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New Numerical Method to Study Phase Transitions

Jooyoung Lee and J. M. Kosterlitz

Department of Physics, Brown University, Providence, Rhode Island 02912

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We present a new numerical method to identify the nature of a phase transition. When combined with finite-size scaling, the method can identify unambiguously a weak first-order transition even when accessible system sizes are $L/\xi < 0.05$ as in the five-state Potts model. At a continuous transition, exponents can be determined surprisingly accurately and the computational effort required is moderate. The method is tested on the 2D Potts and 3D Ising models, but should be quite generally applicable.

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Monte Carlo (MC) simulations have been used for many years to study the properties of models of physical systems. The behavior near phase transitions has been one of the main objectives of such studies but a correlation length ξ greater than accessible system sizes L may lead to many difficulties. Finite-size-scaling ideas[1-3] help to extract critical exponents, amplitude ratios, etc., but this requires prior knowledge of at least the nature of the transition. When the system undergoes a weak first-order transition with $\xi \gg L$, as in the five-state Potts model[4] where $\xi > 10^3$ lattice spacings,[5] it becomes very difficult to identify its nature even with large-scale computations.[5,6] This problem is worse when one is faced with a new system in which nothing is known.

This Letter deals with the purely numerical study of phase transitions supplemented by very general finite-size-scaling ideas, assuming that almost nothing is known. There are two separate issues here: first, the identification of a continuous or first-order transition which is a prerequisite for the second, the detailed evaluation of physical quantities such as critical exponents, latent heats, etc. Moreover, to perform an accurate extrapolation to the thermodynamic limit of, say, the latent heat at a first-order transition, it is essential to use system sizes $L > \xi$, which may be completely inaccessible. As an example of this, Fig. 1 shows a plot of the deviation of the latent heats from the exact values[4] $\Delta l = [l(L) - l(\infty)]/l(\infty)$ against ξ/L for the $q = 5,6,8$ Potts model for $L \leq 60$ using estimated values of $\xi(q)$. It is clear from the figure that it is impossible to extrapolate accurately the five-state data because of the rapid decrease of $l(L)$ for $L > \xi$. It has so far proved impossible to verify the first-order nature of the transition by purely numerical methods.

Binder[7] has suggested using the fourth cumulant of energy or order parameter, but, although this has a known nontrivial thermodynamic limit, it suffers from severe crossover effects. Our method exploits the finite-size-scaling properties of a quantity $\Delta F(L)$ which are

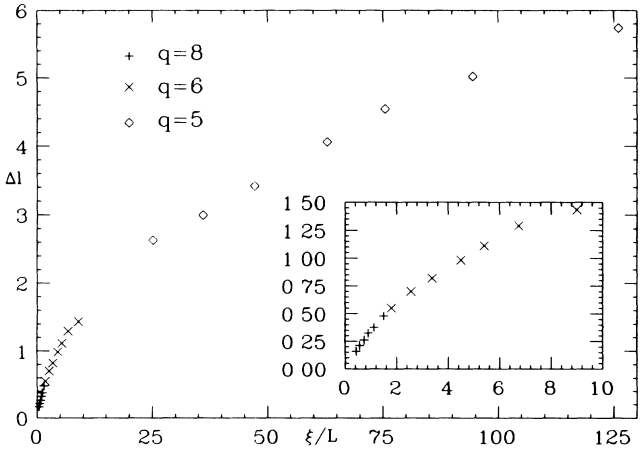

FIG. 1. Deviation of latent heats $\Delta l = l(L)/l(\infty) - 1$ of $q = 5,6,8$ Potts models. Correlation lengths $\xi(q) = 1512$, 108,18 are chosen to collapse data on a single curve.

unambiguous even when $L \ll \xi$ and, more importantly, can be implemented with reasonable computational effort.

All our simulations were performed on an IBM3090 without techniques such as multispin coding, and most were done using a standard single-spin-flip Metropolis algorithm. Some were repeated using the Swendsen-Wang algorithm[8] to reduce critical slowing down which reduced statistical errors, but the two methods agree within numerical errors. We tested the method on the 2D q-state Potts models with $q=2,4,5,6,8$ with $L \leq 60$ and on the 3D models with $q=2,3$ with $L \leq 14$. The expected first-order nature for $q \geq 5$ in 2D and $q=3$ in 3D is unambiguously confirmed and, as a by-product, we have been able to obtain surprisingly accurate values of the Ising correlation-length exponent $\nu(2)=1.003(10)$ and $\nu(3)=0.634(6)$. The exponent $2\beta/\nu$ is obtained with rather less accuracy, with the results 0.247(8) and 1.02(3).

