Provable first-order transitions for liquid crystal and lattice gauge models with continuous symmetries.

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Abstract: We consider various sufficiently nonlinear sigma models for nematic liquid crystal ordering of RP^{N-1} type and of lattice gauge type with continuous symmetries. We rigorously show that they exhibit a first-order transition in the temperature. The result holds in dimension 2 or more for the RP^{N-1} models and in dimension 3 or more for the lattice gauge models. In the two-dimensional case our results clarify and solve a recent controversy about the possibility of such transitions. For lattice gauge models our methods provide the first proof of a first-order transition in a model with a continuous gauge symmetry.

In [10], it was shown that a class of ferromagnetic N-vector models with a sufficiently nonlinear nearest-neighbour interaction – meaning that the nearest neighbour interaction has the shape of a deep and narrow well – show a first-order transition in temperature. An example of a model which could be treated is given by the Hamiltonian

$$H = -J \sum_{<i,j>\in\mathbb{Z}^2} \left(\frac{1+\cos(\phi_i - \phi_j)}{2} \right)^p ,$$

with p large. These results confirmed earlier numerical work [9, 6]. The main ingredient of the proof was a similarity between such models and high-q Potts models, which allows one to adapt proofs for Potts models, first developed in [17], and based on [8], to prove first-order transitions in the temperature parameter for these N-vector models.

In this paper we extend our analysis to include RP^{N-1} (liquid-crystal) models (such as were first introduced by Lasher and Lebwohl [23, 22]) and lattice gauge models. We can then employ techniques for showing the existence of first-order transitions, such as have been used for Potts ferromagnets in d at least 2, as well as for Potts lattice gauge models in d at least 3 [17], to conclude that the corresponding nonlinear liquid-crystal and lattice gauge models, (with either abelian or non-abelian symmetries) have 1st order transitions.

The standard N-vector models are either believed or sometimes rigorously known to have 2nd order transitions in $d = 3$ or higher, a "Kosterlitz-Thouless" transition in $d = 2, N = 2$, and no transition for $d = 2$ and higher N [1]. In the XY-model ($N = 2$) for either $d = 2$ or high d these results are rigorous, for the other models there is a consensus based on both numerics and heuristic arguments.

In contrast, for the standard versions of the liquid crystal and lattice gauge models, as well as for very non-linear σ-models, both numerics and high temperature series suggested the existence of 1st order transitions, despite some theoretical analyses originally either suggesting 2nd order transitions, no transitions at all, or Kosterlitz-Thouless type transitions. For some of this literature, see e.g. [20, 23, 22, 11, 2, 32, 26, 28, 31] and references therein. Moreover, in the limit where N approaches infinity (the spherical limit) 1st order transitions were found, in dimension 2 or more [19, 33, 31]. This spherical limit result also holds for our nonlinear interactions in the ferromagnetic case [7]. Whether such a first-order transition can also occur for finite N larger than 3 in $d = 2$, or whether it might be an artefact of the spherical limit has for a long time been a matter of controversy (see for example [31, 33]). In fact, Sokal and Starinets described the existence of such a first-order transition as a "pathology". Our result finally settles this question: first-order phase transitions for models with continuous symmetry in $d = 2$ can occur, despite the conjecture to the contrary of [31]. Our results are essentially in agreement with the analysis of [33]. In contrast to what was suggested in most earlier analyses, the symmetry or the low-temperature properties of the model do not play a role of any great importance, and in fact for our nonlinear choice of interaction the spin-dimensionality N does not need to be large and can be as small as 2. The lattice dependence of the phenomenon found in [33] seems somewhat of an artifact, however, which disappears if one varies the nonlinearity parameter.

The fact that our proofs are insensitive to the nature of the phases between which the transition takes place implies that, similarly to the ferromagnetic cases, one might have in the liquid-crystal models a transition between a disordered high-temperature phase and either a nematically-ordered, a Kosterlitz-Touless or a disordered phase at low temperatures. Similarly one might find a transition either between a confining and a nonconfining – Coulomb-like – phase or between two confining phases in the lattice gauge models. Which one occurs in a particular case should depend on dimension and/or symmetry of the system.

