Linear transverse susceptibility of Ising systems

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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-\(1/2\) 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 and two dimensions. In three dimensions, experimental work finds cusplike behavior, which cannot be explained by simple approximations, such as mean-field theory, which ignore fluctuations. Some progress has been made by 1/2 expansions, with the number of nearest neighbors, and, especially, by linked-cluster expansions. 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-\(1/2\) and spin-1 Ising systems on three-dimensional lattices ranging from \(3^3\) to \(20^3\) sites. For the spin-1 (Blume-Capel) model, the peak in the susceptibility at \(T_c\) is studied for several Ising-like anisotropies.

For the spin-\(1/2\) Ising model, \(H = -\sum S_i^y S_j^y\), the transverse susceptibility is

\[
\chi^y = \frac{1}{N} \sum_{i,j} \int_0^\beta d\tau \langle S_i^y(\tau) S_j^y(0) \rangle .
\]

The effect of both \(S_i^y\) and \(S_j^y\) 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 \(\chi^y\) becomes

\[
\chi^y = \frac{1}{N} \sum_{m} \int_0^\beta d\tau \frac{\text{Tr}(e^{-(\beta-\tau)H^m} e^{-\tau H^m})}{\text{Tr}(e^{-\beta H})}
= \frac{1}{4N} \sum_{m} \int_0^\beta d\tau \frac{e^{-\beta E_m} \pi_{E=0}}{\sum_m e^{-\beta E_m}} ,
\]

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

\[
\chi^y = \frac{1}{4} \frac{e^{\beta E_m,i} - 1}{\Delta E_{m,i}} .
\]

where \(\Delta E_{m,i} = E_m - E_{m,i} = -2m^i \gamma_i\) and \(\gamma_i = \sum_\delta m^i_{\delta + \delta}\) is the sum of the nearest-neighbor spins.

Unfortunately, this estimator is exponentially dependent on both \(\gamma_i\) and \(\beta\), 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." In effect, we sum over the different states at site \(i\) given the nearest-neighbor configuration. Thus,

\[
\chi^y = \frac{1}{4} \left( e^{-\beta \gamma_i} - 1 + e^{\beta \gamma_i} - 1 \right) \frac{\tanh(\beta \gamma_i/2)}{\gamma_i/2} ,
\]

where, of course, \(P(S^y) \propto \exp(\beta S^y \gamma)\). 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 \(\gamma\), 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 \(\beta\) 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 \(5.96 \times 10^{-2}\), whereas the old estimator has a standard deviation of \(2.64 \times 10^{-2}\). For the same lattice at \(0.50T_c\), the standard deviations are \(2.098 \times 10^{-3}\) and \(4.28 \times 10^{-2}\) for the new and old estimators, respectively. Thus as \(\beta\) 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. 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. $\chi_1(T)/\chi_1(0)$ 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\textsuperscript{8}) model $H = -\sum S_i^z S_j^z + D \sum (S_i^x)^2$ to produce a low-variance estimator. In the diagonal basis of $S_i^z$ use

\[
\frac{\text{Tr}e^{-(\beta - \gamma)H}S_i^x e^{-\tau H}S_i^x}{\text{Tr}e^{-\beta H}} = \frac{\text{Tr}e^{(\beta - \gamma)S_i^y}S_i^x e^{\tau S_i^y}S_i^x}{\text{Tr}e^{\beta S_i^y}},
\]

(5)

with

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

(6)

and

\[
S_i^x = \begin{bmatrix}
0 & \frac{1}{\sqrt{2}} & 0 \\
\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\
0 & \frac{1}{\sqrt{2}} & 0
\end{bmatrix}
\]

(7)

to find

\[
\chi_1 = \frac{1}{D - \gamma_i} (e^{BD} - e^{-\beta \gamma_i}) + \frac{1}{D + \gamma_i} (e^{BD} - e^{-\beta \gamma_i})
\]

\[
e^{BD} + 2\cosh(\beta \gamma_i)
\]

(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, 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.\textsuperscript{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. 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 $\omega$ is given by the Fourier transform of the retarded Green's function:

$$\chi_{\omega} = i \left( \tanh(\beta \gamma / 2) \left[ \frac{1}{\omega + \gamma} - \frac{1}{\omega - \gamma} \right] - i \pi \delta(\omega + \gamma) - \delta(\omega - \gamma) \right),$$

with $\epsilon$ 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

$$\langle S^z(\tau) S^z(0) \rangle = \frac{1}{2} \langle S^+(\tau) S^+(0) + S^-(\tau) S^-(0) + S^+(\tau) S^-(0) + S^-(\tau) S^+(0) \rangle,$$

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

$$S^\pm(\tau) = e^{\tau H} S^\pm e^{-\tau H} = e^{-\gamma S^z} S^\pm e^{\gamma S^z}$$

$$= S^\pm + \frac{(-\gamma)^2}{2!} [S^z, [S^z, S^\pm]] + \cdots$$

$$= e^{-\gamma S^z}.$$

The resultant expression for the transverse susceptibility will involve

$$\langle S^z(\tau) S^z(0) \rangle = s(s+1) - \langle (S^z)^2 \rangle \pm \langle S^z \rangle,$$

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

$$\chi_{\omega} = \frac{1}{2\gamma} \left( (2s+1) \coth[\beta \gamma (s + \frac{1}{2})] + \coth(\beta \gamma / 2) \right).$$

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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10The method used to produce the low variance estimator is sometimes called the method of expected values, and is often used in the transport Monte Carlo method. Earlier references to its use may be found in G. Goertzel and M. H. Kalos, in Progress in Nuclear Energy, edited by P. J. Hughes, J. E. Sanders, and J. Horowitz (Pergamon, New York, 1958), Ser. I, Vol. II, p. 315.