The method depends on two key ideas: the identification of a quantity $\Delta F(L)$ which has characteristic behavior as a function of L at a first-order or second-order transition or in a single-phase region, and a technical advance by Ferrenberg and Swendsen[9] enabling this to be computed accurately. The central quantity is the restricted probability distribution for a system of size L with periodic boundary conditions. In N MC sweeps, standard probability theory implies that the number of times an observable X, such as energy or order parameters, is realized is

$$\exp[-A(X,L,N)] = NZ^{-1}(\beta)\sum_{E_1}\Omega(E_1,X)\exp(-\beta E_1)\,, \tag{1}$$

where $\Omega(E_1,X)$ is the number of states with energy E_1 and $Z(\beta)$ is the partition function. For a field-driven first-order transition, X is chosen as the order parameter M and for a temperature-driven one X is the energy E, with $\Omega(E_1,E)=\Omega(E)\delta(E_1,E)$. $A(X,L,N)$ differs from the bulk free energy $F(X,L)$ by a temperature- and N-dependent additive quantity but, at fixed β,L,N, the shape of $A(X,L,N)$ will be identical to that of $F(X,L)$ and also $A(X)-A(X')=F(X)-F(X')$. This last point is important since a measurement of ΔA gives a direct evaluation of the corresponding ΔF. Since the shapes of A and F are identical and we shall use free-energy differences for quantitative purposes, we shall refer to free energies in the following.

At a transition, $F(X,L)$ has pronounced double minima corresponding to two coexisting phases at $X=X_{1,2}$ separated by a maximum at X_m corresponding to a domain wall between the two phases. The other variable of interest is a scaling field g which moves the system along the phase boundary. The critical point is at $g=0$, the first-order line is at $g<0$, and $g>0$ is the disordered region with the field h conjugate to X fixed at its critical value. For a magnetic system undergoing a field-driven first-order transition $g \propto T-T_c$ and $X=M$, while for the q-state Potts model undergoing a temperature-driven first-order transition, $X=E$, $h \propto T-T_c$, and $g(q)$ is a measure of the distance from $q=4$.[10]

In the thermodynamic limit, $F(X)L^{-d}$ is independent of X for $X_1 \leq X \leq X_2$ at a first-order transition, but for finite L, the bulk free energy $F(X,L)$ has a double-minima structure with an expansion

$$F(X,L)=L^d f_0(X,g)+L^{d-1}f_1(X,g)+\cdots\,. \tag{2}$$

The bulk free-energy density f_0 is minimum and constant for $X_1 \leq X \leq X_2$ and the surface term f_1 has a maximum at X_m.[3,11] Then it is obvious F has minima at $X_1(L)=X_1-O(L^{-1})$ and $X_2(L)=X_2+O(L^{-1})$ with a maximum of height

$$\Delta F(L)=F(X_m,L)-F(X_1,L)=B(g)L^{d-1}+O(L^{d-2})\,.$$

This is true at any first-order transition provided $L \gg \xi$, but, when $g \simeq 0$ and $L \ll \xi$, $F(X,L)$ is dominated by its singular part and is a universal function of the scaling variables $x=XL^{\lambda_x}$ and $y=gL^{\lambda_g}$. At the transition, defined by equal depths of the minima, ΔF is a universal increasing function of $-y$ in a first-order regime since the minima become more pronounced. For the 2D $q>4$ Potts models, g is a marginally relevant variable[10] so $\lambda_g=0$, but y increases with L so that ΔF also increases.

Although we have been unable to calculate the explicit form of $\Delta F(y)$ it is clear that, as L increases, if we are in a first-order regime, ΔF must also monotonically increase as the minima develop, eventually crossing over to L^{d-1} behavior. Of course simulations of $\Delta F=\Delta A$ for $L \leq L_{\max}$ cannot determine completely and unambiguously the presence or absence of a first-order transition. However, if one assumes that all irrelevant variables have scaled to zero and the system is not crossing over to another critical point where ΔF is also finite, then a growing ΔF implies a first-order transition,[12] a constant ΔF a critical point, and a decreasing ΔF, vanishing at $L=O(\xi)$, a disordered phase (see Fig. 2). These arguments constitute a sensitive test for the nature of a transition by simulations. In Fig. 3 are shown a typical set of simulations for $q=5,6,8$ Potts models and in Fig. 4 the results for $\Delta F(L)$. The monotonic increase is obvious for all three.

