Monte Carlo Calculation of Free Energy, Critical Point, and Surface Critical Behavior of Three-Dimensional Heisenberg Ferromagnets

M. P. Nightingale
Department of Physics, University of Rhode Island, Kingston, Rhode Island 02881

and

H. W. J. Blöte
Laboratorium voor Technische Natuurkunde, 2600 GA Delft, The Netherlands
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A transfer-matrix Monte Carlo technique is developed to compute the free energy of three-dimensional, classical Heisenberg ferromagnets. From the free energy of systems with periodic and antiperiodic boundary conditions, helicity moduli are calculated. From these the critical couplings for simple cubic (sc) and face-centered cubic lattices are estimated, by use of finite-size scaling. For the sc lattice, the critical dimension of the surface magnetization is estimated with standard Monte Carlo methods, yielding a result in excellent agreement with the ϵ-expansion work of Diehl and Nüsser.

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Transfer matrices are widely used in numerical studies of statistical mechanical systems in two dimensions with discrete microscopic degrees of freedom.[1] In three dimensions, numerical calculation of eigenvalues of transfer matrices become intractable already for small systems: a $5\times5\times\infty$ Ising model in 2+1 dimensions seems to be the current upper limit.[2] Systems with continuous degrees of freedom, with the exception of linear chains, are even more of a challenge.

Here, we combine Monte Carlo (MC) and transfer-matrix techniques to tackle a three-dimensional Heisenberg model and directly calculate free energies in terms of the transfer-matrix eigenvalues for lattices up to $10\times10\times\infty$. The method is a variant of the Green's-function MC method,[3] of which there have been some preliminary applications to the three-dimensional Ising model.[4]

Consider a lattice in three dimensions with N sites: n_z layers of $m=n_xn_y$ sites each. We chose helical boundary conditions to obtain a single, sparse transfer matrix, and label the sites with one index $i=1,\ldots,N$. Sites $1,\ldots,m$ and $N-m+1,\ldots,N$ form the bottom and top surfaces. For a general lattice, each nearest-neighbor bond features precisely once in the list $(i,i-d_\alpha)$, $i=1,\ldots,N$, and $\alpha=1,\ldots,c$, up to end effects. The c displacements d_α define the lattice: $c=3$ with $d_1=1$, $d_2=n_x$, and $d_3=m$ yields the simple cubic (sc) lattice; for the face-centered cubic (fcc) lattice, add $d_4=m-1$, $d_5=m-n_x$, and $d_6=m-n_x-1$. At each site i there is a spin, a three-component unit vector $\mathbf{s}_i$. The reduced Hamiltonian is

$$-\beta\mathcal{H}=\sum_{i=1}^{N}\sum_{\alpha=1}^{c}\mathbf{s}_i'\cdot\mathbf{s}_{i-d_\alpha}', \tag{1}$$

where $\mathbf{s}_i'=\mathbf{s}_i\sqrt{K}$ for coupling constant K ($\mathbf{s}_i'=0$ for $i<0$). Integration of the Boltzmann weights over all $\mathbf{s}_i$ with $i\leqq N-m$ gives a partition function:

$$Z_N(S_N^{N-m+1})=\int\cdots\int dS_1^{N-m}\,e^{-\beta\mathcal{H}}, \tag{2}$$

where $S_i^j=(\mathbf{s}_i,\ldots,\mathbf{s}_j)$. With general m-uples of spins $U=(\mathbf{u}_i,\ldots,\mathbf{u}_m)$ and V, we define a transfer matrix T that adds one site to the lattice:

$$\mathsf{T}(U\,|\,V)=\exp\left(\mathbf{u}_1\cdot\textstyle\sum_\alpha\mathbf{v}_{d_\alpha}\right)\displaystyle\prod_{i=2}^{m}\delta(\mathbf{u}_i,\mathbf{v}_{i-1}),$$

where the δ functions are normalized such that

$$Z_{N+1}(U)=\int\cdots\int\mathsf{T}(U\,|\,V)Z_N(V)dV. \tag{3}$$

As $N\to\infty$, the dimensionless free energy (f) per site is given in terms of the dominant eigenvalue (λ_0) of T by $f=-\ln\lambda_0$.

