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Using the Lee–Kosterlitz Method to Detect First–Order Transitions in Models with Continuous Symmetries

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Abstract

Recent simulations of phase transitions using the properties of the free energy on various sized lattices have shown that it is possible to detect first order transitions in models with discrete symmetries. This report tests this technique on models with continuous symmetries using a three–dimensional non–linear sigma model with $SU(n)$ and $U(n)$ symmetries. This model is known to have either a first or second order phase transition depending on the order of the group. The results from these simulations are compared to the known information for the non–linear sigma model.

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In recent years there has been a strong research program to improve the techniques used to identify the order of a phase transition in numerical simulations. One numerical method that has recently been proposed by Lee and Kosterlitz [1] involves using the free energy combined with finite sized scaling. By relating the shape of the curve for the restricted probability distribution to the free energy, they have designed a way to measure the signature of a first order transition for discrete symmetry systems on the lattice.

Standard probability theory states that the number of times an observable X is realized after N iterations in a Monte Carlo simulation on a lattice of size L is given by the restricted probability distribution in eq. (1).

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

The $\Omega(E)\delta(E_1,E)$ represents the number of states with energy E_1 and $Z(\beta)$ is the partition function. The quantity $A(E,L,N)$ differs from the bulk free energy $F(E,L)$ by a temperature and an additive quantity proportional to the sample size N. However, at fixed β, L, N the shape of $A(E,L,N)$ will be identical to that of the bulk free energy F. From the above correspondence between $A(E,L,N)$ and the bulk free energy $F(E,L)$, Lee and Kosterlitz have argued that a relationship between the differences in these quantities can also be constructed as in eq. (2).

$$A(E,L) - A(E',L) = F(E,L) - F(E',L) \tag{2}$$

Not only will the shapes of $A(E,L,N)$ and $F(E,L)$ be identical, but any differences in these quantities should be directly related to each other.

This relationship can be exploited in numerical simulations through direct measurements of the energy near a first order transition. If the minima in the free energy are labelled E_a and E_b, then, in the thermodynamic limit, the quantity $F(E)L^{-d}$ is independent of E in the region where $E_a \leq E \leq E_b$. Because all numerical simulations, involve finite lattices of size L, the bulk free energy will have a double minima with the form eq. (3)

$$F(E,L) = L^d f_0(E) + L^{d-1} f_1(e) + ... \tag{3}$$

where f_0 is the bulk free energy that is minimum and constant and f_1 is a surface term that acquires a maximum value at E_m in the transition region $E_a \leq E \leq E_b$. From this information, the bulk free energy has two minima, one at $E_1(L) = E_1 - \mathcal{O}(L^{-1})$ and the second minima at $E_2(L) = E_2 + \mathcal{O}(L^{-1})$ and some maximum value between these values given by eq. (4).

$$\Delta F(L) = F(E_m, L) - F(E_1, L) \tag{4}$$

In a first order phase transition [2], the bulk free energy has a pronounced double minimum separated by a maximum value at E_m in the transition region. This double minima corresponds to the two co–existing phases with the maximum at E_m representing a domain wall between them. This first order behavior should also be observed when the system is modelled on a lattice. By measuring the energy probability distribution at some coupling near the transition and using the Ferrenberg Swendsen technique, it is possible to construct a plot of the free energy versus the internal energy. From these graphs the barrier ΔF can be measured for each lattice size.

The original work by Lee and Kosterlitz used a Potts model with a discrete symmetry. In their paper the authors raised the question of whether their method might also be applicable to systems with a continuous symmetry. This work extends their proposed technique to a continuous symmetry system. The model chosen for these simulations is the three dimensional non–linear sigma model, or chiral Heisenberg model. This model was originally chosen because of its suitability in the study of the finite temperature chiral phase transition in high energy physics. The model incorporates the properties of chiral symmetry by modelling the right and left-handed transformations characteristic of the $U(n)\times U(n)$ or $SU(n)\times SU(n)$ flavor groups. The model also shares with quantum chromodynamics the property of asymptotic freedom in an appropriate dimension.