In particular, we emphasize that our proof is also insensitive as to whether the symmetry group of the lattice gauge model is abelian – in which case it is expected that in 4 dimensions a transition between a confined and a Coulomb-like phase occurs [16, 12] –, or nonabelian, in which case both states are expected to confining, (this is also expected in general in $d = 3$). For a heterodox discussion on the difference between what is to be expected in abelian and nonabelian models, including some history of this problem cf [25].

We consider a lattice $\mathbb{Z}^d$, and either spin models in which the random variables live on the sites, or lattice gauge models where the variables live on the bonds (or links) of the lattice. The parameters of our models are the spatial dimension d, the spin-dimension N, and the nonlinearity parameter p. The "standard" versions of the models are obtained by taking $p = 1$.

For ferromagnetic models the variables are N-component unit vectors living on the N-sphere. We will discuss the argument in the 2-component case, in the general case the proof is essentially the same. The ferromagnetic models treated in [10] were given by

$$H = -J \sum_{<i,j>\in\mathbb{Z}^2} \left(\frac{1+\cos\left(\phi_i-\phi_j\right)}{2}\right)^p. \tag{1}$$

For liquid crystal RP^{N-1} models either one considers variables – usually denoted n_i – which live on the projective manifold obtained by identifying a point on the N-sphere with its reflection through the origin, or equivalently one can consider ordinary spins on the N-sphere, and divide out this "local gauge symmetry" afterwards. The last approach is the route we will pursue, as it allows us to literally transcribe the proof of [10]. Thus we consider Hamiltonians of the form

$$H = -J \sum_{<i,j>\in\mathbb{Z}^2} \left(\frac{1+\cos^2\left(\phi_i-\phi_j\right)}{2}\right)^p. \tag{2}$$

In [10] we call a bond "ordered" if the angle θ between two neighboring sites is small enough. Here we call it ordered if the angle $\theta \mathrm{mod} \pi$ is small enough. Then the argument of [10], based on [29] and [17] goes through without any changes. There is a first-order phase transition for p chosen large enough (in general the values of p for which the proof works depend on N and d) between a high-temperature regime in which most nearest neighbor bonds are disordered, and a low-temperature regime in which most nearest neighbor bonds are ordered. This holds for each dimension at least 2, and whereas the Mermin-Wagner theorem excludes nematic long-range order in $d = 2$ [24], in $d = 3$ and higher long-range order will occur [3]. Between the ordered and the disordered phase(s) free energy contours occur, whose probabilities are estimated to be uniformly small via a contour estimate valid over a whole temperature interval. In the contour estimate use is made of the Reflection Positivity [27] of the model. We remark that at low temperatures percolation of ordered bonds holds [14]; it follows from our results that the associated percolation transition is first order.

For lattice gauge models the variables are elements of a unitary representation of a compact continuous gauge group, e.g. $U(1)$, $SU(n)$, or sums thereof [30]. Here we present the argument in the simplest case of a $U(1)$-invariant interaction in 3 dimensions.

$$H = -J \sum_{plaquettes\ P\in\mathbb{Z}^3} L\left(U_P\right), \tag{3}$$

with $L(U_P) = \left(\frac{1+\cos(\phi_{e_1}+\phi_{e_2}-\phi_{e_3}-\phi_{e_4})}{2}\right)^p$. Here the e_i denote the 4 edges making up the plaquette P.

The effect of choosing the nonlinearity parameter p high is that the potential, although it still has quadratic minima, becomes much steeper and narrower. In this way one constructs in a certain sense a "free energy barrier" between ordered and disordered phases.

The lattice gauge model proof becomes similar to the arguments from [17]. When the product over the link variables is sufficiently close to unity, we'll call the plaquette "ordered", "disordered" otherwise. This distinction corresponds to unfrustrated and frustrated plaquettes in the Potts case. We will sketch the argument for the toy model where the potential $L(U)$ is chosen to be 1 if the sum ϕ_P of the oriented angles along the plaquette P is between $-\frac{\varepsilon}{2}$ and $+\frac{\varepsilon}{2}$ and zero otherwise. The generalization to the non-square well potentials can then be done in the same way as in [10]. The correspondence, as in [10], is that ε is of order $O(\frac{1}{\sqrt{p}})$.

