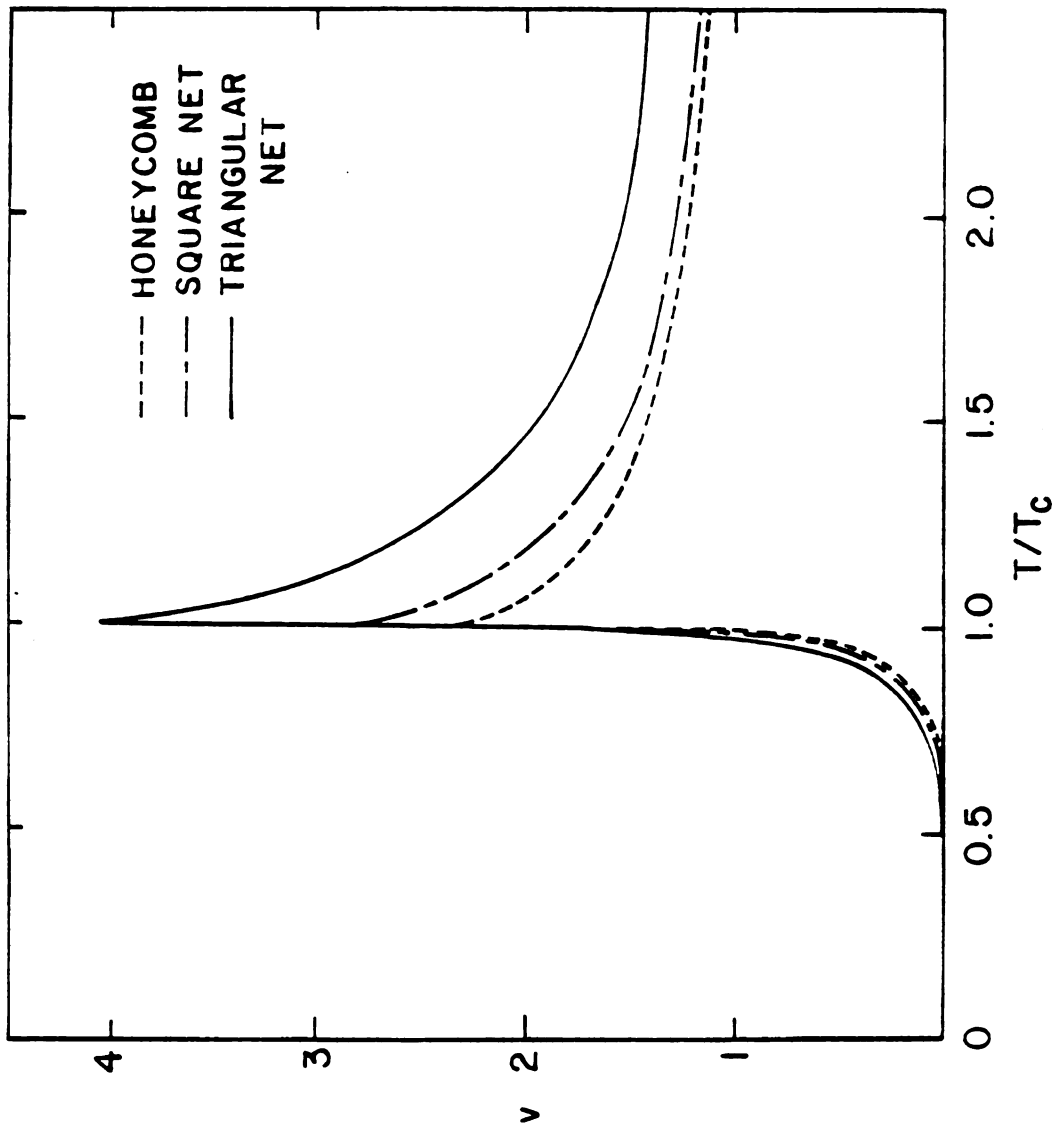Figure 3

HONEYCOMB
SQUARE NET
TRIANGULAR
NET

T/T_c

Figure 4

Appendix B. Some 2D Correlations

In this appendix, some details are given for the calculation
of correlation functions needed in Chapter 5. First the calculation
of a four spin correlation on the square net will be discussed
and then the second part of this appendix will discuss the one honey-
comb correlation needed.

As mentioned in Chapter 5, most of the square net correlations
needed are found in Montroll, Potts, and Ward (1963), the exception
being the four spin correlation. Rather than rederive or rewrite
what has already appeared in MPW, their notation will be adopted here
and then enough information will be presented so that in conjunction
with MPW, the interested reader can calculate this particular
correlation.

