Transverse susceptibility for Ising systems: Direct calculation from the local magnetic field distribution

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It has previously been reported that, for Ising systems, the energy, magnetization, and neutron scattering function can be calculated directly from $P(h)$, the local magnetic field distribution. In this paper it is shown that, in addition, one may also calculate the linear transverse susceptibility $\chi_\perp$ directly from $P(h)$. With the use of earlier calculations of $P(h)$, $\chi_\perp$ for the Sherrington-Kirkpatrick model is obtained analytically above T_g and is obtained below T_g from Monte Carlo simulations, where T_g is the spin-glass transition temperature. It is speculated that $\chi_\perp$ may be nearly linear in temperature below T_g. Simple cubic ferromagnetic Ising systems in two, three, and four dimensions are also discussed.

I. INTRODUCTION

The local-magnetic-field distribution, $P(h)$, has been shown to contain detailed thermodynamic information about Ising[1] and classical m-vector[2] systems. In addition, for Ising systems, the neutron scattering function, $S(\mathbf{k},\omega)$, is given by the product of the symmetric part of $P(h)$ and a thermal factor.[1] A neutron polarized perpendicularly to the Ising system's ordering direction interacts with a spin by attempting to flip it, the difficulty in flipping being directly related to the local field acting on that spin. The close relationship between $S(\mathbf{k},\omega)$ and $P(h)$ is thus not surprising. However, a small external transverse field interacts with individual spins in much the same way, and hence one might expect to find information about the transverse susceptibility, $\chi_\perp$, contained in $P(h)$. In this paper, a relationship between these two functions is developed.

Fisher showed that $\chi_\perp$ can be expressed in terms of a finite number of local correlation functions for a spin-$\frac{1}{2}$ Ising model.[3] It also has been demonstrated that a combination of linear-response theory with transfer matrix techniques will yield $\chi_\perp$ for Ising chains of arbitrary spin S.[4] More recently, Wang *et al.*[5] have developed a linked-cluster-expansion calculation of $\chi_\perp$ for $S=\frac{1}{2}$ systems and have applied it to a ferromagnetic fcc system.

In Sec. II of this paper, it is shown that linear-response theory can be used with the $P(h)$ formalism previously developed[1] and the result is a simple expression for $\chi_\perp$, which makes the explicit the origin of the particular combinations of correlation functions appearing in earlier calculations of this susceptibility. In Sec. III, $\chi_\perp$ is examined for a pure ferromagnetic system on a square net, a simple cubic lattice, a four-dimensional hypercubic lattice, and in the mean-field limit. While in two dimensions results have been obtained[3] analytically by Fisher, in three and four dimensions $\chi_\perp$ is now obtained numerically using results from Monte Carlo calculations of $P(h)$ presented in an earlier paper.[2] Section IV contains a discussion of $\chi_\perp$ for the Sherrington-Kirkpatrick spin-glass model.

II. ANALYTIC DEVELOPMENT

For simplicity, a spin-$\frac{1}{2}$ model will be considered although analogous equations can be developed for $S>\frac{1}{2}$ systems. The Hamiltonian is of the form

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

where

$$H_0=-\tfrac{1}{2}\sum_{i,j}J_{ij}\sigma_i^z\sigma_j^z-\mu_{\parallel}b_{\parallel}\sum_j\sigma_j^z \tag{2}$$

and

$$H_1=-\mu_\perp b_\perp\sum_j\sigma_j^x , \tag{3}$$

and we have assumed $J_{ij}=J_{ji}$ and, for $S>\frac{1}{2}$, $J_{ii}=0$.

It has been shown previously, by using linear-response theory, that to first order in the transverse field, $b_\perp$,[4]

$$\langle\sigma_i^x\rangle=\mu_\perp b_\perp\mathrm{Tr}\{\int_0^\beta d\tau\exp[-(\beta-\tau)H_0]\sigma_i^x\exp(-\tau H_0)\sigma_i^x\}/\mathrm{Tr}[\exp(-\beta H_0)] . \tag{4}$$

As usual, β denotes $(k_BT)^{-1}$.

It is now useful to define formally the local-field *operator* h_i:

$$h_i=\sum_j J_{ij}\sigma_j^z+\mu_{\parallel}b_{\parallel} . \tag{5}$$

The Hamiltonian H_0 can then be split into two pieces,

$$H_0=-h_i\sigma_i^z+H_0' , \tag{6}$$

where H_0' does not contain the operator σ_i^z. Rewriting σ_i^x in terms of raising and lowering operators, and using

$$[H_0',\sigma_i^x]=0 , \tag{7}$$

one finds that

$$\exp(\tau H_0)\sigma_i^x \exp(-\tau H_0)\sigma_i^x = \exp(-2\tau h_i \sigma_i^z) , \quad (8)$$

and hence,

$$\langle \sigma_i^x \rangle = \mu_\perp b_\perp \int_0^\beta \langle \exp(-2\tau h_i \sigma_i^z) \rangle d\tau , \quad (9)$$

where $\langle \cdots \rangle$ indicates a thermal average with respect to H_0.

