A New Numerical Method to Study Phase Transitions

J.M. Kosterlitz[1,*], *J. Lee*[2], *and E. Granato*[3]

[1]Department of Physics, McGill University,
Montreal, Quebec, H3A 2T8, Canada
[2]Materials Science Division, Argonne National Laboratory,
Argonne, IL 60439, USA
[3]INPE, 12201-Sao José dos Campos, S.P., Brazil
*Permanent address: Department of Physics, Brown University,
Providence, RI 02912, USA

Abstract. A powerful method of detecting first order transitions by numerical simulations of finite systems is presented. The method relies on simulations and the finite size scaling properties of free energy barriers between coexisting states. It is demonstrated that the first order transitions in d = 2, q = 5 and d = q = 3 Potts models are easily seen with modest computing time. The method can also be used to obtain quite accurate estimates of critical exponents by studying the barriers in the vicinity of a critical point. Some new results on exponents and conformal charge in frustrated XY models and a related coupled XY-Ising model in d = 2 are presented. These show that the transitions in these models are in new universality classes and that the conformal charge varies with a parameter.

1. Introduction

One of the main goals of numerical simulations of statistical mechanical systems is to elucidate the behavior near a phase transition. At such a point there may be a first order transition with discontinuities in quantities like the internal energy manifested as a latent heat or in the order parameter. The transition may be continuous with associated non-analytic behavior of the order parameter which vanishes as $(T_c - T)^{\beta}$ or the susceptibility which diverges as $|T - T_c|^{-\gamma}$. In general, these non-analyticities are characterised by a set of critical exponents and amplitudes which determine the universality class.

When faced with an unknown system for which available analytic methods and brain power fail, one is forced either to give up or to resort to numerical simulations. At a putative transition, the object of the simulations is two fold: first to identify its nature (first order or continuous) and second to evaluate thermodynamic quantities such as latent heat, susceptibilities, etc. Unless the simulations can answer the first question there is little point in attempting the second. The essential difference between first order and continuous transitions is that the correlation length ξ is finite in the former case and infinite in the latter. At a weak first order transition, as in the two dimensional 5-state Potts model [1], $\xi > 10^3$ lattice spacings [2] which is larger than accessible system sizes L. In a simulation of a system with $L < \xi$, it is rather difficult to distinguish between a first order and continuous transition because the fluctuations

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are limited by L rather than ξ. One therefore expects the behavior of thermodynamic quantities to be very similar in the two cases making it difficult to distinguish the type of transition, even in large scale simulations [2-5].

Older methods for identifying a first order transition [6] have not been very successful as they are subject to ambiguity. For example, hysteresis in the evolution of a thermodynamic quantity as the system is heated and then cooled has been popular. However, in a finite system, the presence or absence of hysteresis caused by barriers depends on the cooling or heating rate. At a very strong first order transition one may be able to identify its nature correctly by a very careful analysis of the hysteresis effect [7-9], but as the transition becomes weaker the effect becomes more ambiguous. The time dependence of the order parameter or internal energy at the transition point has also been used [4]. In the thermodynamic limit, a system prepared in one bulk phase will remain there as the tunneling time is infinite but for finite L it is finite. Again, as the transition becomes weaker the tunneling behavior becomes indistinguishable from that at a continuous transition.

More recently, Binder introduced the fourth cumulant of energy [10] which, in principle, can distinguish between a continuous and temperature driven first order transition. He defined

$$V(L) = 1 - < E^4 > /3 < E^2 >^2 \tag{1}$$

which has the useful property that $V(\infty) = 2/3$ at all T if the transition is continuous. At a first order transition, on the other hand, $V(L) \rightarrow 2/3$ above and below the transition, but in a temperature range of $O(L^{-d})$ of the bulk T_c, it tends to a known non-trivial value [11]

$$V(L)|_{min} = 2/3 - (e_1/e_2 - c_2/e_1)^2/12 - O(L^{-d}) \tag{2}$$

which corrects some earlier work [3,10]. Here e_1 and e_2 are the energies of the bulk ordered and disordered phases. At first sight this looks very good but the difference between the value of eq. 2 and 2/3 may be very small. For the 5-state Potts model in two dimensions $V(L)_{min} = .66622..$ which is rather close to 2/3. Moreover, one needs exact analytic results to find the limiting value which may be difficult to obtain in more complicated cases. It also suffers from the fact that it approaches this value from below as L^{-d} but with a coefficient which depends on the bulk specific heats. To make the situation even worse, the L^{-d} approach sets in only for $L >> \xi$ [11]. Attempts to measure the latent heat and order parameter discontinuity suffer from similar difficulties.