To implement the power method to obtain this eigenvalue, the matrix multiplication in Eq. (3) is represented by a random process, the so-called transfer-matrix MC method. Introduce a sequence of random walkers $R_\iota=(S_\iota,w_\iota)$, $\iota=1,\ldots,r$: $S_\iota=(\mathbf{s}_1^\iota,\ldots,\mathbf{s}_m^\iota)$ represents a layer configuration of statistical weight $w_\iota\geqq0$. We maintain r within a few percent of a target r_0; the weights are kept in the range $b_l<w_\iota<b_u$, with $b_l\approx\frac{1}{2}$ and $b_u=2$. Rewrite $\mathsf{T}(S'\,|\,S)=P(S'\,|\,S)D(S)$, with a normalization $D(S)$ independent of S', such that $P(S'\,|\,S)$ is a probability density for a transition from S to S'. An MC run consists of sweeps $t=1,\ldots,M$ over all random walkers. At time t there are two steps. Affixing primes to variables at time $t+1$, we define step (1): For $\iota=1,\ldots,r$ change R_ι to $R_\iota'=(S_\iota',w_\iota')$ according to $P(S_\iota'\,|\,S_\iota)$, with $w_\iota'=D(S_\iota)w_\iota/c'$. With $\hat\lambda_0$ a running estimate of λ_0, choose $c'=\hat\lambda_0 r/r_0$ to maintain r close to r_0 in step (2): From the R_ι' construct a new sequence

using each walker precisely once: (a) If $w_t' > b_u$, add two random walkers $(S_t', \frac{1}{2} w_t')$ to the new sequence; (b) form pairs (S_t', w_t') and (S_κ', w_κ') with $w_t' < b_l$ and $w_\kappa' < b_l$, and add $(S_\lambda', w_t' + w_\kappa')$, where $S_\lambda' = S_t'$ or $S_\lambda' = S_\kappa'$ with relative probabilities w_t' and w_κ'; (c) if $b_l < w_t' < b_u$, or if R_t is left unpaired in step (b) add R_t'. The walkers represent a vector Φ with components

$$\Phi(U) = \sum_{t=1}^{r} w_t \delta(\mathbf{s}_1^t, \mathbf{u}_1) \cdots \delta(\mathbf{s}_m^t, \mathbf{u}_m). \tag{4}$$

Denote the vector realized in sweep t by $\Phi_t(U)$. The crux of the method is that

$$\left\langle \prod_{b=1}^{\tau} c_{t+b} \Phi_{t+\tau}(U) \right\rangle = \mathbf{T}^\tau \Phi_t(U), \tag{5}$$

where the angle brackets denote the average over all processes starting from the vector $\Phi_t(U)$. An estimator[5] of the dominant eigenvector Ψ_0 of the transfer matrix is

$$\Psi_0(U,\tau) = \frac{1}{M} \sum_{t=1}^{M} \left(\prod_{b=0}^{\tau} c_{t-b} \Phi_t(U) \right). \tag{6}$$

This is the iterate of order τ in the power method, and as such it has a bias for any $\tau < \infty$; its variance increases with τ. As a compromise we chose the largest τ with a statistically significant nonzero estimate of the autocorrelation at lag τ of c_t. The dominant eigenvalue of the transfer matrix is given by $\lambda_0 \approx W_0(\tau+1)/W_0(\tau)$, where W_0 is the integral of $\Psi_0(U,\tau)$ over U. As $\Psi_0(U)$ for $N \to \infty$ is the probability density of a surface configuration U, the multiplication of Eq. (6) through by a spin function and integration over U yields surface correlations.

We applied the same method to systems with antiperiodic boundary conditions: Each of the n_z planes had two seams related by translations by a vector between sites 0 and $n_x n_y$. One seam was in the y direction, the other in the x direction, except for a single step in the y direction forced by the helical boundary conditions. Along bonds across the seam the coupling was $-K$, instead of K.