The properties of the σ^z operator allow Eq. (9) to be written as

$$\langle \sigma_i^x \rangle = \mu_\perp b_\perp \int_0^\beta \langle \cosh(2\tau h_i) - \sigma_i^z \sinh(2\tau h_i) \rangle d\tau . \quad (10)$$

It has been shown in earlier papers (see, e.g., Ref. 1) that σ_i^z in the thermal average on the right-hand side of Eq. (10) can be replaced by $\tanh(\beta h_i)$. After this replacement, integration and some simplification yield

$$\langle \sigma_i^x \rangle = \mu_\perp b_\perp \langle \tanh(\beta h_i)/h_i \rangle \quad (11)$$

so that the linear transverse susceptibility is

$$\chi_\perp / \mu_\perp^2 = \sum_i \langle \tanh(\beta h_i)/h_i \rangle . \quad (12)$$

The temperature-dependent local magnetic field distribution is defined by[1]

$$P(h) = \frac{1}{N} \sum_i \langle \delta(h - h_i) \rangle , \quad (13)$$

where N is the number of spins in the system. With this definition,

$$\chi_\perp / N\mu_\perp^2 = \int dh\, P(h) \tanh(\beta h)/h . \quad (14)$$

Equation (14) is the desired expression for $\chi_\perp$. One can see that all of the local correlation functions which determine $\chi_\perp$ are contained in $P(h)$. This result is quite general, holding for finite parallel field and arbitrary interactions J_{ij}, provided only that $J_{ij} = J_{ji}$.

For the case of general spin S and total Hamiltonian,[6]

$$H = -\tfrac{1}{2} \sum_{i,j} J'_{ij} S_i^z S_j^z - \mu'_\parallel b'_\parallel \sum_j S_j^z - \mu'_\perp b'_\perp \sum_j S_j^x , \quad (15)$$

where we must now also require $J_{ii} = 0$, one finds

$$\chi_\perp / N(\mu'_\perp)^2 = \int dh\, P(h) \mathscr{B}_S(\beta h)/h , \quad (16)$$

where $\mathscr{B}_S$ is the modified Brillouin function which is defined by[1]

$$\mathscr{B}_S(x) = (S + \tfrac{1}{2}) \coth[(S + \tfrac{1}{2})x] - \tfrac{1}{2}\coth(\tfrac{1}{2}x) . \quad (17)$$

To avoid confusion with factors of 2 involved in switching between σ notation and the $S = \frac{1}{2}$ case of Eq. (16), the rest of this paper shall focus on spin-$\frac{1}{2}$ Ising systems in the σ notation, and hence Eq. (14) will be used for the transverse susceptibility.

As might be expected, $\chi_\perp$ can be directly related to the neutron scattering function. Using the previously established result,[1]

$$S(\mathbf{k},\omega) = \frac{N}{2} \frac{P(\omega/2) + P(-\omega/2)}{1 + \exp(-\beta\omega)} , \quad (18)$$

it follows that

$$\chi_\perp / \mu_\perp^2 = \int dh \frac{1 - \exp(-2\beta h)}{h} S(\mathbf{k}, 2h) . \quad (19)$$

Various limiting expressions for the susceptibility can be obtained from Eq. (14). From the normalization property of $P(h)$ it is straightforward to show that the high-temperature limit of $\chi_\perp$ is the Curie susceptibility,

$$\lim_{T \to \infty} \chi / N\mu^2 = \beta . \quad (20)$$

If at zero temperature there is not a macroscopic number of local fields of zero magnitude, then the zero-temperature limit yields

$$\lim_{T \to 0} \chi_\perp / N\mu_\perp^2 = \langle 1/|h| \rangle . \quad (21)$$

For a uniform (nearest-neighbor) ferromagnet (or an antiferromagnet on a bipartite lattice) of coordination q and in zero external field,

$$\lim_{T \to 0} \chi_\perp / N\mu_\perp^2 = 1/|J|q . \quad (22)$$

The last expression is, in fact, valid for general S.