2. The Free Energy Barrier and Finite Size Scaling [12]

It is clear that detecting a first order transition from finite size simulations is a non-trivial task and to make any progress we have to focus on the fundamental cause rather than the outcome. The essential features of a discontinuous transition are (i) a set of coexisting bulk phases and (ii) free energy barriers between them. It turns out that, at least for systems with a discrete symme-

try, the finite size scaling [13,14] properties of these barriers provides a very sensitive test of the order of a transition and, as a useful by product, can be used to obtain quite accurate estimates of critical exponents at a continuous transition. The general idea is very simple and just consists of the observation that, for sufficiently large L, there will be barriers between coexisting states and that these will change in some characteristic fashion with L.

We first consider a strongly first order transition with $L >> \xi$. Boundary conditions are an important consideration at this point since they can affect the existence of a free energy barrier and in the following we assume periodic boundary conditions on a d-dimensional cube of side L. For simplicity, consider the simplest situation of a ferromagnet in an external field h with a critical point at $h = 0$ and $t = \beta_c/\beta - 1 = 0$ when $t << 0$, there is a strong field driven first order transition at $h = 0$ and the bulk free energy F as a function of the magnetization M and β may be written as [6,14]

$$F(M, \beta, L) \simeq L^d f_0(M, \beta) + L^{d-1} f_1(M, \beta) + ... \tag{3}$$

where $f_0(M, \beta)$ is the free energy density in the thermodynamic limit and $f_1(M, \beta)$ is related to the free energy per unit area of a domain wall between the coexisting bulk phases. Note that the form of eq.3 is relevant for systems with a discrete order parameter such as the Ising or Potts models. In the case of an order parameter with a continuous symmetry such as an XY or Heisenberg model, the domain wall term is replaced by $L^{d-2} f_1(M, \beta)$ as the order parameter change is gradual. The bulk free energy density $f_0(M)$ will be a minimum and constant for $M_1 \leq M \leq M_2$ but $f_1(M)$ will have a maximum at some M_m where $M_1 < M_m < M_2$. the resulting bulk free energy in a system of volume L^d will then have a characteristic structure with minima at $M_i(L)$ and local maxima separating them of height

$$\Delta F(t, L) = A(t) L^{d-1} + O(L^{d-2}) \tag{4}$$

Here, $t = \beta_c/\beta - 1$ is the field which drives the system along the transition line at $t < 0$ through the critical point at $t = 0$ into the disordered phase $t > 0$.

For a temperature driven first order transition, the role of the driving field is played by β which is fixed at the transition at β_c and the conjugate density is the internal energy E. There may be another field g which drives the system along the transition line with the first order transition at $g < 0$ and a critical or multicritical point at $g = 0$. For the q-state Potts models in two dimensions, the field g(q) vanishing at $q = 4$ will determine the order of the transition. In this case, the quantity corresponding to the "free energy" of eq. 3 is F(E, g, L) which behaves in exactly the same way as F(M, β, L).

If one were able to simulate arbitrarily large systems, the free energy barrier $\Delta F(L)$ would suffice as one would simply have to demonstrate that this grows as L^{d-1} on the transition line. However, in a weakly first order transition, one is limited to $L < \xi$ but the L^{d-1} behavior does not set in until $L >> \xi$. Thus, it is necessary to understand the behavior of $\Delta F(L)$ in the vicinity of a critical point where the free energy is dominated by its singular part.

Finite size scaling theory tells us that F(X,g,L) may be written in terms of the scaling variables $x = XL^{\lambda_x}$, $y = gL^{\lambda_g}$ and that [14,15] F(X, g, L) $\simeq$ B(x,y) where, for small x and y, B(x,y) has an analytic expansion in x and y. At a first order transition, $y < 0$, B(x,y) must have a set of minima of equal depth at $x = x(y)$ so that the barriers $\Delta F(y) \equiv B(0,y) - B(x(y),y)$ will grow with increasing $-y$, eventually crossing over to the strongly first order behavior L^{d-1}. The simplest possible scenario, which holds for such simple systems as those q-state Potts models which have continuous transitions at some temperature, is, with $y = tL^{1/\nu}$ and $x = ML^{\beta/\nu}$

$$\Delta F(t, L) \simeq a - btL^{1/\nu} \tag{5}$$

Here a and b are positive constants independent of L [15]. An assumption has been made in this general discussion which is that the system size L is sufficiently large so that all irrelevant variables may be ignored. Given this, it follows that $\Delta F(g, L)$ increases with L in the first order regime ($g < 0$), is an L-independent constant (possibly zero) at the critical point ($g = 0$) and decreases with L in a disordered regime ($g > 0$).

