Linear transverse susceptibility of Ising systems

Mark Jarrell and E. Loh, Jr.
Department of Physics, University of California, Santa Barbara, California 93106
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The transverse susceptibility of Ising systems is measured using Monte Carlo methods and low-variance estimators. Data are given for a spin-$\frac{1}{2}$ model on an fcc lattice and for a spin-1 (Blume-Capel) model, with different local anisotropies, on a cubic lattice. In each case a sharp peak is found just above the transition temperature. Real-time dynamics may also be studied. A low-variance Monte Carlo estimator is given for an Ising system having an arbitrary spin and lattice structure.

Ising systems have been studied quite thoroughly as model systems for a variety of classical phenomena and as nontrivial examples for testing theoretical techniques. Surprisingly, however, little work has been done on measuring the transverse susceptibility of such systems. Analytic solutions exist in one[1] and two[2] dimensions. In three dimensions, experimental work[3,4] finds cusplike behavior, which cannot be explained by simple approximations, such as mean-field theory, which ignore fluctuations. Some progress has been made by $1/z$ expansions,[5] with z the number of nearest neighbors, and, especially, by linked-cluster expansions.[6,7] The problem is of particular interest since it involves a quantum observable (transverse susceptibility) in a clearly classical system (zero transverse field). In this paper the linear transverse susceptibility is measured for both spin-$\frac{1}{2}$ and spin-1 Ising systems on three-dimensional lattices ranging from 8^3–20^3 sites. For the spin-1 (Blume-Capel[8]) model, the peak in the susceptibility at T_c is studied for several Ising-like anisotropies.

For the spin-$\frac{1}{2}$ Ising model, $H=-\sum S_i^z S_j^z$, the transverse susceptibility is

$$\chi_\perp=\frac{1}{N}\sum_{i,j}\int_0^\beta d\tau \langle S_i^x(\tau)S_j^x(0)\rangle \ . \tag{1}$$

The effect of both S_i^x and S_j^x is to flip the spins on sites i and j, respectively. Thus, the only nonzero contributions to the sum occur when $i=j$. Denoting the states of the trace sum as m, the expression for $\chi_\perp$ becomes

$$\chi_\perp=\frac{1}{N}\sum_i\int_0^\beta d\tau\frac{\mathrm{Tr}(e^{-(\beta-\tau)H}S_i^x e^{-\tau H}S_i^x)}{\mathrm{Tr}(e^{-\beta H})}$$
$$=\frac{1}{4N}\sum_i\int_0^\beta d\tau\frac{\sum_m e^{-\beta E_m}e^{\tau(E_m-E_{m_i})}}{\sum_m e^{-\beta E_m}} \ , \tag{2}$$

where m_i is the same state as m except with spin i flipped. Performing the integration over τ and using importance sampling to generate the states m according to $\exp(-\beta E_m)$, the transverse susceptibility is

$$\chi_\perp=\frac{1}{4}\left\langle\frac{e^{\beta\Delta E_{m,i}}-1}{\Delta E_{m,i}}\right\rangle , \tag{3}$$

where $\Delta E_{m,i}=E_m-E_{m_i}=-2m_i^z\gamma_i$ and $\gamma_i=\sum_\delta m_{i+\delta}^z$ is the sum of the nearest-neighbor spins.

Unfortunately, this estimator is exponentially dependent on both γ_i and β, giving it intolerable fluctuations either for lattices with many near neighbors, such as an fcc lattice, or for low temperatures. The method we choose to rectify this situation is described in a paper by Parisi.[9,10] In effect, we sum over the different states at site i given the nearest-neighbor configuration. Thus,

$$\chi_\perp=\frac{1}{4}\left\langle\frac{e^{-\beta\gamma_i}-1}{-\gamma_i}P_i(\tfrac{1}{2})+\frac{e^{+\beta\gamma_i}-1}{\gamma_i}P_i(-\tfrac{1}{2})\right\rangle$$
$$=\frac{1}{4}\left\langle\frac{\tanh(\beta\gamma_i/2)}{\gamma_i/2}\right\rangle , \tag{4}$$

where, of course, $P(S^z)\propto\exp(\beta S^z\gamma)$. The form of this estimator is the same as that which is found in mean-field theory. The difference is that in mean-field theory the average would be over a mean field γ_i which is chosen self-consistently while here the average is performed numerically over fluctuations of a function of this field. This Parisi estimator does not diverge as the temperature goes to zero. In fact, the variance of this estimator actually decreases as β increases. This is because the estimator depends only on the sum of the near neighbors, whose variance decreases as the temperature decreases and the system becomes more ordered.

Numerical calculations provide evidence of the superiority of this estimator. For 100 sweeps of a 10^3 cubic lattice at $T=0.75T_c$ the lower-variance estimator has a standard deviation of 5.96×10^{-3}, whereas the old estimator has a standard deviation of 2.64×10^{-2}. For the same lattice at $0.50T_c$, the standard deviations are 2.098×10^{-3} and 4.28×10^{-2} for the new and old estimators, respectively. Thus as β increases the new estimator improves but the old declines in quality.