MPW number the spins using rectangular coordinates so that
in their notation, what is needed is

$$C_4 \equiv \langle \sigma_{12} \sigma_{10} \sigma_{21} \sigma_{01} \rangle \quad . \tag{1}$$

It is useful to rewrite this as

$$C_4 = \langle \sigma_{12} \sigma_{11} \sigma_{11} \sigma_{10} \sigma_{21} \sigma_{11} \sigma_{11} \sigma_{01} \rangle \quad . \tag{2}$$

In analogy to MPW equation (49), one obtains the form

$$C_4 = z^4 \, P(Y^{-1} + Q) \, P(Y) \tag{3}$$

where

$$z = \tanh(\beta J) \quad , \tag{4}$$

$P(A)$ stands for the Pfaffian of matrix A, and Y and Q are matrices

which are defined below. It can easily be shown, as in MPW equation (50), that

$$P(Y) = x^4 \qquad (5)$$

where

$$x = z^{-1} - z \qquad . \qquad (6)$$

The matrix $(Y^{-1}+Q)$ can be written down almost directly. The columns and rows of the matrix are labelled in MPW's notation to aid the reader in seeing how this particular form came about:

$$(Y^{-1}+Q) = \qquad (7)$$

	(0,1)U	(1,1)D	(1,1)U	(2,1)D	(1,0)R	(1,1)L	(1,1)R	(1,2)L
(0,1)U	0	A	0	B	C	D	-D	-C
(1,1)D	-A	0	F	0	-D	E	E	-D
(1,1)U	0	-F	0	A	-D	-E	E	D
(2,1)D	-B	0	-A	0	C	-D	-D	C
(1,0)R	-C	D	D	-C	0	A	0	B
(1,1)L	-D	-E	E	D	-A	0	F	0
(1,1)R	D	-E	-E	D	0	-F	0	A
(1,2)L	C	D	-D	-C	-B	0	-A	0

The six different entries are defined by:

$$A = (1-3z^2)F_{10} - z(1+z^2)F_{00} - x^{-1} \qquad (8)$$

$$B = (1-z^2)F_{20} - z(1+z^2)F_{10} - 2z^2F_{11} \qquad (9)$$

$$C = 2zF_{10} + z^2F_{00} - F_{11} \qquad (10)$$

$$D = (1-z^2)F_{10} - zF_{11} - zF_{00} \qquad (11)$$

$$E = -F_{00} + 2zF_{10} + z^2F_{11} \qquad (12)$$

$$F = z(1+z^2)F_{10} + 2z^2 F_{11} - (1-z^2)F_{00} \qquad (13)$$

The F_{ij}'s depend on elliptic integrals and are defined in the appendix of MPW. In practice they are calculated numerically before the Pfaffian is taken. Since the Pfaffian is the square root of the determinant, the desired correlation is

$$C_4 = z^4 x^4 [DET(Y^{-1}+Q)]^{\frac{1}{2}} \quad . \qquad (14)$$

Turning to the honeycomb lattice, one starts with the partition function (Green and Hurst 1964)

$$Z = c \cdot [\cosh^3(\beta J)]^N \cdot Z' \qquad (15)$$

or

$$\ln Z = \ln c + 3N \ln \cosh(\beta J) + \ln Z' \qquad (16)$$

where c is a constant and

$$\ln Z' = \frac{1}{8\pi^2} \int_0^{2\pi} d\theta \int_0^{2\pi} d\phi \; \ln\{1 + 3y^4$$
$$- 2y^2(1-y^2)[\cos\theta + \cos\phi + \cos(\theta-\phi)]\} \; ; \qquad (17)$$
$$y \equiv \tanh(\beta J) \quad . \qquad (18)$$

Noting that, unlike the convention used in Chapter 5, Green and Hurst double count their bonds,

$$\langle \sigma_0 \sigma_1 \rangle = \tanh(\beta J) + \frac{1}{3} \frac{\partial \ln Z'}{\partial(\beta J)}$$
$$= \tanh(\beta J) + \frac{1}{3} \operatorname{sech}^2(\beta J) \frac{\partial \ln Z'}{\partial y} \quad . \qquad (19)$$