The importance of the above general arguments is that they constitute a sensitive test of the nature of a transition by numerical simulations of $\Delta F(L)$. Perhaps the most important feature of $\Delta F(L)$ is that it shows very definite qualitative trends depending on the nature of the transition rather than tending to some finite value as $L \rightarrow \infty$ as, for example, Binder's cumulant [10]. However, a note of caution is in order. One may safely argue that, if $\Delta F(L)$ is found to increase with L, then the transition is first order but, if no peak structure is seen it may merely mean that L is too small for the peak to be noticeable above numerical noise or that irrelevant variables have not scaled away.

3.1 Simulations of Temperature Driven First Order Transitions

The free energy itself is rather difficult to obtain from simulations but we can find the free energy barrier by simulating the appropriate probability distribution or histogram. To study a temperature driven first order transition, one simulates the histogram of events at values of the density conjugate to β, namely energy. Elementary probability considerations tell us that in N tries the number of times the energy E occurs is

$$H(E, \beta, L) = NZ^{-1}(\beta, L)\Omega(E, L)e^{-\beta E} \equiv \exp - A(E, \beta, L) \tag{6}$$

Here N is the number of MC sweeps, Z is the partition function and Ω(E,L) is the number of states of energy E. Provided we compare the number of events at different E but at the same N, β and L we immediately obtain the crucial result

$$\Delta F_E(\beta_c, L) = \Delta A_E(\beta_c, L) \tag{7}$$

as the unknown partition function etc. cancel out. Exactly the same argument

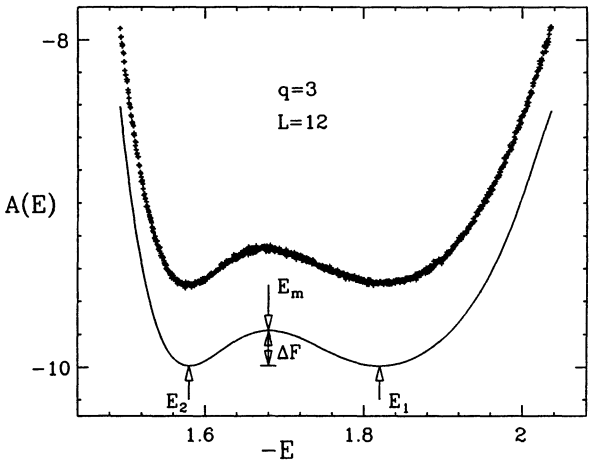

Fig. 1. A typical form of A(E,β,L) at $\beta = \beta_c(L)$ for a temperature driven first order transition. The crosses are extrapolated data for the q = d = 3 Potts model for L = 12 and the solid line is an eighth order polynomial fit.

holds for the order parameter histogram H(M,β,L) at the critical value of the field conjugate to M.

The function $A_E(\beta, L)$ will have minima of equal depth at the pseudo-critical temperature $\beta_c(L)$ corresponding to the coexistence of ordered and disordered states. Provided one has simulated this sufficiently accurately, one can obtain $\Delta F_E(L)$ by simply measuring the height of the barrier and, if it grows with L, one concludes that the transition is first order. The technical problem of computing A(E,β,L) at the transition has been solved by the histogram method as used by Ferrenberg and Swendsen [16] who showed how to extrapolate data from one value of β to nearby values. Since such extrapolations are accurate only for $\delta\beta \sim O(L^{-d})$, one must first locate $\beta_c(L)$ defined by $A(E_1, \beta_c, L) = A(E_2, \beta_c, L)$ reasonably accurately by hand and then, for each size, perform one long simulation of about 5 x 10^6 MCS to obtain reasonable statistics. One then extrapolates to the true $\beta_c(L)$ and measures $\Delta F_E(L)$. In practice we also smoothed the data by a polynomial fit. A typical curve of A(E,β,L) is shown in fig. 1 after extrapolation to $\beta_c(L)$ for the q = d = 3 Potts model. At some stage, one may also want the order parameter histogram so it is convenient to measure the double histogram H(E,M,β) and extrapolate by

$$H(EM\beta') = NH(EM\beta)e^{(\beta-\beta')E} / \sum_{EM} H(EM\beta)e^{(\beta-\beta')E} \qquad (8)$$

We note that a reasonably efficient algorithm is required so that many tunnelings between metastable states at $E_1(L)$ and $E_2(L)$ are realised which limits the system size L. Many of our early simulations [12] were performed using a standard single spin flip Metropolis algorithm but for q $\geq$ 6 state Potts models the Swendsen-Wang algorithm [17] was used to reduce slowing down.