The transverse susceptibility for a 20^3 fcc lattice is plotted in Fig. 1. The circles are Monte Carlo data using the low-variance estimator and the triangles are linked-cluster data.[6] The agreement is very good. The difference between the two data sets near the peak is due to finite-size effects since the linked-cluster data is for an infinite-lattice system while the Monte Carlo data is for a 20^3 lattice.

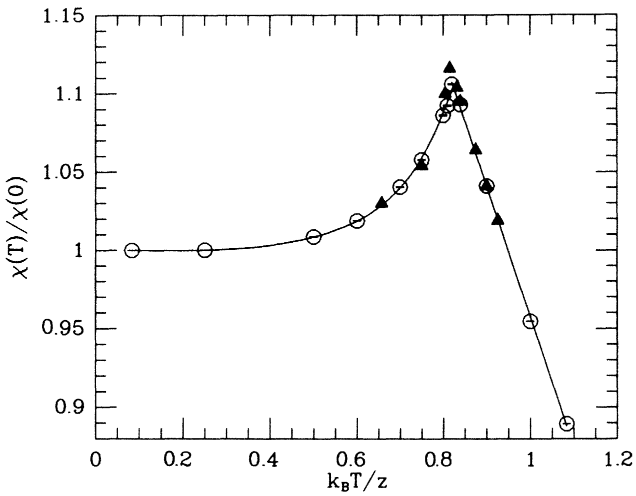

FIG. 1. $\chi_\perp(T)/\chi_\perp(0)$ for a spin-$\frac{1}{2}$ Ising Hamiltonian on a fcc lattice. Circles are Monte Carlo results for a 20^3 lattice and triangles are the result of a linked-cluster series expansion. The solid line is a guide to the eye. The difference between the two data sets near the peak is due to finite-size effects.

A similar analysis may be done for the spin-1 (Blume-Capel[8]) model $H=-\sum S_i^z S_j^z + D\sum (S_i^z)^2$ to produce a low-variance estimator. In the diagonal basis of S_i^z, use

$$\frac{\mathrm{Tr}\, e^{-(\beta-\tau)H} S_i^x e^{-\tau H} S_i^x}{\mathrm{Tr}\, e^{-\beta H}} = \frac{\mathrm{Tr}\, e^{(\beta-\tau)S_i^z\gamma_i} S_i^x e^{\tau S_i^z \gamma_i} S_i^x}{\mathrm{Tr}\, e^{\beta S_i^z \gamma_i}} , \tag{5}$$

with

$$e^{-\tau H} = \begin{bmatrix} \exp[\tau(\gamma_i - D)] & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \exp[\tau(-\gamma_i - D)] \end{bmatrix} \tag{6}$$

and

$$S_i^x = \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 \end{bmatrix} \tag{7}$$

to find

$$\chi_\perp = \left\langle \frac{\frac{1}{D-\gamma_i}(e^{\beta D} - e^{\beta\gamma_i}) + \frac{1}{D+\gamma_i}(e^{\beta D} - e^{-\beta\gamma_i})}{e^{\beta D} + 2\cosh(\beta\gamma_i)} \right\rangle . \tag{8}$$

Here D is the local anisotropy and the average is over all lattice sites i in zero field. Data from this estimator is plotted against temperature in Figs. 2(a) and 2(b) for 8^3 and 20^3 cubic lattices, respectively, for three different values of the local anisotropy D. For the larger lattices,