For the special case of the Ising model with $X=M$, one can show explicitly[13]

$$\Delta F(L)=a-by+O(y^2)\,, \tag{3}$$

where a,b are positive constants of order 1 and estimates of the critical exponents may be obtained using Eq. (3). In particular, the exponent $\nu=1/\lambda_g$ is obtained by comparing $S=\partial\Delta F/\partial g \sim L^{1/\nu}$ for different L values (Fig. 5). This yields quite accurate estimates of ν and does not need an accurate location of T_c. Moreover, because ΔF

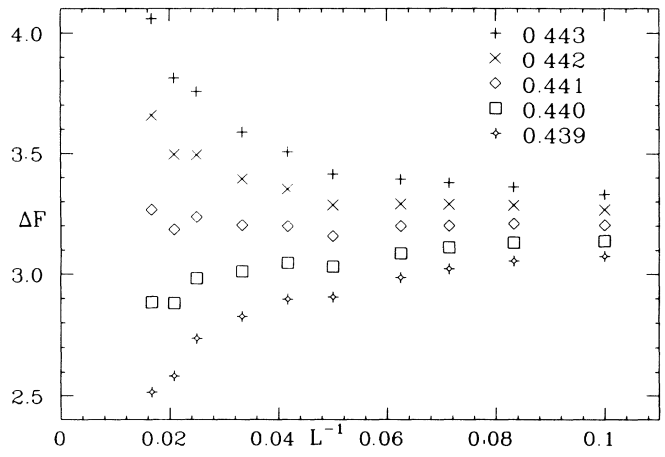

FIG. 2. Peak height $\Delta F(L)$ for various values of J/kT in critical region of 2D Ising model. The values at fixed L are all generated by doing one simulation at $J/kT=0.44069$ and then extrapolating.

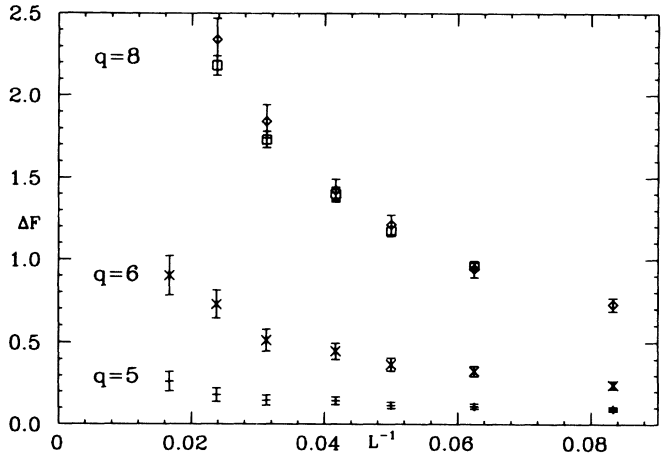

FIG. 4. Peak height $\Delta F(L)$ for $q=5,6,8$ Potts models. Open squares for $q=8$ were obtained by Swendsen-Wang algorithm; all others by Metropolis algorithm.

is linear in g near the critical point, there is a built-in check for the importance of corrections to scaling. The exponent β/ν can be obtained by measuring the separation of the minima X_1-X_2 at T_c which behaves as $L^{-\beta/\nu}$ (see Fig. 6). The main errors arise from the location of T_c, about 0.1%.

The technical problem of computing $F(X,g,L)$ on the transition line for several values of L and g is solved by the methods of Ref. 9. For the $q>4$ Potts models, $X=E$ and g is fixed by the value of q. For $q\leq 4$, g is taken to be zero since the system scales to a Gaussian theory.[10] It is necessary to be at $T_c(L)$ defined by $F(E_1,L)=F(E_2,L)$. This is done by finding $T_c(L)$ reasonably accurately and performing one long simulation of 5×10^6 MC steps to obtain good statistics. The data were smoothed by fitting with an eighth-order polynomial and extrapolated to $T_c(L)$.[9] System sizes were limited to $L\leq 60$ in 2D and $L\leq 14$ in 3D by the computer time available since good statistics are much more important than large system sizes. The statistics and the errors are worst for $q=8$ since that has the strongest first-order nature and the system cycles over the available states less frequently. We repeated the simulations for this case using the Swendsen-Wang algorithm[8] and obtained identical results for ΔF within numerical accuracy. As an additional check, we also studied the $q=3$ Potts model in 3D and found an unambiguous increase in ΔF with increasing L, verifying the first-order nature of the transition.[14]

The Ising-model simulations for $F(M;g,L)$ are carried out in the same way at $h=0$ because of symmetry. The simulation at each L was done close to the critical point $g=0$ and data at nearby g found by extrapolation.[9] This procedure yields very good estimates of ν but some error