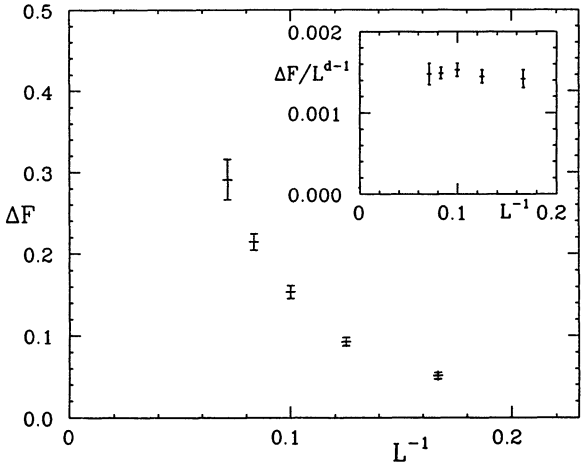

Fig. 2. Variation of $\Delta F_E(L)$ with 1/L for the q = d = 3 Potts model. The inset shows that $\Delta F(L) \sim L^2$. Note that $\Delta F(L) < 1$ for our $L \leq 14$ and L^{-d} finite size scaling predictions cannot hold.

Fairly extensive testing of temperature driven first order transitions was carried out for Potts models in two and three dimensions. The simulations in d = 2 were performed for quite small systems L < 60 for q = 4,5,6,8,10 to see if it could detect the very weak transition in q = 5,6 and whether the behavior could be distinguished from that of q = 4 which is known to undergo a continuous transition. Small system sizes were used to obtain good statistics and to check that useful information could be obtained with reasonable amounts of computing time. These tests were successful in that the first order nature of the q = 5 transition was unambiguous despite $L/\xi < \cdot 05$.

The L dependence of the barrier $\Delta F(L)$ also gives a measure of a correlation length ξ which may be defined by $\Delta F(\xi) = 1$. This definition gives a measure of a typical domain size of one phase at β_c and also serves as a criterion for distinguishing between weak and strong first order transitions. Since the tunneling time is $O(e^{\Delta F})$, for systems with $L < \xi$ the bulk state is short lived while for $L >> \xi$, the bulk state is in a deep free energy well and is long-lived. If one should wish to analyze data by standard finite size scaling theory [14] which predicts that scaling is in terms of L^d, this method provides a numerical criterion for strong first order finite size scaling. Extensive tests of analytic predictions have been performed for the q = 8,10 state Potts models [11].

The method was also applied to the q = d = 3 Potts model for system sizes up to L = 14. From some earlier work it was concluded that the transition was weakly first order. Apply this technique, the first order nature is obvious as an unambiguous and rapid increase in $\Delta F(L)$ is seen [18] which, already for these small values of L, seems to obey $\Delta F \sim L^2$ as shown in fig. 2. As a by product of the Swendsen-Wang algorithm, one can also extrapolate in the number of Potts states q from simulation data at q = 2 and 3. This can be done by working the partition function $Z(q, \beta)$ as

$$Z(q,\beta) = \sum_{E,N_C} \Omega(E,N_c)\exp(N_c \ell nq - \beta E) \tag{9}$$

where N_c is the number of percolation clusters generated by the algorithm. This allows us to extrapolate in ℓnq just as in β, remembering the limitation $\delta q \sim L^{-d}$. If we take the extrapolated data seriously it can be fitted to a very reasonable scaling form [18]

$$\Delta F(q,L) \sim (q - q_c)^2 L^{2/\nu q} \tag{10}$$

with $q_c = 2.45 \pm 0.1$ and $\nu_q = .85 \pm .1$.

3.2 Simulations of Field Driven Transitions Near the Critical Point

As a by product, the general method when applied to systems near a continuous transition provides an easy and surprisingly accurate way of obtaining the correlation length exponent ν and, somewhat less accurately, the order parameter exponent β/ν. As discussed in section 2, one can show that, for a field driven situation, the free energy barrier $\Delta F_M(L)$ is given by eq.5 [15] which summarizes one's intuition that, when the ordering field is fixed to its critical value, there will be a barrier between the ordered states. $\Delta F_M(L)$ increases with L for $T < T_c$, is a constant for $T = T_c$, and decreases with L for $T > T_c$, vanishing at $L \sim \xi$. A plot of $\Delta F_M(L,t)$ against $1/L$ is shown in fig. 3 for the $q = 3$, $d = 2$ Potts model. A very similar structure is seen for Ising models in $d = 2$ and 3.