It has been previously noted that for certain systems, e.g., the antiferromagnet triangular net,[7] the one-dimensional antiferromagnet in a compensating field,[8] and dilute one-dimensional systems,[9] the transverse susceptibility diverges at zero temperature. These systems all share the common property of a finite fraction of sites, W_0, having a local field of zero at $T = 0$. For such systems, it is this fraction of sites, W_0, which dominate the low-temperature behavior of the susceptibility:

$$\lim_{T \to 0} \chi_\perp / N\mu_\perp^2 = W_0 \beta . \quad (23)$$

III. FERROMAGNETIC SYSTEMS

The transverse susceptibility for Ising systems with uniform nearest-neighbor interactions on a linear chain and on a square net may be obtained analytically from Eq. (14) and previously published exact calculations of $P(h)$.[1] These reproduce the results obtained earlier by Fisher.[3] Since $P(h)$ can be calculated explicitly on ferromagnetic Bethe lattices of coordination z up to ten,[2] $\chi_\perp$ can also be obtained for these systems. In practice, however, the calculation increases rapidly in complexity with increasing z. The mean-field limit,[10] however, can be quickly calculated. Taking as the Hamiltonian,

$$H = \frac{\tilde{J}}{N} \sum_{i=1}^{N} \sum_{j(\neq i)} \sigma_i \sigma_j \quad (24)$$

which has a phase transition at

$$k_B T_c = \tilde{J} , \quad (25)$$

the mean-field magnetization is given by

$$\begin{aligned} m &= \tanh(\beta \tilde{J} m), \quad T < T_c \\ &= 0, \quad T > T_c . \end{aligned} \quad (26)$$

It has been shown that[2]

$$P(h) = \delta(h - \tilde{J} m) , \quad (27)$$

from which follows

$$\chi_\perp / N\mu_\perp^2 = \beta, \quad T > T_c$$
$$\chi_\perp / N\mu_\perp^2 = \tilde{J}^{-1}, \quad T < T_c . \tag{28}$$

Returning to the case of finite dimension, Monte Carlo simulations have been developed to obtain numerical results for $P(h)$ for three- and four-dimensional simple cubic systems with nearest-neighbor ferromagnetic interactions.[2] Using these results, $\chi_\perp$ may be calculated directly. Figure 1 shows $\chi_\perp$, normalized by its zero-temperature value, as a function of temperature for these generalized simple cubic systems in 2, 3, 4, and infinite dimensions, the latter being the mean-field limit. While a singularity in the slope at T_c is expected, these simulations in three and four dimensions are not sufficiently precise to study this region in detail. It is clear that the peak in $\chi_\perp$ is moving towards a lower temperature as the dimension is increased, although it may never cross T_c. Finally, the decrease in peak height and the sharpening of the peak with increasing dimension are both consistent with the approach to the mean-field limit.

IV. THE SHERRINGTON-KIRKPATRICK MODEL

The Sherrington-Kirkpatrick (SK) model[11] is an infinite-range spin-glass model with Hamiltonian

$$H = -\sum_{(ij)} J_{ij}\sigma_i\sigma_j , \tag{29}$$

where the sum is over all pairs (ij). The J_{ij} are independently distributed random bonds with mean J_0/N, taken to be zero here, and variance J^2/N, N being the number of sites.

A transition from the paramagnetic phase to the spin glass occurs at

$$k_B T_g = J . \tag{30}$$

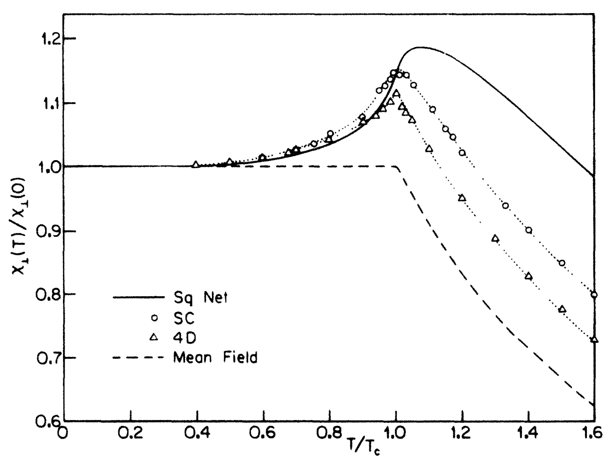

FIG. 1. The transverse susceptibility as a function of temperature for simple cubic (SC) lattices in 2, 3, and 4 dimensions and in the mean-field limit. The results in 3 and 4 dimensions are approximate (see the text) and the dotted lines are to guide the eye.

Above T_g, $P(h)$ is given by[12]

$$P(h) = \frac{1}{\sqrt{2\pi}}\frac{1}{J}\cosh(\beta h)\exp(-h^2/2J^2)\exp(-\beta^2 J^2/2) . \tag{31}$$

Inserting this into Eq. (14) and using

$$\frac{\sinh(\beta h)}{h} = \int_0^\beta d\beta' \cosh(\beta' h) \tag{32}$$

to transform the integral over all h to a finite integral over β', one finds[13]

$$\chi_\perp / N\mu_\perp^2 = \exp(-\beta^2 J^2/2) \int_0^\beta d\beta' \exp(\beta'^2 J^2/2) . \tag{33}$$

As has previously been noted,[12] the temperature derivative of $P(h)$ is expected to be continuous at T_g in the SK model. Thus continuity in the temperature derivative of $\chi_\perp$ is also expected, and one can use the derivative at T_g to approximate $\chi_\perp$ below T_g. It is interesting to note that

$$\left.\frac{\partial}{\partial(k_B T)}\frac{J\chi_\perp}{N\mu_\perp^2}\right|_{T=T_g} = \frac{\chi_\perp(T_g)}{N\mu_\perp^2} - \frac{1}{J} \tag{34}$$

so that a straight line extrapolation of $J\chi_\perp / N\mu_\perp^2$ from T_g would intersect the $T=0$ axis at 1.