Our strategy is to find bounds for free energy contours between ordered phases, in which one has mainly cubes with 6 ordered plaquettes, and disordered phases, in which most cubes have 6 disordered plaquettes. We need thus to estimate the weights of contours consisting of cubes which are neither ordered nor disordered. The number of possibilities for such cubes includes the 7 possibilities given in [17], except that now we have the additional 8th possibility of having cubes with one disordered plaquette on one side, and five ordered ones.

For the partition function Z_L on a cube B_L of size L^3 we use the (quite rough) lower bound

$$Z_L \geq max(Z_L^d, Z_L^o), \tag{4}$$

where Z_L^d (resp., Z_L^o) is part of the partition function, calculated over all configurations which have all plaquettes disordered (resp., mostly ordered). For the disordered partition function Z_L^d we obtain the lower bound $(1-4\varepsilon)^{3L^3}$ (we take a normalized reference measure, giving a weight 1 to each link).

For the ordered partition function Z_L^o we proceed as follows: we first choose a set of bonds T_L in B_L, which is a tree, passing through every site. For example, we can put into T_L all vertical bonds – z-bonds – except these connecting sites with z-coordinates 0 and 1, plus all y-bonds in the plane $z = 0$, except these connecting the sites with y-coordinates 0 and 1, plus all x-bonds of the line $y = z = 0$, except the one between the sites $(0, 0, 0)$

and $(1,0,0)$. The site $(0,0,0)$ can be taken as a root of T_L. Note that the number of bonds in T_L is L^3-1. Therefore it is not surprising (and easy to see) that for every edge configuration $\phi=\{\phi_b, b\in T_L\}$ there exists a unique site configuration $\psi=\psi_\phi=\{\psi_x, x\in B_L\}$, such that the following holds:

1. Let $\mathfrak{g}^\psi$ denote the gauge transformation, defined by the configuration ψ. Then $\left(\mathfrak{g}^\psi\circ\phi\right)\Big|_b=1$ for every bond $b\in T_L$;

2. $\psi_{(0,0,0)}=1$.

For every family of bonds $S\subset B_L$ let us define a bigger family $C(S)$, by the rules:

1. $S\subset C(S)$,

2. for every four bonds $\{b_1,...,b_4\}$, making a plaquette, such that three of them are in S, we have $\{b_1,...,b_4\}\subset C(S)$.

Then we can consider also the sets $C^2(S)=C(C(S))$, $C^3(S)$, and so on. Define $\mathfrak{C}(S)=\cup_k C^k(S)$. Note that the number of plaquettes in $\mathfrak{C}(T_L)$ is $3L^3-O(L^2)$. We claim now that for every configuration $\phi_{T_L}=\{\phi_b, b\in T_L\}$ one can specify (in a continuous way) a collection of arcs
$\left\{I_b=I_b(\phi_{T_L})\subset S^1, b\in\mathfrak{C}(T_L)\setminus T_L, |I_b|=\frac{\varepsilon}{4}\right\}$, such that for every configuration ϕ on B_L, which coincides with ϕ_{T_L} on T_L, and for which the values ϕ_b on the bonds $b\in\mathfrak{C}(T_L)\setminus T_L$ belong to the above segments I_b, all the plaquettes that fall into $\mathfrak{C}(T_L)$ are non-frustrated. That would imply that

$$Z_L^o\geq\left(\frac{\varepsilon}{4}\right)^{2L^3}\exp\left\{3J\left(L^3-O\left(L^2\right)\right)\right\}$$