The temperature derivative

$$S(L) \equiv -\partial \Delta F(t,L)/\partial t \sim L^{1/\nu} \tag{11}$$

provides a numerical method of obtaining $1/\nu$ by $\ell nS = \nu^{-1}\ell nL +$ const from a one parameter fit. The important aspect is that, although one can obtain T_c very accurately (·1% for the $d = 2$ Ising model) it is not necessary for the estimate of ν. One requires only the L - dependence of the slope of ΔF at T_c so, provided corrections to scaling are small, a small error in T_c will not affect the exponent. The slope S of the barrier is computed either by a numerical derivative of $\Delta F(t,L)$ by extrapolation or by [19]

$$S(L,t) = < E >_0 - < E >_M \tag{12}$$

where $< E >_M$ is the average internal energy at fixed M. The order parameter exponent β/ν is obtained by measuring the separation of the minima of A(M,T,L) at T_c which scales as $L^{-\beta/\nu}$. The major source of error here is the small uncertainty in T_c. Our results for the Ising model in $d = 2$ are $\nu = 1.003(10)$, $2\beta/\nu = 0.247(8)$ and in $d = 3$, $\nu = 0.634(6)$ and $2\beta/\nu = 1.02(3)$ which are quite good considering the modest amount of computer time involved and the simplicity of our analysis. For the 3-state Potts model in $d = 2$ we obtain $\nu = 0.84(2)$ from the data of fig. 4.

One may argue that the exponent ν could be just as easily be obtained from a study of Binder's cumulant $U_L = 1 - < s^4 > /3 < s^4 >^2$ whose derivative

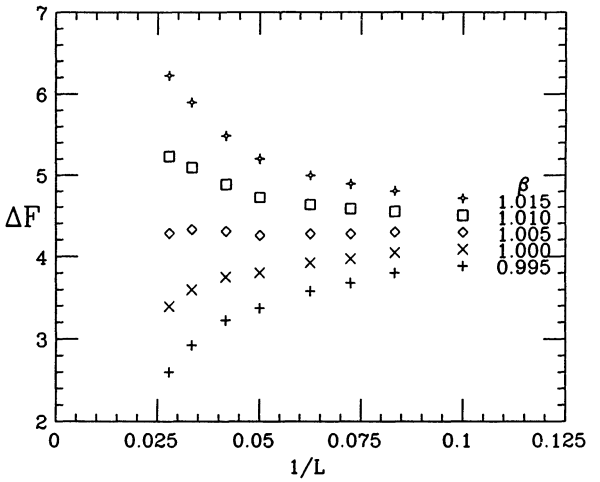

Fig. 3. Plots of $\Delta F_M(\beta, L)$ in the vicinity of a continuous transition for the q = 3, d = 2 Potts model. All points at fixed L are obtained from the same data by extrapolation.

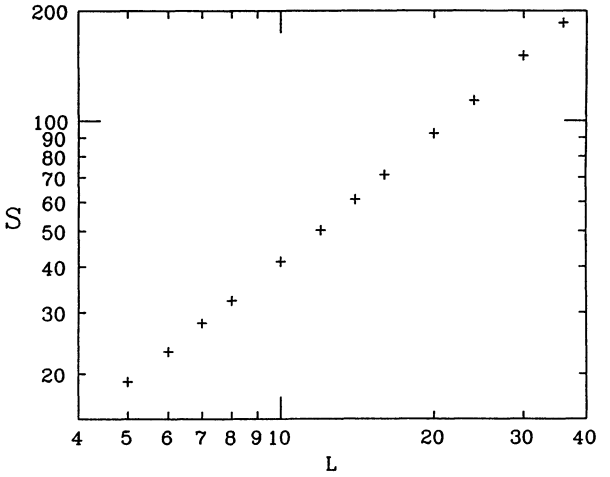

Fig. 4. S(L) data from fig. 3 used to obtain $1/\nu$. Note curvature for L < 10 indicating an irrelevant variable.

$\partial U_L/\partial\beta$ also behaves as $L^{1/\nu}$. However, using the same data as for $\Delta F(L)$, we find that $\partial U_L/\partial\beta$ is much more sensitive to temperature variations than S(L) and gives much larger uncertainties. For example, the variation of S(L) over a temperature range of ·02 T_c is about 8% while it is about 50% for $\partial U_L/\partial\beta$.

The method is very successful when applied to simple models but a word of caution is necessary. First, in these models it is known that the transition

is continuous so this style of numerical analysis will yield a good estimate of the exponents which are known to exist. However, the transition may be so weakly first order that this cannot be detected with accessible system sizes and the exponent estimates are meaningless. Also, the presence of slowly decaying irrelevant variables may effect the estimates, as the example below shows. Suppose the free energy is a function of the scaling variables $x = mL^{\beta/\nu}$, $y = tL^{1/\nu}$ and $z = gL^{-\lambda}$ with $\lambda > 0$ but small, and has the form

$$B(x,y,z) \sim -ax^2 + bx^4 + cyx^2 + dzx^2 + ... \tag{13}$$

Then, a simple calculation yields the effective exponent $1/\nu(L)$

$$1/\nu(L) \simeq 1/\nu + C\lambda(L/\xi g)^{-\lambda} \tag{14}$$

For the $q = 3$ Potts model in $d = 2$, there seems to be an irrelevant variable whose affect leads to curvature in $S(L)$ up to about $L = 10$, while for the Ising model there is no noticeable effect even for the smallest system sizes. It is also entirely possible that an irrelevant variable may obscure the peak in $\Delta F(L)$ as in eq. 13 when $dz > a - by$, thus hiding the fact that for $y = tL^{1/\nu} < 0$ there is a field driven transition for small values of L.

