Direct Calculation of Absolute Free Energy for Lattice Systems by Monte Carlo Sampling of Finite-Size Dependence

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It is shown that the absolute free energy of lattice spin systems can be calculated directly by a novel application of Monte Carlo sampling of finite-size dependence. Results are obtained for the two- and three-dimensional Ising models at T_c and are consistent with recent finite-size scaling-theory predictions. The free energy is in excellent agreement with Onsager's exact solution for two dimensions and with series expansions for three dimensions. The U_0 is measured for the first time. Results are consistent with the proposed universality.

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Despite the extensive applications and contributions made by Monte Carlo simulations[1] to the understanding of a wide range of physical problems involving many degrees of freedom, a long-standing problem of obtaining directly the absolute free energy by efficient Monte Carlo sampling continues to be of significant interest[1] to the understanding of phase transitions, critical phenomena, lattice gauge theory, and similar problems. Standard techniques[1] for obtaining free energy or related quantities such as entropy[1,2,3] have been the application of the thermodynamic integration method,[4] which depends on linking the point of interest to regions of the phase diagram where free energy can be calculated accurately by other approximate methods. Although such methods usually involve rather large numbers of Monte Carlo simulations, there are a number of advantages,[4] such as being able to obtain various properties of interest for the region of the phase diagram covered by the paths of integration. These methods, however, cannot be used to obtain information on the singular part of the free-energy density f_s at the critical point. In this paper, I propose a solution to this problem by showing that the absolute free energy of lattice systems at criticality can be calculated directly by a novel Monte Carlo method. The method has been applied to the ferromagnetic Ising model at criticality and is in excellent agreement with Onsager's exact solution[5] for two dimensions and the high-temperature series expansion results for the simple cubic (sc) and body-centered cubic (bcc) lattice for three dimensions. The finite-size scaling amplitude U_0 for the singular part of the critical free energy[6] is measured for the first time for both sc and bcc lattices. It is consistent with the recent proposal of universality for such amplitudes. The method has also been applied to the Ising model away from criticality with excellent agreement with the exact solution and will be presented elsewhere.

The method is based on two observations: First, the free energy for sufficiently small systems can be calculated exactly, and second, Monte Carlo sampling can be used to obtain directly the finite-size dependence of the absolute free energy. Although the first observation may be considered trivial, the second observation when shown to be practical is novel and quite useful. The method is also especially relevant in view of recent discussions on universal critical amplitudes[6] related to the singular part of the free energy near the critical point. These authors define the singular part of the finite-size free-energy density for an N^d lattice in d dimensions as

$$f_s(T,h,N) = f(T,h,N) - f_\infty(T,h), \tag{1}$$

with

$$f(T,h,N) = F(T,h,N)/(kTN^d).$$

$f_\infty(T,h)$ is the analytic "background" part of the free-energy density. In the asymptotic limits at T_c and zero field, it was proposed that

$$f_s \cong U_0 N^{-d}, \tag{2}$$

with scaling amplitude U_0. With the present method, one can obtain the finite-size dependence of the free energy and calculate U_0 for the first time.

For simplicity, I describe the method in two dimensions; extensions to three dimensions are straightforward. We consider a nearest-neighbor ferromagnetic Ising model on a $2N\times 2N$ square lattice. The system is considered under two sets of boundary conditions. The first is the usual periodic boundary conditions for a $2N\times 2N$ lattice and will be denoted by the Hamiltonian H_{2N}. In the second set, we divide the $2N\times 2N$ lattice into four separate $N\times N$ square lattices, each with the standard periodic boundary conditions, and denote the composite system by $\overline{H}_N$. The partition functions of the two systems are related by

$$\frac{Z_{\bar{H}_N}}{Z_{H_{2N}}}=\frac{\mathrm{Tr}\exp(-\beta\bar{H}_N)}{\mathrm{Tr}\exp(-\beta H_{2N})}$$

$$=\langle\exp[-\beta(\bar{H}_N-H_{2N})]\rangle_{H_{2N}}, \quad (3)$$

where $\beta=1/kT$ and $\langle\,\rangle_{H_{2N}}$ is an ensemble average generated by H_{2N}. The free-energy-density difference between a $2N\times2N$ and an $N\times N$ lattice can be obtained as

$$f_{2N}-f_N=\frac{\ln\langle\exp[-\beta(\bar{H}_N-H_{2N})]\rangle_{H_{2N}}}{4N^2}. \quad (4)$$

This allows the calculations of size dependence of the free-energy density directly as a Monte Carlo ensemble average. The extension to three-dimensional sc would be to partition a $2N\times2N\times2N$ system into eight $N\times N\times N$ separate systems. The bcc lattice is treated as a sc lattice with a two-sites basis. Although except for very small systems, such ensemble averages cannot in practice be evaluated directly by standard Monte Carlo methods,[1] I have been able to obtain very efficient sampling even for large systems (24×24) by applying the ratio method.[7] The ratio method is based on obtaining the ensemble average as a ratio of two ensemble averages. Equation (4) can be rewritten as[8]

$$\langle\exp[-\beta(\bar{H}_N-H_{2N})]\rangle_{H_{2N}}=\frac{\langle g[\beta(\bar{H}_N-H_{2N})]\rangle_{H_{2N}}}{\langle g[\beta(H_{2N}-\bar{H}_N)]\rangle_{\bar{H}_N}}, \quad (5)$$

