First-order transitions for very nonlinear sigma models.

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Abstract. In this contribution we discuss the occurrence of first-order transitions in temperature in various short-range lattice models with a rotation symmetry. Such transitions turn out to be widespread under the condition that the interaction potentials are sufficiently nonlinear.

In memory of John Lewis, who by his kind guidance and excellent scientific and professional sense has always been a stimulus and an inspiration.
1 Introduction

One of the main predictions of the Renormalisation Group (RG) theory is what is called “universality”. This means that in great generality the nature of the phase transition between high-temperature and low-temperature phases and the corresponding critical exponents depend only on dimension, symmetry and the range of the interaction. Here range means short-range (finite-range or sufficiently fast decaying with distance) or long-range (slowly decaying at large distances). The classical Landau mean-field theory similarly predicts that the nature of the spontaneously broken symmetry determines the order of the transition. Although in many cases such RG predictions have been confirmed, there are some examples where, somewhat unexpectedly, first-order instead of the predicted second-order (or absence of any) transitions were observed, see e.g. [5, 30, 45, 46].

In some cases, such as the nearest-neighbour $q$-state Potts models, one might think that it is the nature of the broken (permutation) symmetry which governs whether there is a first-order (at high $q$) or a second-order (at low $q$) transition. But the generalization of this statement is hard to make. Indeed, as Onsager [20] already knew, there seems to be no general method to predict whether a transition is first-order or second-order. For example, it was shown in [25] (which extended the related work of [5]) that a 3-state Potts model in dimension two, with an interaction of finite but large range, has a first-order transition, while for the nearest-neighbour model the transition is of second order.

In this contribution, we review results from [17, 18] where we exhibited a different class of models. Though they possess global rotation symmetries, they undergo first-order transitions, whereas the universality predictions of the RG suggest second-order transitions. More precisely, for short-range ferromagnetic, $d$-dimensional, rotation-invariant $n$-vector models standard lore [1] (which as we here show can be violated) predicts the following (“universal”) behaviour:

- If $d = 2$, there is a unique Gibbs measure at any positive temperature. For $n = 2$ (classical XY spins – or the “nonlinear sigma model” in field theoretical language) there is nevertheless an infinite-order transition between a low-temperature Kosterlitz-Thouless phase with slowly decaying correlations and a high-temperature phase with exponential correlation decay. For higher $n$ there is no phase transition.

- If $d = 3$ or higher, there is a second-order transition between a magnetized low-temperature phase and a high-temperature phase. If $d = 3$, one has $n$-dependent critical exponents, in higher dimensions one obtains mean-field exponents.
Below we present a rather wide class of models in which this standard lore is violated.

2 Notation and some background

For general background on the theory of Gibbs measures we refer to [16, 23, 24, 43, 42]. We will consider spin models defined on the lattice $\mathbb{Z}^d$ with spins taking values on the $n$-dimensional unit sphere.

We will use small Greek letters $\sigma, \eta, \ldots$ to denote spin configurations in finite or infinite boxes. The nearest-neighbour Hamiltonians in a box $\Lambda$, for which we take a $d$-dimensional torus, will be given by

$$H^\Lambda(\sigma) = \sum_{\langle i,j \rangle \subset \Lambda} U(\sigma_i \cdot \sigma_j) + \sum_{i \in \Lambda} h \cdot \sigma_i.$$  \hspace{1cm} (1)

Associated to these Hamiltonians $H^\Lambda(\sigma)$ are Gibbs measures

$$\mu^\Lambda(d\sigma) = \frac{1}{Z^\Lambda} \exp\left[-H^\Lambda(\sigma)\right] \mu^\Lambda_0(d\sigma)$$  \hspace{1cm} (2)

Here $\mu^\Lambda_0(d\sigma)$ denotes the rotation-invariant product measure. The choice of the function $U$ of the inner product between the spins at neighbouring sites will determine our model. We will study only the case of nearest-neighbour interactions. The reason is that our method is based on the use of certain correlation inequalities, called chessboard estimates, see below. These inequalities hold once the measures $\mu^\Lambda$ have the Reflection Positivity (RP) property, see again below, which RP holds for the n.n. interactions, see [23, 58].