The critical coupling K_c was obtained as follows. Denote the dimensionless free energies per site of the periodic and antiperiodic systems by f_+ and f_-; write $\Delta = K_c - K$. For $n_x = n_y = n$ and small $|\Delta|$ one has the scaling relation

$$n^d (f_+ - f_-) = H(n^{y_T} \Delta) \approx H_0 + H_1 n^{y_T} \Delta$$

in $d=3$ dimensions[6]; H is the *helicity* scaling function, and the correlation length diverges as $\Delta^{-\nu}$, where $y_T = \nu^{-1}$. With K_c, H_0, and H_1 as parameters, we made least-squares fits to data for several K and n values. In most runs the target number r_0 was 2500. With a number of sweeps that added roughly 5000 layers, this amounts to 12.5×10^6 flips per spin in total.

Figure 1 shows H vs n on an n^{y_T} scale for various K,

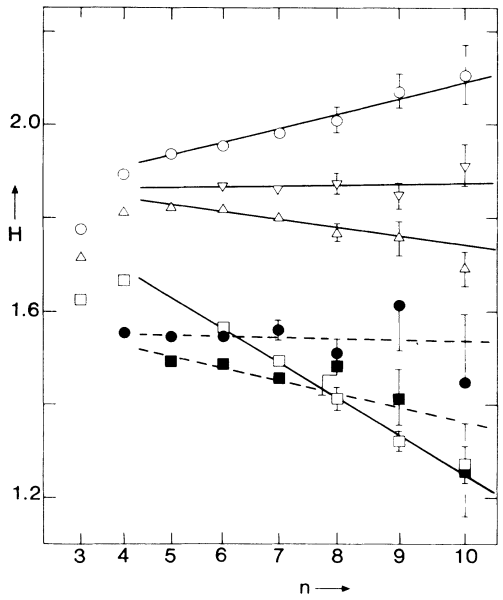

FIG. 1. Helicity modulus scaling function vs $n^{1.418}$ for various coupling strengths K. Open symbols represent data for the sc lattice: $K=0.695$ (circles), 0.6922 (inverted triangles), 0.6904 (triangles), and 0.68236 (squares); filled symbols are fcc data: $K=0.316$ (circles) and 0.31489 (squares). For $n=10$, two squares almost coincide; the fcc datum point has the longer error bars. Solid (sc) and dashed (fcc) lines illustrate linear behavior near criticality for $n > 5$.

for both the sc and fcc lattices. To check for finite-size effects, we systematically increased the size of the smallest system included in the fits. The results (and standard errors) are as follows: For the sc lattice, $K_c = 0.6922(2)$ and 0.6925(3), for sizes 5 and up and 6 and up, respectively; for the fcc lattice, $K_c = 0.3162(3)$, 0.3160(2), and 0.3170(5), for sizes 4 and up, 5 and up, and 6 and up. In the fits we used[7] $y_T = 1.418$. The K_c for the sc case agrees well with results of Ritchie and Fisher,[8] and of Ferer[9] obtained from eight- and twelve-term series. Agreement is less satisfactory with a ten-term-series estimate of Ohno, Okabe, and Morita[10] who find $K_c \approx 0.68236$. For the fcc lattice the agreement with the result[11] $K_c = 0.3149(2)$ is reasonable. The values of K around K_c were not chosen optimally to estimate the bulk thermal exponent, yet we have data for the sc lattice over a sufficiently wide range of couplings to obtain least-squares estimates: $y_T = 1.406(55)$ and 1.396(78) for sizes 5 and up and 6 and up, respectively.