by Fubini's theorem. To see the validity of our claim, consider first the case when the configuration $\phi_{T_L}\equiv\mathbf{1}\in S^1$ (here 1 is the neutral element). Then the choice of the segments I_b is easy: $I_b(\mathbf{1})=\left[-\frac{\varepsilon}{8},\frac{\varepsilon}{8}\right]$ for every $b\in\mathfrak{C}(T_L)\setminus T_L$. For a general ϕ_{T_L} let us take the corresponding gauge transformation $\mathfrak{g}^{\phi_{T_L}}$ (which is the identity for $\phi_{T_L}\equiv\mathbf{1}$), and we define our segments by

$$I_b(\phi_{T_L})=\left(\mathfrak{g}^{\phi_{T_L}}\right)^{-1}I_b(\mathbf{1}).$$

This provides a lower bound

$$Z_L \geq \max\left[(1-4\varepsilon)^{3L^3}, \left(\frac{\varepsilon}{4}\right)^{2L^3} \exp\left\{3J\left(L^3 - O\left(L^2\right)\right)\right\}\right]. \tag{5}$$

This bound on the partition function as the maximum of the ordered and disordered term is similar to the argument in [10]. It plays the same role as the bound in terms of a fixed energy partition function given in [17].

To obtain our contour estimates, by Reflection Positivity we need to estimate the partition functions of configurations constrained to have a "universal contour". The estimates of the 7 types of universal contours mentioned in [17] are of a similar form as in that paper with the number of Potts states q up to some constants replaced by $\frac{1}{\varepsilon}$. The universal contour due to the new case of cubes with one disordered plaquette consists of configurations in which the horizontal plaquettes in every other plane are disordered, and all the other ones are ordered. These configurations have a similar entropy contribution to the partition function as the ordered configurations, but the energy per cube is $\frac{5}{6}$ of that of a cube in the fully ordered situation. For ε small enough (which corresponds to p large enough) also such a contour is suppressed exponentially in the volume. The combinatorial factor in the contour estimate changes by some finite constant, which choosing ε small enough takes care of.

To summarize we have obtained the following results:

Theorem 1 *For any nonlinear RP^{N-1} model in dimension 2 or more and p high enough, there is a first order transition, that is, there exists a temperature at which the free energy is not differentiable in the temperature parameter.*

Theorem 2 *For lattice gauge models with plaquette action $\left(\frac{1+L(U_P)}{2}\right)^p$, (where $L(U_P) = Tr(U_P + U_P^*)$) in dimension 3 and more and p high enough, there is a first order transition, that is there exists a temperature at which the free energy is not differentiable in the temperature parameter.*

Here U_P^* denotes the adjoint operator of U_P.

This seems to be the first case in which a first order transition for a lattice gauge model with a continuous gauge symmetry group is rigorously obtained. Whereas the example of the Potts lattice gauge model in $d = 3$ or higher is between a confining and a nonconfining phase [18, 21], in our theorem this is to be expected in $d = 4$, with $U(1)$ symmetry only. For $d = 3$ and also for

$SU(n)$ in $d = 4$ we conjecture that confined phases exist on both sides of the phase transition.

Our proof only gives results for very high p. We will discuss some further aspects of what may actually be the p-values for which to expect first-order transitions, and what one might hope to prove. The recent work of Biskup and Chayes [4] shows that if a reflection positive model has a phase transition in mean field theory, then also at sufficiently high dimension a first-order transition occurs. They include in their discussion the RP^{N-1} model for $N = 3$, for which even for $p = 1$, a first-order transition is derived. The mean field analysis of [5] indicates that a similar result for the ferromagnetic case holds if $p = 3$. For lattice gauge models also the standard actions lead to first order transitions in mean-field theory [35], section 34.4, which indicates a first order transition in sufficiently high dimension.

If one believes that here the spherical (N to infinity) limit is not singular (which has been a matter of controversy itself), then for the square lattice, N large and p larger than 6 the ferromagnet might have a first order transition, while for the RP^{N-1} case on the square or triangular lattice even for $p = 1$ a first order transition occurs, while for the hexagonal lattice one presumably needs a higher value of p [31, 33].

As mentioned before, numerical work suggests that in the standard ($p = 1$) Lebwohl-Lasher model with $N = 3$ as well as in the $U(1)$-lattice-gauge model a first order transition should occur; however, this seems far away from any provable result.

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