The choice

$$U(x) = -x$$  \hspace{1cm} (3)

provides the standard classical XY and Heisenberg models. Equivalently, as a function $W$ of the difference angle $\theta$ between neighbouring spins, this means choosing

$$W(\theta) = U(\cos(\theta)) = -\cos(\theta)$$  \hspace{1cm} (4)

3 Results, and some remarks on proofs.

In this section we describe our results on the nonstandard $n$-vector models.
We start with the case of zero field \( h = 0 \) and \( d = 2, n = 2 \), so we have classical \( XY \) spins in two dimensions. This seems to be the first case which was considered in the literature \cite{15} as an example of the phenomenon we display. However, the arguments in that paper – which we here prove to be correct – were later contested \cite{28,26}. The original choice of \cite{15} was

\[
W(\theta) = -\left(\frac{1}{2}(1 + \cos\theta)\right)^p
\]

with \( p \) large enough. A simpler but essentially similar model was introduced in \cite{3}:

\[
W(\theta) = \begin{cases} 
-1 & \text{if } |\theta| < \varepsilon, \\
0 & \text{otherwise},
\end{cases}
\]

where the parameter \( \varepsilon \) is small enough.

Both these potentials have the form of a deep (depth = 1) and narrow (width \( \sim \frac{1}{\sqrt{p}} \), cf width = \( 2\varepsilon \)) well, compared to the standard, rather shallow-well, cosine shape.

The second model is a square well (or a top hat) potential, in which the distinction between being in or out of the well is unambiguous, in the first model there is a slight arbitrariness, and one has to make a choice to fix it.

First we notice that by the Mermin-Wagner theorem \cite{35,14,27,36}, all Gibbs measures are rotation-invariant, so that the spontaneous magnetisation is necessarily zero. This does not prevent, however, the presence of multiple Gibbs measures (as was known already from the model of \cite{41}, where a discrete, chiral, symmetry was shown to be broken).

Our first result is about the square-well model:

**Theorem**

For \( \varepsilon \) small enough, there is a transition temperature where two Gibbs measures, an “ordered” one and a “disordered” one, coexist. In the ordered state most bonds are ordered, in the sense that the two spins at its ends have a difference angle smaller than \( 2\varepsilon \) (they are in the well), in the disordered state the opposite is true.

**Remarks about the proof:** The proof is a fairly straightforward application of the Reflection Positivity, chessboard estimates method, which was developed by Dyson, Fröhlich, Israel, Lieb and Simon \cite{38}. For the benefit of the reader we recall these concepts.

Let \( R_L \) be a reflection of our torus \( \Lambda \) in some plane \( L \) passing through its sites. (To have such a symmetry plane, \( \Lambda \) has to be of even size.) Then \( L \) cuts \( \Lambda \) into two halves, \( \Lambda_+ \) and \( \Lambda_- \), so that \( R_L(\Lambda_\pm) = \Lambda_\mp \). Let \( \Lambda_0 = \Lambda \cap L \); in the case \( d = 2 \) this intersection is a pair of meridians of \( \Lambda \). Let us consider the conditional distribution
of the measure $\mu^\Lambda$ under condition that the restriction $\sigma_{\Lambda_0} \equiv \sigma \mid_{\Lambda_0}$ is fixed. Then it is easy to see that for every value of $\sigma_{\Lambda_0}$ the conditional measure $\mu^\Lambda (\cdot \mid \sigma_{\Lambda_0})$ splits into a product of two identical measures, $\mu_{\Lambda^\pm, \sigma_{\Lambda_0}}^\Lambda$, living on corresponding halves, with $R_L (\mu_{\Lambda^\pm, \sigma_{\Lambda_0}}^\Lambda) = \mu_{\Lambda^{\mp, \sigma_{\Lambda_0}}}^\Lambda$. From that it follows immediately that for every function $C (\sigma_\Lambda) = C (\sigma_{\Lambda^+})$, depending only on the “left” variables $\sigma_{\Lambda^+}$, we have

$$\int C R_L C \, d\mu^\Lambda \geq 0. \quad (7)$$

The Reflection Positivity property is precisely the validity of this inequality. The details can be found in [23], Theorem 17.21. Note that one can choose the symmetry plane $L$ arbitrary, so in fact we have many such inequalities, and one corollary of this set of inequalities is the following chessboard estimate.

To describe the simplest example of such an estimate let us consider a random variable $D (\sigma_\Lambda)$, which depends on just one spin value, $\sigma_0$, where $0 \in \Lambda$ is the origin. Then for its expected value $\langle D (\sigma_0) \rangle_{\mu^\Lambda} \equiv \int D (\sigma_0) \, R_L (\sigma_\Lambda) \, d\mu^\Lambda (\sigma_\Lambda)$ we have

$$\langle D (\sigma_0) \rangle_{\mu^\Lambda} \leq \left[ \prod_{x \in \Lambda, x \text{ is even}} D (\sigma_x) \right]_{\mu^\Lambda}^{\frac{4}{|\Lambda|}} . \quad (8)$$

Here $D (\sigma_x)$ is the same function $D$, computed at value $\sigma_x$, and we take a product over all sites $x$ with both coordinates even. Note that if the interaction $U$ is identically zero, then the measure $\mu^\Lambda$ is just the product measure $\mu^\Lambda_0 (d\sigma)$, and the last inequality becomes an equality.