4. Application to More Complex Systems

The original motivation to look for a more sensitive numerical method was the study of fully frustrated Josephson junction arrays. These consist of a two-dimensional regular periodic array of weak links connecting superconducting grains in a magnetic field corresponding to half a flux quantum per plaquette perpendicular to the plane of the array. This problem has been intensively studied for many years both experimentally and theoretically [20] but the results have been rather inconclusive. In its simplest form, the system consists of an array of grains on a square or triangular lattice connected to their nearest neighbors by weak links. Assuming that the BCS temperature, at $T << T_0$, the only important fluctuations are in the relative phases of the grains. In this phase only approximation, by a suitable choice of gauge, the Hamiltonian may be written as

$$H/kT = -\sum_{<ij>} J_{ij} \cos(\theta_i - \theta_j) \tag{15}$$

where the coupling parameters $J_{ij} = \pm J$ are chosen so that each plaquette is frustrated. On a square lattice, this becomes Villain's odd model [21] of a fully frustrated XY model (FFXY) with every horizontal bond ferromagnetic ($J_{ij} = J$) and every alternate vertical bond antiferromagnetic ($J_{ij} = -J$). Despite the fundamental excitations of the system being fairly well understood in many different guises, the nature of the transition has been a mystery. On a triangular lattice, all $J_{ij} = -J$, so this becomes an XY antiferromagnet, which

is equally poorly understood. A few moments reflection will convince one that the ground state of these models is an antiferromagnetic arrangement of $\pm\frac{1}{2}$ vortices on each plaquette. The ground state is thus doubly degenerate so there are the usual Ising - like excitations coupled to fluctuations in the overall phase [20-23].

Attempts to treat phase transitions by analytic methods in these systems have been a complete failure. Earlier simulations [20,22] came to the conclusion that the system orders via an XY transition and an Ising transition occurring together, within numerical uncertainty. This conclusion was reached by performing a finite size analysis of the specific heat peak and finding consistency with $C_{max}(L) \sim \ell nL$ while the XY nature was deduced from the jump in the helicity modulus. There is some disagreement whether this is consistent with the universal XY value but general agreement on the Ising nature, which is strengthened by some large scale MC work [24].

Since these systems have a discrete part to the order parameter, the chirality of a plaquette, our method seems ideal to revisit this system with a view to evaluating ν and β/ν for chirality. This may be defined on plaquette P by

$$\chi_P = DJ^{-1} \sum J_{ij} \sin(\theta_i - \theta_j) \tag{16}$$

where the directed sum is over the bonds of the plaquette and $D = 2/3\sqrt{3}$, $1/2\sqrt{2}$ for the triangular and square lattices respectively. Despite the XY fluctuations being inaccessible to our simulations, the chiral exponents will decide if the transitions happen together or in a decoupled fashion. If the XY order parameter and the chirality are decoupled, the exponents of the latter will take on Ising values of $\nu = 1$ and $2\beta/\nu = 1/4$ while, if they turn out different, then the transition is non-Ising and must occur simultaneously with the XY part. We note that, if all the couplings are of equal strength, chiral disorder implies XY disorder.

Unfortunately, for the FFXY systems we were unable to construct an efficient algorithm and had to resort to a standard Metropolis algorithm with all the difficulties of equilibrating the phase fluctuations. We simulated system sizes $10 \leq L \leq 40$ with periodic boundary conditions and about 5×10^6 MCS [25,26]. Strictly speaking, the systems were never properly equilibrated and, especially for $L = 40$, the statistics were not very good. However, by studying $A_E(\beta, L)$, no trace of a first order transition was found so it is assumed continuous. The behavior of $\Delta F_M(\beta_c L)$ is very similar to that of the discrete models discussed earlier, although the L values are somewhat small and we do not seem to have quite reached the asymptotic limit. An estimate of $1/\nu$ from the temperature derivative S(L) yields $1/\nu = 1.18 \pm .03$, $2\beta/\nu = 0.31 \pm .03$ and $T_c/J = .455 \pm .002$ for the FFXY on a square lattice. The value of T_c is slightly lower than that of other workers [24] but agrees with estimates from MC transfer matrix (MCTM) [27]. The slope of ℓn S(L) against ℓnL is increasing steadily indicating we are not quite in the asymptotic scaling regime but that our estimate for $1/\nu$ is a lower bound and is inconsistent with the pure Ising value (see fig.5). Additional support for the unusual nature of the transition was obtained from MCTM methods which, although rather prelim-