The transfer-matrix method was also used to calculate surface correlations for the Heisenberg system. Only for small systems was a variance obtained smaller than with a standard MC algorithm,[12] and so only results of the latter will be discussed here. We used finite sc lattices with sites (x,y,z), with x, y, and z ranging from 1 to $n_x = n_y = n$ and $n_z = 2n$, respectively, free boundaries at $z=1$ and $z=n_z$, and helical or periodic boundary condi-

tions in x and y directions. Up to boundary effects, the Hamiltonian was that of Eq. (1). Also, couplings with and within the surface were redefined via $\mathbf{s}_i' = \mathbf{s}_i \sqrt{K_s}$, where $K_s = \epsilon K$ with enhancement factor ϵ. We calculated the surface susceptibility

$$\chi_{11} = n^{-2} \left\langle \sum \mathbf{s}_{x,y,z} \cdot \mathbf{s}_{x',y',z} \right\rangle,$$

summing over all sites (x,y,z) and (x',y',z) on one surface; the angle brackets denote the thermal average. We also calculated the surface correlation g_n halfway across the system:

$$g_n = n^{-2} \sum_x \sum_y \langle \mathbf{s}_{x,y,z} \cdot (\mathbf{s}_{x+n/2,y,z} + \mathbf{s}_{x,y+n/2,z} + \mathbf{s}_{x+n/2,y+n/2,z}) \rangle,$$

identifying sites (x,y,z) and (x',y',z), if $|x-x'| = n$, or $|y-y'| = n$. With χ_{11} and g_n we estimated the surface critical exponent y_{H_1}, which, e.g., yields the surface susceptibility exponent with $\gamma_{11} = (d' - 2y_{H_1})/y_T$, where $d' = 2$.

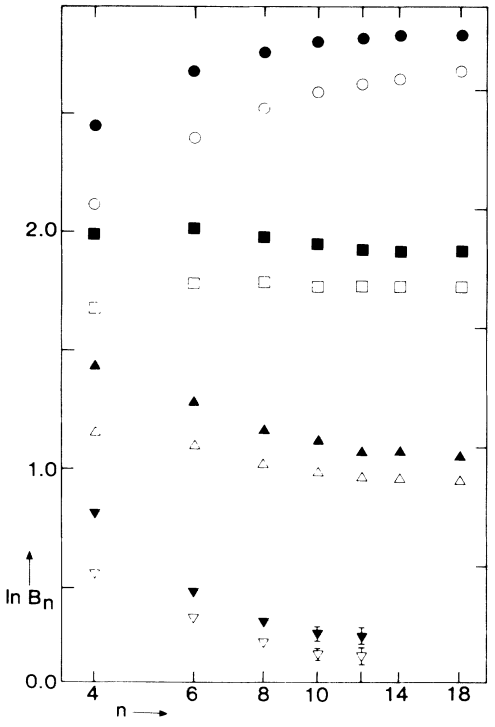

FIG. 2. Scaling behavior of surface correlation function g_n: $\ln B_n$ vs n on a $\ln n$ scale for several values of the surface enhancement ϵ, where $B_n = g_n \exp[(4 - 2y_{H_1}) \ln n]$, with $y_{H_1} = 0.8$ from our numerical analysis. According to scaling, B_n is finite and nonzero for $n \to \infty$. Filled and open symbols are for cylindrical and helical boundary conditions, respectively: $\epsilon = 1.0$ (circles), 0.83 (squares), 0.66 (triangles), and 0.5 (inverted triangles). To avoid overlap, data points for cylindrical systems are shifted upward by 0.1 (see tick marks on the right-hand side). Error bars are shown where they exceed the symbol size.

The MC estimates were obtained from one or several runs of 2×10^5 flips per spin. To obtain a vectorizable algorithm, spins were flipped sequentially on sublattices, such that nearest neighbors were on different sublattices. For periodic lattices of even size this is simple: They are bipartite. Helical systems had p sublattices L_i: L_i consists of sites $i + kp$ $(k = 0,1,\ldots)$, with p the smallest integer relatively prime to n and n^2.