Pisarski and Wilczek [3,4] have investigated the order of the finite temperature chiral transition using the ϵ–expansion in the linear version of the sigma model. Using the most general renormalizable Lagrangian, including terms that describe the behavior of the system in the presence of the anomaly, they have calculated the β functions in $4-\epsilon$ dimensions. The

fixed points were classified as either infrared stable or unstable depending on whether or not the stability matrix had real positive eigenvalues for the given fixed point. They calculated that for two or more flavors, the system did not have an infrared stable fixed point for the coupling constants in the model. Some of these predictions based on the $4-\epsilon$ expansion in the linear σ model have recently been tested by Gausterer and Sanielevici [5]. Their results appear to be in agreement with the $4-\epsilon$ expansion predictions.

Simulations of the chiral phase transition using the non-linear sigma model have been studied with both $SU(n)$ and $U(n)$ flavor symmetries for $n = 2$ and $n = 3$. Early numerical simulation work on the non-linear sigma model and the finite temperature chiral phase transition using this chiral spin model was performed by Kogut, Snow, and Stone [6]. Recently, a far more extensive study of the order of the chiral phase transition has recently been completed. The details of the numerical simulations and results are given in references [7] and [8].

To test the idea of using measurements of the free energy for a system with a continuous symmetry, measurements of the internal energy per site data from the finite temperature chiral phase transition study have been used. This data was generated from a simulation of the chiral spin model using a nearest neighbor lattice action of the partition function

$$Z = \int \prod_k [dU_k] \exp[\frac{1}{2}\beta \sum_{<ij>} \mathrm{tr} U_i^\dagger U_j + h.c.] \tag{5}$$

In eq. (5) i labels the sites, $< ij >$ labels links, U_i is an $SU(n)$ or $U(n)$ flavor matrix and [dU] is the invariant $SU(n)$ or $U(n)$ measure.

The three dimensional non-linear σ model was embedded on the lattice with periodic boundaries in all directions. Monte Carlo simulations with an improved Metropolis algorithm [9] with 10 hits per site for each iteration were used to update the lattice sites. High precision numerical simulations of various lattice sizes were performed for both $SU(3)$ and $U(2)$ flavor symmetries at various values of the coupling near the transition. In this region, the problems associated with critical slowing down seriously impeded the accumulation of data for the larger lattice sizes. To combat this effect and generate an accurate profile of the simulated

quantities near transition, the technique of Ferrenberg and Swendsen [10] was employed on the larger lattices.

The application of the Lee Kosterlitz method was applied to the $SU(3)$ simulations for 16^3, 18^3, and 20^3 lattices, and to the $U(2)$ simulations for the 16^3, 18^3, 20^3, and 22^3 lattice sizes. Both the $SU(3)$ and $U(2)$ groups in the this non–linear sigma model have been shown to have first–order transitions. Plots of free energy versus the internal energy were made with adjustments to the shape of the curve using the Ferrenberg–Swendsen method. Although ΔF=ΔA cannot uniquely determine the presence or absence of a first–order transition, if it is assumed 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, a constant ΔF a critical point, and a decreasing ΔF, vanishing at $L = \mathcal{O}(\xi)$ a disordered phase [11]. If we are in a first–order regime, then as the lattice size increases, then ΔF must also monotonically increase as the minima develop, eventually crossing over to L^{d-1} behavior. Applying their procedure to the $SU(3)$ and $U(2)$ data, it was found that, in both cases, there is evidence that ΔF monotonically increased [Fig. 1, and Fig. 2]. These results are in agreement with both the analytical work of Pisarski and Wilczek and recent numerical simulation work of the 3–dimensional non–linear sigma model, and also indicate that this method can be used to detect first–order transitions in models with continuous symmetries.

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[11] Lee and Kosterlitz point out in their paper that if a slowly decaying irrelevant variable is present, then a growing ΔF may not imply a first–order transition. In this case, they assert that, at some L, the curvature of ΔF must change sign. Therefore, if simulations are done with large lattice sizes this behavior should be detectable.