Applying this kind of chessboard estimate to various observables it is fairly straightforward to show that at low temperatures most bonds are ordered and that at high temperatures most bonds are disordered. The main step then left is to prove that uniformly for all temperatures in a temperature interval, including both high and low temperatures, the probability for two arbitrary bonds to be different (one ordered, one disordered) is small. Indeed, the only way these two properties can hold simultaneously is the existence of an intermediate temperature at which both the ordered and the disordered phase coexist.

We will explain now how an estimate of the probability that a certain bond $b_1$ is ordered, while another one, $b_2$, is disordered, can be obtained. If such an event happens, then there exists a contour $\gamma$, separating $b_1$ and $b_2$, formed by sites which have a pair of orthogonal bonds, one of them being ordered and another disordered. For example, one obtains such a contour by taking the appropriate
component of the boundary of the set of ordered bonds, containing the bond \( b_1 \). Therefore it is enough to obtain a Peierls-type contour estimate, which shows that long contours are improbable. More precisely, we need to show that the probability for the occurrence of a contour \( \gamma \) of size \(|\gamma|\) is exponentially small in \(|\gamma|\).

By using again the chessboard estimate, it is possible to show that it is enough to obtain the desired estimate for just one single contour, \( \Gamma \), called the universal contour. This universal contour contains all bonds of \( \Lambda \): half of them are ordered, and the remaining half are disordered. In our case the event \( \Gamma \) happens iff all the bonds adjacent to sites \( x \) with \( x_1 + x_2 = 0 \mod 4 \) are ordered, while those adjacent to sites with \( x_1 + x_2 = 2 \mod 4 \) are disordered. Since the size \( |\Gamma| = |\Lambda| \), we have to show that

\[
\Pr (\Gamma) \leq \exp \left\{ -c |\Lambda| \right\}
\]  
(9)

with the constant \( c \) sufficiently large. (The concept of a "universal contour" goes back to the pioneering paper by Fröhlich and Lieb [21].

The remaining computations go just as in the proof for the large-\( q \) Potts model, given in detail in [29] or [40]. This similarity with the Potts problem was already remarked upon in [15]. The correspondence is that \( \varepsilon \), and the same holds for \( \frac{1}{\sqrt{p}} \), plays the role of the small parameter \( \frac{1}{q} \). To estimate the probability of the universal contour, one has to integrate over all configurations such that the prescribed arrangement of ordered and disordered bonds occurs. To do it we observe that the total partition function of an \( N \)-by-\( N \) square satisfies

\[
Z_N \geq \max\left[ 1, \left( \frac{1}{2} \varepsilon \exp (2\beta N^2) \right)^N \right].
\]  
(10)

Indeed, on the one hand we use that the potential is positive, and on the other hand we get a lower bound by taking the integral at each site over the interval \([ -\frac{1}{2} \varepsilon, \frac{1}{2} \varepsilon ]\), so that each bond is ordered.

The restricted partition function \( Z_\Gamma \), which is the integral over all configurations compatible with the universal contour satisfies

\[
Z_\Gamma \leq (2\varepsilon)^{\frac{1}{4} N^2} \exp \left\{ \frac{\beta N^2}{2} + O(N) \right\}.
\]  
(11)

From these two estimates the bound (9) follows.

The final conclusion is now, that somewhere inside our temperature interval there is a value \( \beta_t \), at which a first-order transition happens between an ordered and a disordered Gibbs measure, as was first numerically found in [15]. The value of \( \beta_t \) is approximately given by \( 2\beta_t = -\ln \varepsilon \).
The non-square-well model can be treated in a very similar way (see [17, 18] and also [7]). The ordered Gibbs measure has a polynomial spin-spin correlation decay of Kosterlitz-Thouless type.

**Generalisations:**

1) The same method of proof works if either the spin dimensionality $n$ or the dimension $d$ of the lattice is larger than 2 (or both). For the case of Heisenberg spins ($n = 3$) in $d = 2$, the first-order transition was first found numerically [10, 9]. In this case presumably both the low-temperature and the high-temperature phase have exponential decay of the spin-spin correlations. For the $n \to \infty$ spherical limit see also [11, 12].