where $g(X)$ denotes the Fermi function, $g(x)=1/[1+\exp(x)]$. The advantages of this method have been discussed in detail by Bennet[7] and will not be considered here. For three dimensions, even the ratio method failed to be efficient and multistage sampling is needed.[9] For example, Eq. (3) is rewritten for a three-stage sampling,

$$\frac{Z_{\bar{H}_N}}{Z_{H_{2N}}}=\frac{Z_{\bar{H}_N}}{Z_{H'}}\frac{Z_{H'}}{Z_{H''}}\frac{Z_{H''}}{Z_{H_{2N}}}, \quad (6)$$

where each ratio can be evaluated by the ratio method. For example,

$$\frac{Z_{H'}}{Z_{H''}}=\frac{\langle g[\beta(H'-H'')]\rangle_{H''}}{\langle g[\beta(H''-H')]\rangle_{H'}}. \quad (7)$$

H' and H'' are suitable Hamiltonians chosen such that the ratios can be evaluated efficiently. I have used up to six stages with the intermediate stages generated by H', which interpolates between $\bar{H}_N$ and H_{2N}, as $H'=a'H_{2N}+b'\bar{H}_N$ and (a',b') varies between (0,1) and (1,0). Typically, each sampling is averaged over about 50 000 Monte Carlo passes per site and standard block averages are used to obtain the error estimates. For the six-stage sampling, the intermediate Hamiltonians H' are chosen for computational convenience to be $(a',b')=[(1.0,0.0),(0.7,0.3),(0.4,0.6),(0.2,0.8),(0.1,0.9),(0.0,1.0)]$. The size dependences for the square, simple cubic, and body-centered cubic lattices are exhibited in Fig. 1. Observe that the size dependence can be fitted as N^{-d} for the three lattices with d the dimensionality. This is consistent with scaling-theory predictions.[6] I have also obtained the finite-size scaling amplitudes U_0. (See Table I.) Note that the sc and bcc cases are equal within the error estimates, thus providing the first Monte Carlo evidence that the finite-size scaling amplitudes of the singular part of the free energy are universal.

To obtain the absolute free energy, we combine the finite-size dependence results with an exact solution of a 4×4 or $2\times2\times2$ lattice to obtain the free energy for each size considered. The thermodynamic limit $f_\infty(T_c,0)$ is obtained by assuming that Eqs. (1) and (2) hold, which is exhibited in Fig. 1 for the range of sizes considered. The results are summarized in Table I with comparisons to exact results and high-temperature series expansions. The agreements are excellent.[13]

I have shown that the finite-size dependence of the free-energy density for lattice systems can be evaluated directly by the Monte Carlo method at T_c and have obtained the finite-size scaling amplitudes for the singular part of the free-energy density U_0 for the first time in two and three dimensions. By combination of

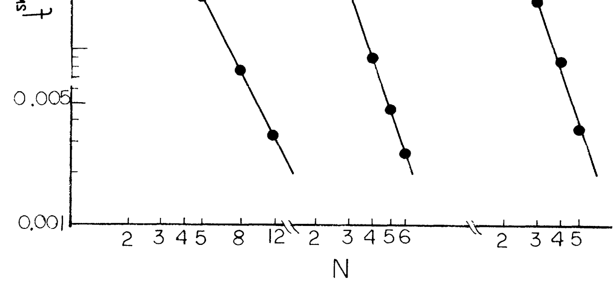

FIG. 1. Finite-size dependence of free-energy density from Monte Carlo simulations. The solid line is a fit to the N^{-d} scaling prediction. d is the dimensionality.

TABLE I. Summary of results for the scaling amplitude U_0 and free-energy density f_{mc} for two- and three-dimensional Ising models with comparison to exact results f_{exact} (Refs. 5,10) and high-temperature series expansion f_{ser} (Ref. 11) at criticality. The critical couplings for the sq, sc, and bcc lattices are 0.440 68 . . . , 0.2217, and 0.157 37 and were taken from Refs. 5 and 12.

	U_0	f_{mc}	f_{exact}	f_{ser}
sq	−0.0669 ±0.006	−0.9283 ±0.002	−0.9296 . . .	
sc	−0.657 ±0.03	−0.7776 ±0.001		−0.777 87
bcc	−0.643 ±0.04	−0.7552 ±0.001		−0.754 03

the finite-size dependence with exact solutions to small systems, the absolute free-energy density can be evaluated directly without thermodynamic integration. The results are in excellent agreement with exact solutions or high-temperature series expansions and consistent with finite-size scaling theory. The proposed method is thus shown to be useful and extensions to other lattice models should be possible. The actual computational efforts needed for accurate results will depend on the particular model and dimensionality.

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[2]Various methods have been proposed to estimate entropy. One interesting method is S. k. Ma, J. Stat. Phys. **26**, 221 (1981). See Ref. 1 for an extensive list of references.

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[8]To obtain Eq. (5), use the identity

$$\mathrm{Tr}\{\exp(-x)/[1+\exp(y-x)]\} = \mathrm{Tr}\{\exp(-y)/[1+\exp(x-y)]\}.$$

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[13]Note that this procedure does not assume that Eqs. (1) and (2) hold for 4×4 and $2\times2\times2$ lattices. Since the free energy for all the system sizes considered is calculated, it is sufficient for the asymptotic behaviors of Eqs. (1) and (2) to be reached by the larger system sizes considered. It turns out that this holds even for the smaller lattices.