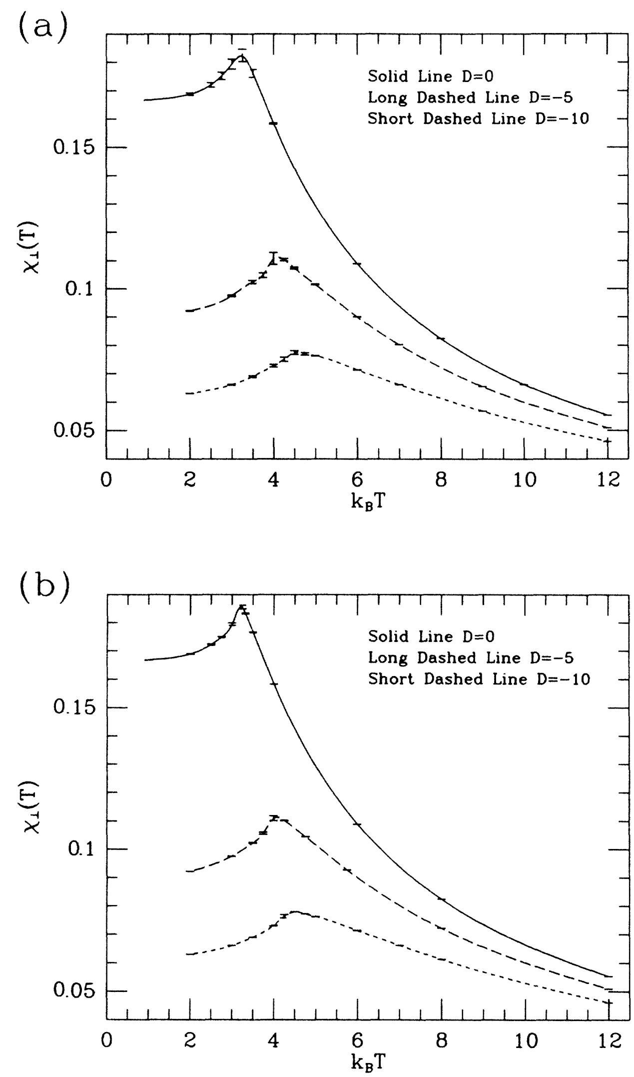

FIG. 2. $\chi_\perp(T)$ for a spin-1, Blume-Capel Hamiltonian on a cubic lattice with local anisotropies $D=0$, -5, and -10. (a) is for a 8^3 lattice and (b) is for a 20^3 lattice. In each case the peak of the curve falls slightly above the critical temperature for the lattice.

the peak becomes sharper while remaining finite. It is found, however, that this peak does not correspond with the peak found in a plot of the parallel susceptibility. The peak of the parallel susceptibility diverges in the limit of an infinite lattice, and its position gives the value of T_c for the lattice. The position of the transverse susceptibility peak is shifted up from T_c by a few percent, as was predicted by Fisher in 1963.[2] For example, for $D=-10$ the transverse susceptibility peak seems to be shifted up from T_c by about 2.5% as determine by extrapolating finite-lattice data. Thus the behavior at the peak of the transverse susceptibility must be analytic and cannot be a cusp.

Typically, quantum Monte Carlo simulations study the evolution of a system in imaginary time. Since analytic continuations of numerical data can be very sensitive to noise, it has proved difficult to obtain information on real-time dynamics.[11] As we have shown, however, the transverse susceptibility of the classical Ising model can be made an entirely classical measurement. The transverse susceptibility of a spin-$\frac{1}{2}$ system to a uniform ac field of frequency ω is given by the Fourier transform of the retarded Green's function:

$$G(t) = -i\frac{1}{N}\langle [m(t), m(0)]\rangle\theta(t) ,$$

where

$$m(t) = e^{iHt}\sum S^x e^{-iHt} .$$

A low-variance estimator for this susceptibility is

$$\chi_\perp(\omega+i\epsilon) = \tfrac{1}{4}\left\langle \tanh(\beta\gamma_j/2)\left[\left[\frac{1}{\omega+\gamma_j} - \frac{1}{\omega-\gamma_j}\right] - i\pi\delta(\omega+\gamma_j) - \delta(\omega-\gamma_j)\right]\right\rangle , \quad (9)$$

with ϵ a positive infinitesimal.

Finally, a low variance estimator will be constructed for the transverse susceptibility of an Ising system of arbitrary spin s. Again, we are interested in quantities of the form

$$\langle S^x(\tau)S^x(0)\rangle = \tfrac{1}{4}\langle S^+(\tau)S^+(0) + S^+(\tau)S^-(0) + S^-(\tau)S^+(0) + S^-(\tau)S^-(0)\rangle , \quad (10)$$

where now the spins are no longer spin $\frac{1}{2}$. The purely quantum pieces $\langle S^+(\tau)S^+(0)\rangle$ and $\langle S^-(\tau)S^-(0)\rangle$ do not contribute to the sum. The remaining time-evolved operators, meanwhile, are

$$\begin{aligned} S^\pm(\tau) &= e^{\tau H}S^\pm e^{-\tau H} = e^{-\tau\gamma S^z}S^\pm e^{\tau\gamma S^z} \\ &= S^\pm + \frac{(-\tau\gamma)}{1!}[S^z, S^\pm] \\ &\quad + \frac{(-\tau\gamma)^2}{2!}[S^z,[S^z,S^\pm]] + \cdots \\ &= e^{-\tau\gamma}S^\pm . \end{aligned} \quad (11)$$

The resultant expression for the transverse susceptibility will involve

$$\langle S^\pm S^\mp\rangle = s(s+1) - \langle (S^z)^2\rangle \pm \langle S^z\rangle , \quad (12)$$

and so will be entirely classical. Summing over all values of S^z with relative probabilities $\exp(\beta\gamma S^z)$ produces the low-variance estimator

$$\chi_\perp = \left\langle \frac{1}{2\gamma_j}\{(2s+1)\coth[\beta\gamma_j(s+\tfrac{1}{2})] + \coth(\beta\gamma_j/2)\}\right\rangle \quad (13)$$

for the transverse susceptibility. The functional form of this estimator is similar to that of the Brillouin functions found in mean-field theory.

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