Although an analytic calculation of $P(h)$ is not available below T_g, numerical results are, having been obtained from Monte Carlo simulations.[12] Numerical estimates of $\chi_\perp$ may therefore be obtained in the spin-glass phase. However, because of the long relaxation time associated with the SK model, it is believed that these simulations overestimate $P(h=0)$. Since $\chi_\perp$ is very sensitive to this value at low temperatures, it is likewise to be expected that these numerical results for $\chi_\perp$ in the low-temperature regime lie above their true values.

In Fig. 2, $\chi_\perp$ as a function of temperature is plotted. As

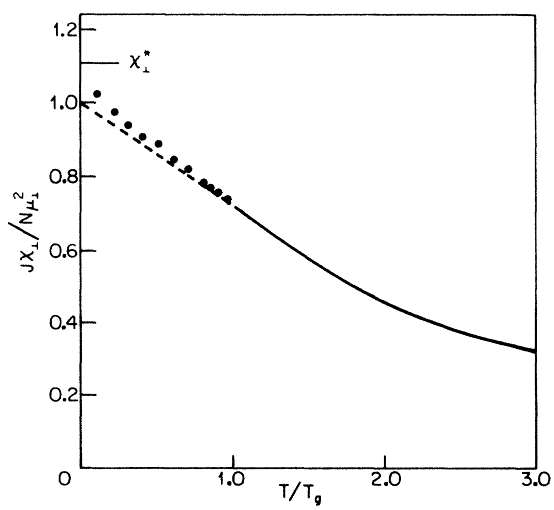

FIG. 2. The transverse susceptibility of the Sherrington-Kirkpatrick model. Results below T_g are approximate and the dashed line shows the linear extrapolation from T_g (see the text). The zero-temperature upper-bound $\chi_\perp^*$ is defined in Eq. (38).

the temperature is lowered below T_g the linear extrapolation provides a reasonable fit to the data until $T < T_g/2$. In light of previous comments, it is not unreasonable to expect the exact function to lie even closer to the extrapolation.

This approximate "freezing" of $\partial \chi_\perp / \partial T$ below T_g is reminiscent of the approximate freezing of $\partial P(0)/\partial T$ below T_g.[12] Given that the latter is believed *not* to be exact and given the close relationship between $\chi_\perp$ and $P(0)$, one might expect that the apparent freezing of $\partial \chi_\perp/\partial T$ is also *not* exact.

Thouless, Anderson, and Palmer have argued that at $T=0$ and for small $|h|$,[14]

$$P(h) \simeq A\,|h|\,, \tag{35}$$

where

$$A = \tfrac{1}{2}[(2\ln 2 + 1)/3 + (\ln 2)^{1/2}]^{-1}\,. \tag{36}$$

An upper bound to $\chi_\perp(0)$ may be obtained from this by assuming

$$\begin{aligned} P(h) &\simeq A\,|h|\,, \quad |h| < A^{-1/2} \\ &\simeq 0, \quad |h| > A^{-1/2}\,. \end{aligned} \tag{37}$$

This yields

$$J\chi_\perp(0)/N\mu_\perp^2 < \chi_\perp^* = 2A^{1/2} \simeq 1.108 \tag{38}$$

or about 10% higher than the value obtained from the linear extrapolation.

V. CONCLUSION

It has been shown that the transverse susceptibility may be obtained from the distribution of local magnetic fields for a quite general class of Ising systems. At sufficiently low temperatures, $\chi_\perp$ can serve as a direct measure of $P(h=0)$. By exploiting previous calculations of $P(h)$, $\chi_\perp$ has been obtained for a variety of Ising systems. Perhaps the most interesting result is the approximate freezing of $\partial\chi_\perp/\partial T$ in the spin-glass phase of the Sherrington-Kirkpatrick model. Whether or not a similar phenomenon will occur in finite-range Ising spin glasses is not yet clear and is the subject of current investigation. A candidate for experimental analysis of this issue is $Fe_{0.55}Mg_{0.45}Cl_2$, an Ising-like system which is believed to exhibit a mixed antiferromagnetic and spin-glass phase.[15]

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