One can show

$$\frac{\partial \ln Z'}{\partial y} = \frac{1}{8\pi^2} \int_0^{2\pi} d\theta \int_0^{2\pi} d\phi \; \frac{A + B\cos\theta}{C + D\cos\theta + E\sin\theta} \qquad (20)$$

with

$$A = 12y^3 \tag{21}$$

$$B = -3(4y - 8y^3) \tag{22}$$

$$C = (1+3y^4) - 2y^2(1-y^2)\cos\phi \tag{23}$$

$$D = -2y^2(1-y^2)(1+\cos\phi) \tag{24}$$

$$E = -2y^2(1-y^2)\sin\phi \quad . \tag{25}$$

Stephenson (1964) pointed out that

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \, \frac{\exp(in\theta)}{C + D\cos\theta + E\sin\theta} = \alpha^n(C^2 - D^2 - E^2)^{-\frac{1}{2}} \quad ; \tag{26}$$

$$\alpha \equiv [(C^2 - D^2 - E^2)^{\frac{1}{2}} - C]/(D - iE) \quad . \tag{27}$$

This relation is used to perform one of the integrals in equation (20), giving

$$\frac{\partial \ln Z'}{\partial y} = \frac{1}{4\pi} \int_0^{2\pi} d\theta \left[A + \frac{BCD}{D^2+E^2} \right] \cdot (C^2-D^2-E^2)^{-\frac{1}{2}}$$

$$+ \frac{1}{4\pi} \int_0^{2\pi} d\theta \, \frac{BD}{D^2+E^2} \quad . \tag{28}$$

Now $\langle \sigma_0 \sigma_1 \rangle$ is expressed (through equations (28) and (19)) in terms of a pair of single integrals, a more suitable form for obtaining numerical results.

Appendix C. Details of Monte Carlo Simulations

The basis for the Monte Carlo simulations of the spin glass and ferromagnetic systems was the algorithm introduced by Metropolis et. al. (1953). Given a system at a temperature T, the algorithm generates an ensemble of <u>states</u> $\{S_i\}$, which can be used to determine the thermal average of properties of the system. From the ith member of an ensemble, S_i, the next member is generated by creating a new state S^t. In Ising systems this is typically done by flipping one spin in S_i. Given

$$E^t = \text{energy of } S^t \qquad (1)$$

$$E_i = \text{energy of } S_i \qquad (2)$$

$$\Delta E = E^t - E_i \qquad , \qquad (3)$$

S_{i+1} is defined in the following way:

1) $\Delta E < 0 \rightarrow S_{i+1} = S^t$

2) $\Delta E > 0$:

   Choose a random number p such that $0 < p < 1$.

   a) $p < \exp(-\Delta E/k_B T) \rightarrow S_{i+1} = S^t$

   b) $p > \exp(-\Delta E/k_B T) \rightarrow S_{i+1} = S_i$.

The initial state, S_1, may be chosen at random or taken to be the last state generated by a simulation at a nearby temperature. In either case, one generally excludes some of the initial members of the ensemble from the averaging process, which is equivalent to allowing the system to come into equilibrium before making

a measurement.

In the simulations described below, a system change consists of flipping a single spin. A Monte Carlo step is defined by N attempted spin flips, where N is the number of spins in the system.

Most of the rest of this appendix will describe the spin glass simulation, with some details of the ferromagnetic simulations appearing at the end.

The Hamiltonian for the Ising Sherrington-Kirkpatrick model is

$$H = -\tfrac{1}{2} \sum_{i \neq j} J_{ij} \sigma_i \sigma_j \tag{4}$$

where as usual the superscript, z, is suppressed for convenience. Let σ_j^p denote the value of σ_j in the pth state of the ensemble. Suppose a trial state is arrived at by flipping the ith spin so that its new value is $\sigma_i^t = -\sigma_i^p$. Then

$$
\begin{aligned}
\Delta E &= -\sum_j J_{ij} \sigma_j^p (\sigma_i^t - \sigma_i^p) \\
&= 2 \left(\sum_j J_{ij} \sigma_j^p \right) \sigma_i^p \\
&= 2 h_i^p \sigma_i^p \quad .
\end{aligned}
\tag{5}
$$

At this point, the difficulties involved in doing a simulation of the SK model are apparent. First one has to have stored in an accessible way, the $N(N-1)/2$ independent values of J_{ij}. Second one must be able to calculate h_i^p, which has N-1 terms, efficiently. Modifying an array packing scheme suggested by Jacobs and Rebbi (1981), these difficulties can be overcome to a degree.

Neglecting the fact that the J_{ii}'s are zero, the information

describing this system is binary in nature:

$$J_{ij} = \pm 1$$

$$\sigma_i^p = \pm 1 \quad .$$

The $J_{ii} = 0$ problem is easily treated separately in the computer program. Rahter than taking an entire computer word, which is sixty bits on a Cyber 750 system, to store one value of, say, σ_i^p, one can store sixty spin values in one word. These individual bits can be accessed and modified through such FORTRAN commands as SHIFT, OR, XOR, and AND. The last three correspond to the logical functions whose operations are defined below.