For $d \geq 3$, the Mermin-Wagner theorem does not apply anymore, and the low-temperature phase now displays a spontaneous magnetisation.

2) In a small external field there still is a first-order transition between an ordered (strongly magnetised in the direction of the field) and a disordered (weakly magnetised in the direction of the field) phase, which now we expect to be both pure phases (extremal Gibbs measures) also in higher dimensions.

3) Instead of a single well, one can also consider potentials having the shape of repeated wells in wells (or a hat-in-a-hat-in-a-hat...), which give rise to possibly infinitely many transitions. A choice of such a Seuss [39] potential is $U(x) = -\sum_n 2^{-n} \varepsilon_n(x)$ with $\varepsilon_n(=\varepsilon^3_{n-1}) = \varepsilon^{3n-1}$, with the first $\varepsilon$ small enough. Such transitions in which one keeps jumping in deeper and deeper wells, can occur either between nonmagnetised-nonmagnetised, magnetised-nonmagnetised or magnetised-magnetised Gibbs measures, and the nonmagnetised measures may display either exponential or Kosterlitz-Thouless decay.

4) Instead of ferromagnetic models the argument also works for nematic liquid crystal $RP^n$ models [32, 33], in which one considers interactions of the form $U(x) = -x^{2p}$ for which there are two minima on the interval $[-1, +1]$. Here even for $p = 1$, and $n = 3$, first-order transitions were found numerically (see e.g. [30, 31, 37]) in $d = 3$, whereas the occurrence of a transition in the limit $n \to \infty$ in $d = 2$ has been a matter of controversy [45, 46]. Additional numerical references are mentioned in [18]. Further models of this type, with a larger number of sharp minima, combined with a term causing a chiral symmetry breaking as in [41], are considered in [34].

5) Similarly as for the Potts gauge model of [29], we can prove the existence of a first-order transition in various nonlinear lattice gauge models with continuous symmetries. In some of these models first-order transitions were initially concluded on the basis of numerical data (see e.g. [19, 2, 44]). In [18] we provide
the first occasion where a first-order transition for a lattice gauge model in the presence of a continuous symmetry can be proven.

6) Instead of the above spin systems with a compact rotation symmetry, one can also consider continuous unbounded-spin systems which possess a non-compact symmetry (that is, they are “massless”). In this case the symmetry describes a shift in the height (average) of the spin. Again a similar construction works [8], now showing coexistence of “gradient Gibbs measures”.

7) For quantum spin systems the ingenious analysis of [6] shows that again a first-order transition occurs, once the potential is sufficiently nonlinear and the spin number is large enough.

4 Conclusions and Comments

In many cases, some of them also of direct physical interest, first-order transitions occur instead of the second-order transition, which a naive universality argument would predict. Such first-order transitions tend to occur more easily when either the nonlinearity parameter \( p \), the spin-dimensionality \( n \) (the spherical limit), or the dimension \( d \) of the lattice (the mean-field limit, [4]) is large.

In this paper we have presented a number of models where we can prove these transitions for sufficiently strong nonlinearities. Furthermore, if one adds an external field, the transition persists. Although the two phases on both sides of the transition can have different characters (breaking other symmetries, having polynomial or exponential decay of the spin-spin correlations, etc), it can be shown that no “intermediate” phases exist (there is a “forbidden gap” for the energy variable [7]).

The method of Reflection Positivity we use here has the disadvantage that one is limited in the interactions one can take, in the sense that they need to be defined on the unit cube. As compared to the more robust Pirogov-Sinai contour methods, RP methods have the advantage, however, that they are more generally applicable in that we need no information about the phases on both sides of the transition. For Pirogov-Sinai methods to work, however, the phases need to be pure and will typically have some kind of exponential decay of correlations. On the other hand, with RP methods it has not been possible up to now to obtain results for surface or interface properties or about the completeness of the phase diagram.

If one varies the nonlinearity parameter in \( d = 2 \), one moves towards a critical point where the second-order transition is expected to have Ising characteristics, in higher dimensions varying the nonlinearity parameter will lead one to a tricritical point.
Although our proofs require a fairly large nonlinearity (that is, a large value of $p$, or a small value of $\varepsilon$), either by numerical methods or in the large-$n$ or large-$d$ limit we expect, and sometimes know, that the type of first-order transitions we studied will occur for much smaller values of $p$, $n$, and/or $d$, especially for the liquid-crystal models.

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