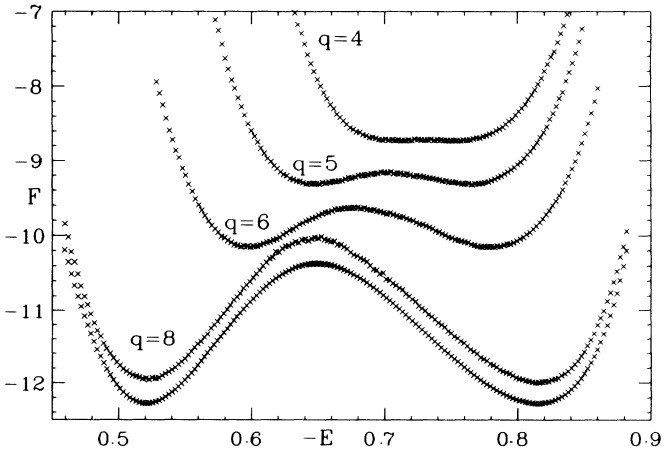

FIG. 3. Free energy $F(T_c(L))$ for $q=4,5,6,8$ Potts models for $L=32$. Bottom curve is $q=8$ data smoothed by polynomial fit. The energy scale is normalized to unity for complete order.

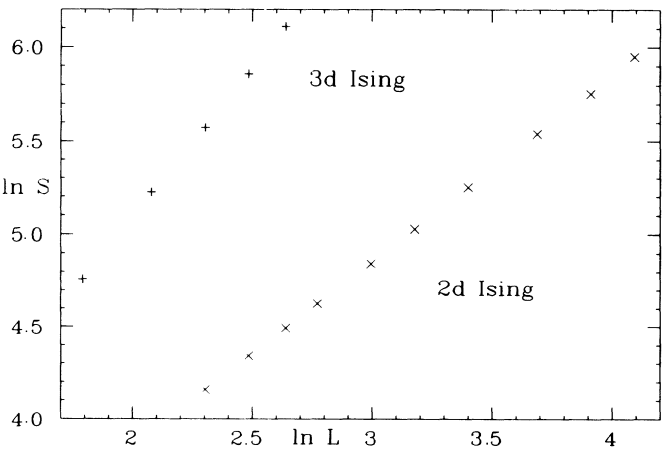

FIG. 5. $S=d\Delta F/dT\sim L^{1/\nu}$ for Ising models in critical region.

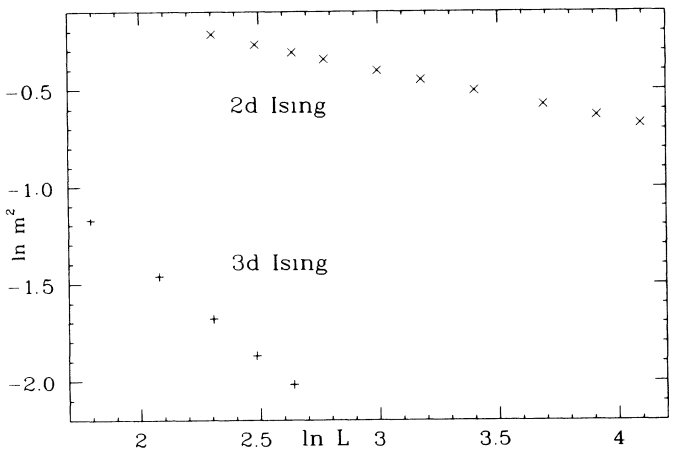

FIG. 6. $M^2(L) \sim L^{-2\beta/\nu}$ at T_c for Ising models.

in T_c and hence in $2\beta/\nu$. This can be reduced at the expense of much more computer effort by doing an independent simulation at each T.

To conclude, we have a powerful numerical method for finding the nature of a transition because the qualitative behavior of $\Delta F(L)$ is characteristic of the type of transition. At a second-order transition, good estimates of the critical exponents can be obtained. Latent heats are not accessible since we have been unable to overcome the crossover problem at $L \sim \xi$. The computer time and power required are moderate. It remains to be seen if the method can be successfully applied to systems with a continuous symmetry.

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[12]A growing ΔF may not imply a first-order transition if a slowly decaying irrelevant variable is present. However, at some L, the curvature of ΔF must then change sign and reasonably large simulations should be able to detect such behavior. This happens on a critical line near a tricritical point in $F(M,L)$ but not in $F(E,L)$.

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