AND(A,B)   OR(A,B)   XOR(A,B)

B\A	0	1
0	0	0
1	0	1

B\A	0	1
0	0	1
1	1	1

B\A	0	1
0	0	1
1	1	0

(6)

The corresponding FORTRAN functions, operating on two words, perform these logical operations on a bit by bit basis. For example,

$$AND(1,7) = 1 \tag{7}$$

because $7 = 111_2$ and $1 = 001_2$. Only in the least significant bit (LSB) do both words have a 1 so that 1 appears only in the LSB of the answer. In fact, a projection operator, projecting out the LSB of a word M, can be defined by

$$P_1(M) = AND(1,M) \quad . \tag{8}$$

The SHIFT(M,N_b) function performs a cyclic permutation of the bits of word M, N_b bits to the left. Hence one can define a projection operator for the Nth LSB of a word M by

$$P_N(M) = AND(SHIFT(1,N-1),M) \quad . \tag{9}$$

Similar use of the OR function will allow the definition of a particular bit in a word. Hence each bit of the sixty bit word is both definable and accessible.

The values of N spins can be stored in an array with N/60 words. This is why N was taken to be a multiple of 60 for the spin glass simulations. Similarly, one could store the $N(N-1)/2$ values of J_{ij} in an array of approximately $N^2/120$ words. However, for ease in calculation of the h_i^p , the full matrix of J_{ij} values was stored in an array of $N^2/60$ words. A simple rescaling of the energy allows one to let a binary 0 represent -1 in the physical system.

The calculation of the h_i^p is achieved by noting that when J_{ij} and σ_j^p have the same value, σ_j^p contributes positively to h_i^p , while negative contributions arise when J_{ij} and σ_j^p have opposite values. Hence the product $J_{ij}\sigma_j^p$ can be represented by the XOR function. Furthermore, the FORTRAN XOR function will perform these multiplications sixty at a time. What remains is to sum up over all j. Apparently there is no easy way of doing this, and so each bit of the product word is projected out separately and the results are added as integers.

The memory limit of the Cyber 750, 127,000 words, is reached for an SK system of about 2400 spins. The practical computation limit, based on cpu time, is 2040 spins, while systems of 1020 spins were sufficiently large for most calculations. A typical measurement at one temperature involved averaging over four 1020 spin systems; that is, four different J_{ij} matrices were generated.

Each system was brought into equilibrium by running for sixty Monte Carlo steps and then thermal averages were performed over two hundred steps. Such a run requires about 37,000 words of storage and five minutes of cpu time on the Cyber 750.

Not all of the advantages to using binary methods for simulating the infinite range spin glass model hold for simulating short range ferromagnetic systems. First, for uniform nearest neighbor systems, it is more efficient to devise a way of locating nearest neighbors than to store the entire J_{ij} array. Secondly, the number of multiplications involved in calculating h_i no longer scales with the system size. However, with long range order being important in ferromagnetic systems, it is useful to be able to work with larger systems, particularly near T_c. Hence the amount of central memory associated with storing the spin configurations becomes important.

There is a trade-off between efficiency of use of storage space and ease with which spin values can be accessed. One compromise between these two optimizations is to utilize the sixty bit length of each word as an extra dimension. As an example, the spin configuration of a 30×30×30 simple cubic lattice was stored in an array of 30×30 words, with each word in the array containing information about 30 spins.

The chief difficulty in programming a Monte Carlo simulation of these ferromagnetic systems is finding an efficient way to locate the nearest neighbors of a spin. For a D dimensional simple cubic system, the method is intuitive. A spin located at

$$(i_1, i_2, \ldots, i_D) \quad ,$$

where i_D refers to the bit number in word

$$(i_1, i_2, \ldots i_{D-1}) \quad ,$$

has nearest neighbors located at

$$(i_1 \pm 1, i_2, \ldots, i_D),$$

$$(i_1, i_2 \pm 1, \ldots, i_D) \quad , \quad \ldots.$$

A body centered cubic lattice, in three dimensions, can be represented by two interpenetrating simple cubic lattices. Locations on the BCC lattice are thus described by four integers:

$$(L, i_1, i_2, i_3)$$

where $L=1,2$ is the sublattice number and

$$(i_1, i_2, i_3)$$

locates the position on that sublattice. With this decomposition it is straightforward to write out a table which describes the nearest neighbors of a given spin. Similarly, a face centered cubic structure can be decomposed into four simple cubic sublattices and a diamond structure into eight. The nearest neighbor locations which are obtained in this decomposition are shown in Table 2. The periodic boundary conditions used in these simulations are imposed with the aid of modular arithmetic.