FIGURES

FIG. 1. ΔF versus L^{d-1} for $SU(3)$ data.

FIG. 2. ΔF versus L^{d-1} for $U(2)$ data.

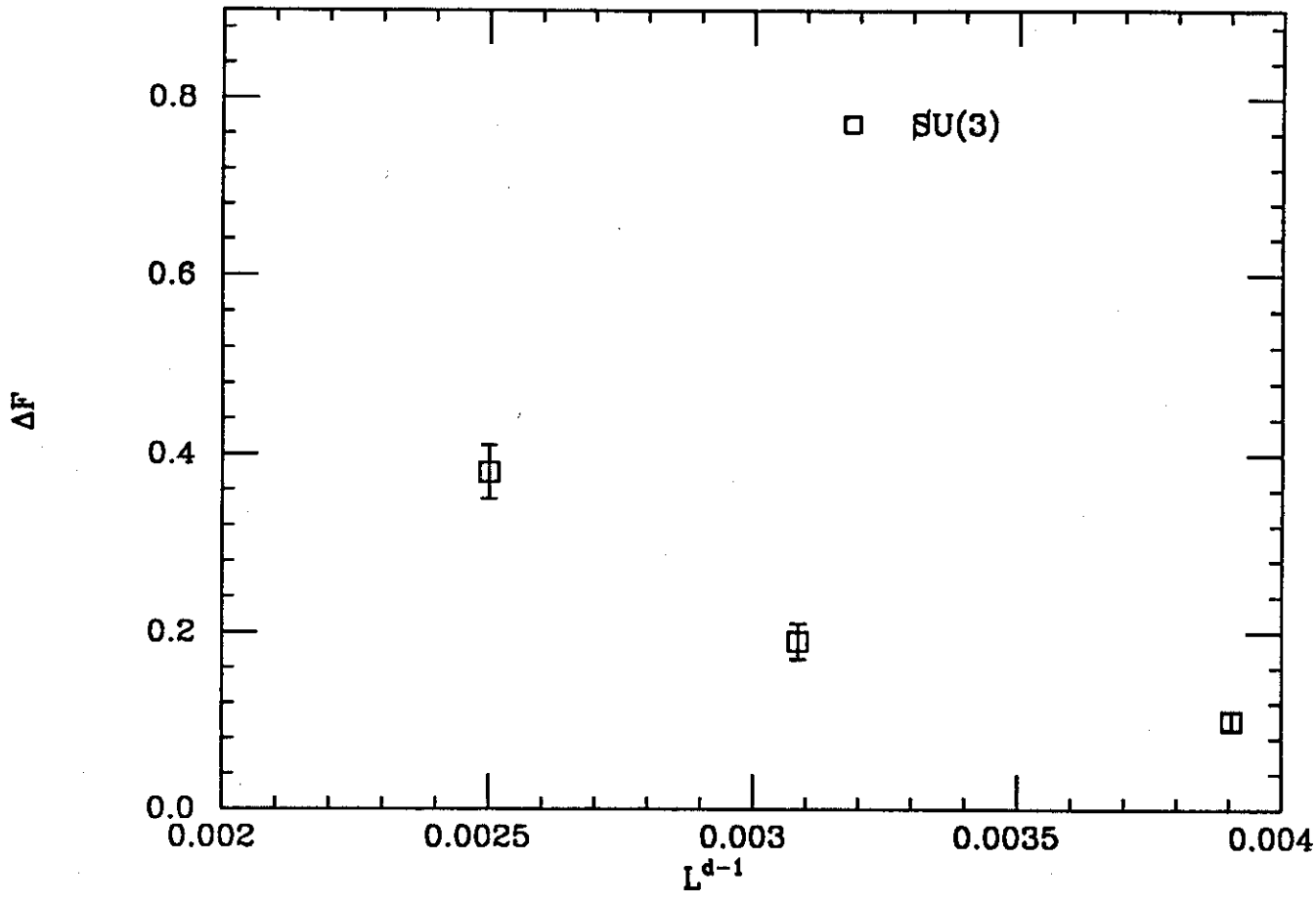

Fig. 1

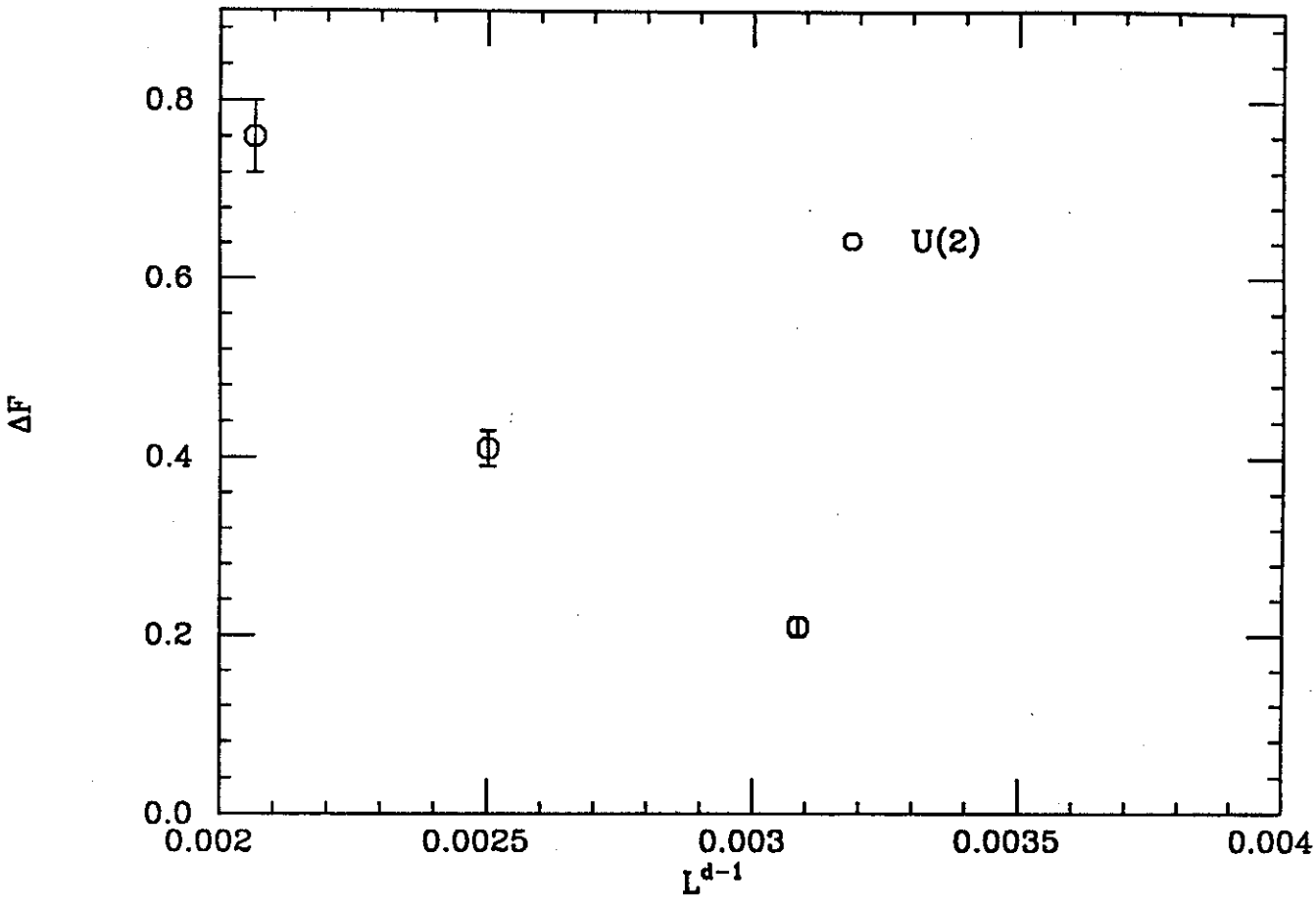

Fig. 2