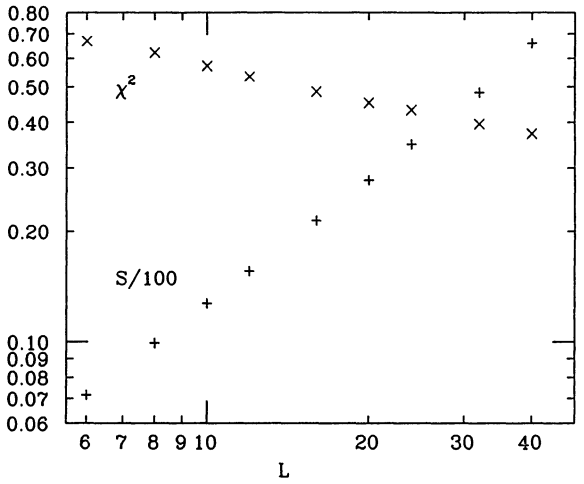

Fig. 5. Plots of S(L) and χ^2(L) for FFXY on square lattice. Upward curvature implies $1/\nu$(L) has not reached asymptotic value for L values used.

inary, are more consistent with this estimate of $1/\nu$ than unity. This is to be contrasted with a recent analysis [27] which concluded that $\nu = 1$ but our finite size scaling analysis is not the same.

Since earlier MC work concentrated on the specific heat peak as evidence of the Ising nature, we repeated the analysis with the same data used for the estimates of $1/\nu$. We find that assuming a a power law $C(L)|_{max} \sim L^{\alpha/\nu}$ yields a better fit to the data than a ℓnL behavior. We obtain $\alpha/\nu \simeq 0.5 \pm .1$ as an upper bound which is consistent with the hyperscaling estimate $\alpha/\nu = 2/\nu - 1$.

The same analysis was also carried out for the FFXY model on a triangular lattice and find $T_c/J = .513 \pm .002$ agreeing with earlier estimates [22] but disagreeing with the Ising value of 1 [22] for the chirality exponent. This latter is consistent with the FFXY on the square lattice although there are reasons for believing that the two models may be in different universality classes. Unfortunately, owing to the inefficiency of the algorithm, our data are not good enough to distinguish between them but do show that both are definitely not Ising-like.

5. A Generic Model

The two FFXY models of the previous section have a U(1)xZ(2) symmetry which are broken simultaneously at the transition. However, in principle there is no particular reason why they should be [28,29]. To study this aspect of the problem, the FFXY models may be mapped via an approximate Hubbard-Stratonovich transition into a coupled XY-Ising model of the form [25]

$$\beta H = -A \sum_{<ij>} (1 + s_i s_j) \cos(\theta_i - \theta_j) - C \sum_{<ij>} s_i s_j \qquad (17)$$

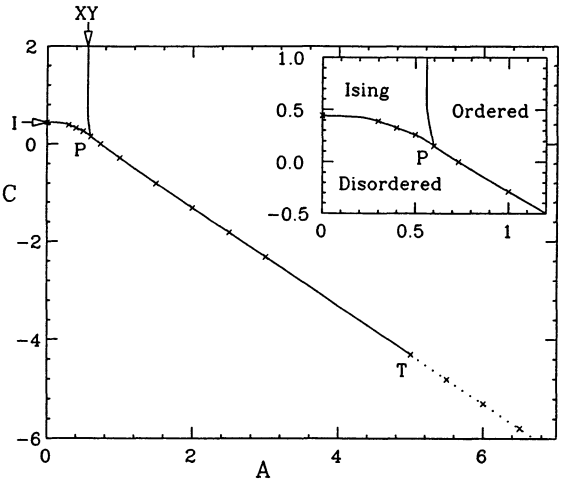

Fig. 6. Phase diagram of coupled XY-Ising model in A,C plane from MC. Solid (dotted) lines indicate continuous (first order) transitions. The location of T is uncertain.

where $s_i = \pm 1$ represents the chirality of a plaquette and θ_i its phase. Although the mapping is somewhat approximate, the structure of the resulting action of eq. 17 is consistent with all symmetries [23] of the original models. Anisotropy in the coupling strengths result in an extra operator of the form $B\sum_{<ij>} \cos(\theta_i - \theta_j)$ destroying some of the symmetry. In this generic model of coupled U(1) and Z(2) order parameters, the constants A,C depend on the original model and will differ for a triangular and square FFXY.