Typical runs on ferromagnetic systems began with 1000 Monte Carlo steps to bring the system into equilibrium. This was followed by 1000 steps (2000 steps at T_c) during which thermal averages were computed.

Table 2. Nearest neighbor locations for three dimensional lattices.

BCC

Site	Nearest Neighbors
$(1,i,j,k)$	$(2,i,j,k)$ $(2,i-1,j,k)$ $(2,i,j-1,k)$ $(2,i,j,k-1)$ $(2,i-1,j-1,k)$ $(2,i-1,j,k-1)$ $(2,i,j-1,k-1)$ $(2,i-1,j-1,k-1)$
$(2,i,j,k)$	$(1,i,j,k)$ $(1,i+1,j,k)$ $(1,i,j+1,k)$ $(1,i,j,k+1)$ $(1,i+1,j+1,k)$ $(1,i+1,j,k+1)$ $(1,i,j+1,k+1)$ $(1,i+1,j+1,k+1)$

FCC

Site	Nearest Neighbors
$(1,i,j,k)$	$(2,i,j,k)$ $(2,i-1,j,k)$ $(2,i,j,k-1)$ $(2,i-1,j,k-1)$ $(3,i,j,k)$ $(3,i-1,j,k)$ $(3,i,j-1,k)$ $(3,i-1,j-1,k)$ $(4,i,j,k)$ $(4,i,j-1,k)$ $(4,i,j,k-1)$ $(4,i,j-1,k-1)$
$(2,i,j,k)$	$(1,i,j,k)$ $(1,i+1,j,k)$ $(1,i,j,k+1)$ $(1,i+1,j,k+1)$ $(3,i,j,k)$ $(3,i,j-1,k)$ $(3,i,j,k+1)$ $(3,i,j-1,k+1)$ $(4,i,j,k)$ $(4,i+1,j,k)$ $(4,i,j-1,k)$ $(4,i+1,j-1,k)$
$(3,i,j,k)$	$(1,i,j,k)$ $(1,i+1,j,k)$ $(1,i,j+1,k)$ $(1,i+1,j+1,k)$ $(2,i,j,k)$ $(2,i,j+1,k)$ $(2,i,j,k-1)$ $(2,i,j+1,k-1)$ $(4,i,j,k)$ $(4,i+1,j,k)$ $(4,i,j,k-1)$ $(4,i+1,j,k-1)$
$(4,i,j,k)$	$(1,i,j,k)$ $(1,i,j+1,k)$ $(1,i,j,k+1)$ $(1,i,j+1,k+1)$ $(2,i,j,k)$ $(2,i-1,j,k)$ $(2,i,j+1,k)$ $(2,i-1,j+1,k)$ $(3,i,j,k)$ $(3,i-1,j,k)$ $(3,i,j,k+1)$ $(3,i-1,j,k+1)$

DIAMOND

Site	Nearest Neighbors
$(1,i,j,k)$	$(5,i,j-1,k)$ $(6,i-1,j-1,k-1)$ $(7,i-1,j-1,k)$ $(8,i,j-1,k-1)$
$(2,i,j,k)$	$(5,i,j-1,k)$ $(6,i,j-1,k)$ $(7,i,j-1,k)$ $(8,i,j-1,k)$
$(3,i,j,k)$	$(5,i,j,k)$ $(6,i,j,k-1)$ $(7,i,j-1,k)$ $(8,i,j-1,k-1)$
$(4,i,j,k)$	$(5,i,j,k)$ $(6,i-1,j,k)$ $(7,i-1,j-1,k)$ $(8,i,j-1,k)$
$(5,i,j,k)$	$(1,i,j+1,k)$ $(2,i,j+1,k)$ $(3,i,j,k)$ $(4,i,j,k)$
$(6,i,j,k)$	$(1,i+1,j+1,k+1)$ $(2,i,j+1,k)$ $(3,i,j,k+1)$ $(4,i+1,j,k)$
$(7,i,j,k)$	$(1,i+1,j+1,k)$ $(2,i,j+1,k)$ $(3,i,j+1,k)$ $(4,i+1,j+1,k)$
$(8,i,j,k)$	$(1,i,j+1,k+1)$ $(2,i,j+1,k)$ $(3,i,j+1,k+1)$ $(4,i,j+1,k)$

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