The MC data (see Figs. 2 and 3) were analyzed with finite-size scaling. The γ_{11} were fitted[13] with $\chi_{11}(n) \approx \chi_{11}(\infty) + An^g$, where $g = d' - 2y_{H_1}$. The g_n have strong corrections to scaling and were fitted with $g_n \approx (B + C/n)n^h$, where $h = 2(y_{H_1} - d')$. A renormalization-group argument suggests the origin and sign of this correction. Simply assume that the surface fixed point[14] is characterized by a single, nearest-neighbor interaction K_s^*. At bulk criticality K_s will tend towards K_s^* under renormalization. As the number of renormalizations required to calculate correlations grows with distance, they will decay with an effective exponent y_{H_1} which decreases with distance for $K_s > K_s^*$ and vice versa. Scaling[15] and ϵ-expansion[16] arguments suggest the naive

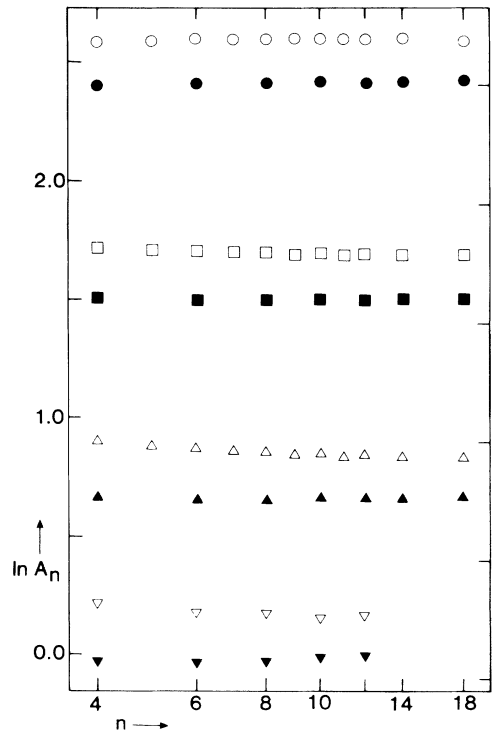

FIG. 3. Scaling behavior of surface susceptibility χ_{11}: $\ln A_n$ vs n on a $\ln n$ scale for several values of the surface enhancement ϵ, where $A_n = [\chi_{11}(\infty) - \chi_{11}(n)] \exp[(2y_{H_1} - 2) \ln n]$, with $y_{H_1} = 0.8$ and $\chi_{11}(\infty) = 11.25$, 6.05, 3.65, and 2.50 for $\epsilon = 1.0$, 0.83, 0.66, and 0.5 from our numerical analysis. For the key to the symbols see Fig. 2. To avoid overlap, data points for cylindrical systems are shifted upward by 0.1 (see tick marks on the right-hand side). The statistical errors in the data do not exceed the size of the symbols.

TABLE I. Estimates of surface critical exponent y_{H_1} obtained from least-squares fits to surface susceptibility and correlation data for both helix and cylinder boundary conditions. Results are labeled by n, the smallest system size included in the various fits.

	χ_{11}		g_n	
n	Helix	Cylinder	Helix	Cylinder
4	0.804(11)	0.778(07)	0.696(11)	0.685(12)
5	0.809(10)			
6	0.792(11)	0.806(11)	0.753(14)	0.770(18)
7	0.793(17)			
8	0.774(21)	0.791(24)	0.785(23)	0.784(32)
9	0.801(36)			
10	0.776(50)	0.699(49)	0.823(36)	0.821(72)

value -1 for the correction-to-scaling exponent. The analysis of χ_{11} required no such correction. Estimates of y_{H_1} were obtained from χ_{11} and g_n for several enhancements ϵ, both for cylinders and helices. Table I summarizes the results. We attribute the deviations at the top and bottom of Table I to finite size and too small a range of system sizes, respectively, and find $y_{H_1}=0.80\pm0.03$. This confirms the ϵ-expansion value[17] $y_{H_1}=0.809\pm0.014$, the series estimate[10] $y_{H_1}=0.85\pm0.06$, a previous MC result[18] $y_{H_1}=0.87\pm0.14$, and the experimental value[19] $y_{H_1}=0.83\pm0.06$.

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