In the appropriate ferromagnetic range of parameters, $A > 0$ and $A+C > 0$, this model has three possible phases – disordered, fully ordered and partially (Ising) order. The fourth possibility, XY order and Ising disorder is excluded by the vanishing of the XY coupling across an Ising domain wall when $1+s_is_j = 0$. It is clear that for $A \simeq 0$, there must be a pure Ising transition at $C = C_c(A)$ and for $C > C_c$, as A increases there is a pure XY transition at $A \simeq 1/\pi$ to complete the ordering. However, when $C << 0$, but $A + C > 0$, the XY and Ising ordering must take place simultaneously and the questions of universality class and order of transition along the line of single transitions arise.

Again, on the single line, analytic methods fail so we simulated systems up to $L = 50$, again by a somewhat inefficient Metropolis algorithm, but used our method to obtain the phase diagram and exponents by monitoring the Ising variables only. The phase diagram is shown in fig. 6. Note that all possibilities discussed earlier – single transition or double transition [29] – are present, but the former is of particular interest.

By studying the energy distribution, we find for $C << 0$ a first order transition while along the segment PT we were unable to detect any sign of one so we assume it is continuous. The Ising exponents were measured from the order parameter distribution and find they vary continuously along PT. At

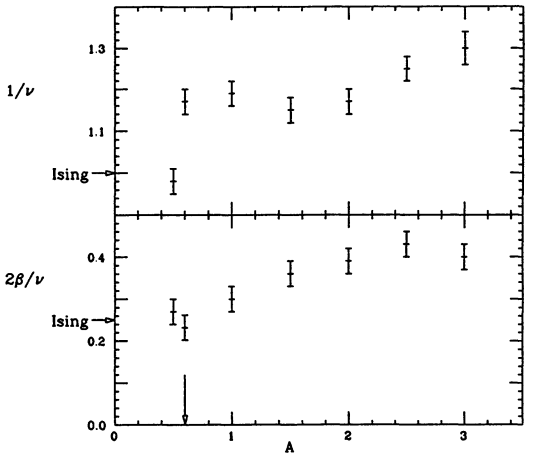

Fig. 7. Ising exponents ν and $2\beta/\nu$ on line PT of single transitions. Arrow on A axis denotes bifurcation point.

the bifurcation pont P, $1/\nu$ changes abruptly from its Ising value to about 1.2 reaching 1.3 at A = 3, while $2\beta/\nu$ increases steadily from 0.25 at P to 0.4. Unfortunately, our algorithm leaves much to be desired but was sufficient to establish the non-Ising character on the single line, the continuous variation of exponents as shown in fig. 7 and the existence of a first order regime. We conclude that the original FFXY models are described by eq. 17 at A $\simeq$ 1.

These results are interesting in themselves but more so is the conformal charge c along the line. The c-theorem of Zamalodchikov [30] tells us that $1.5 \leq c \leq 2$ on this line as the model of eq. 17 may be obtained by adding a relevant operator to two decoupled XY models ($c \leq 2$) or an irrelevant operator to a decoupled Ising and XY model ($c \geq 1.5$). Using MCTM methods [25] we find that c increases continuously from 1.5 at P to 2.0 at A $\simeq$ 3. We identify this as a tricritical point, which disagrees with the MC estimate but there is no real inconsistency when one recalls that the absence of double minima in A(E,L) does not exclude first order. Also, the value of c at A $\simeq$ 1 is consistent with those of the FFXY models of section 4.

6. Conclusions and Open Problems

We have developed a remarkably powerful method for numerically detecting first order transitions by studying the appropriate probability distribution. As a bonus, provided the transition is continuous (which cannot be unambiguously shown by these methods), the method provides very good estimates of critical exponents. Extensive tests were carried out on known systems and also compared to results on some 3D systems. Some interesting new results were obtained on FFXY systems, relevant to junction arrays, and strong evidence found which contradicts the long held belief that the transition is partly Ising-

like. It is shown that a coupled XY-Ising model captures much of the important physics of the FFXY models and that different representations of these may behave quite differently, showing either single or double transitions. Finally, some recent surprising results obtained by MCTM methods were presented for the conformal charge of the generic model.

There are many obvious directions to go at this point. We have not yet studied systems with a continuous symmetry such as O(n) models. There seems to be no particular difficulty in principle, provided one uses a sufficiently powerful algorithm which can simulate the function $A(M^2, \beta, L)$. As far as the FFXY models and its generalisations are concerned, one should should try to invent much more powerful algorithms so that larger systems with better statistics may be simulated. On the analytic side, one really needs a theory for $A(E,\beta,L)$ in the vicinity of a tricritical point as these are notoriously difficult to locate by numerical methods. The appropriate distribution for non-trivial systems at their lower critical dimension and its finite size scaling properties would be very useful.

It would be of interest to develop analogous methods to treat random systems such as random field and spin glass systems. With the present interest in flux flow in HTC superconductors and the hypothetical vortex glass phase such a study would be of some use. Finally, our results for the conformal charge of the coupled XY-Ising model need some explanation if they are real.

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