First-order transitions for some generalized XY models

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Abstract. In this note we demonstrate the occurrence of first-order transitions in temperature for some recently introduced generalized XY models, and also point out the connection between them and annealed site-diluted (lattice-gas) continuous-spin models.

1 Introduction

In some recent papers [28, 8, 25, 24] a class of *generalized* XY models was introduced and studied. These models are ferromagnetic and, in the simplest case, restricted to a nearest-neighbour XY - type interaction. In contrast to the *plane rotator* interaction, they involve 3-component spins (just as the classical Heisenberg model does) and they possess an $O(2)$ symmetry with respect to the X and Y components. This part is multiplied by a product of single-site terms, depending on the third (Z) component only, which is raised to an exponent $p > 0$. In the following, this factor will be simply called "single-site term".

For $p = 1$ one recovers the standard ferromagnetic XY model, in which the interaction is defined by the scalar product of the nearest neighbour spin projections on the XY - plane.

With the help of some correlation inequalities it was found [28] that in $d = 2$ there is a transition between a low-temperature Berezinskiĭ-Kosterlitz-Thouless (BKT) phase and a high-temperature phase, whereas, in $d \geq 3$ dimensions, the existence of magnetic order at low temperatures was established.

The nature of this transition, however, was left open in these works. In $d = 2$ one might expect either a BKT scenario (an infinite-order transition between the BKT phase and a high-temperature phase), which was found when this exponent p is small, or a first-order one between the BKT phase and the high-temperature phase , and in $d = 3$ there may be an ordinary second-order transition (again found for small p), or a first-order transition. Recall that the first-order transition means coexistence of different infinite-volume Gibbs measures. Here this implies a jump in the energy density, in $d \geq 3$ (but not in $d = 2$) accompanied by a jump in the magnetisation.

In this note we point out that, by a minor adaptation of the reflection positive chessboard-estimates analysis for free-energy contours (which goes back to [9, 21] and which was recently applied to study magnetic transitions for *nonlinear* classical vector spin models in [12, 13, 14, 4, 22]), the occurrence of a first-order transition for sufficiently *large* values of the exponent p can be proven. Such a transition was already suspected to occur in $d = 2$, based on the numerical data of [24]. In the last part of our paper we compare this result with further numerical data.

We remark that with some small modifications our analysis covers also the case of the first-order instead of e.g. a BKT infinite-order transition in some *annealed* diluted lattice-gas models (see [6], [18], Sect. 2.4, and [7]), and even in some *continuum* magnetic systems [19]. In this case the role of the nonlinearity is played by terms involving either the lattice-gas particle occupation numbers [6, 18, 7], or the particle density [19]. This becomes in particular evident, when we consider the model of [28] in the *square-ditch* approximation, see (2). Then the generalized XY model reduces to an annealed site-diluted *plane rotator* model.

With minor modifications we can also treat generalized (3-component Heisenberg interactions for n-vector spins with $n \geq 4$) or annealed dilute Heisenberg models. In that case we expect that in $d = 2$ there will be a transition between two phases with exponentially decaying correlations, similarly to what is expected for the nonlinear models of [12, 13].

2 Model, proofs and results

For general background on the theory of Gibbs measures on lattice systems we refer to [11, 16, 17, 32, 31]. The method of reflection positivity and chessboard estimates [27] is reviewed in [30] and in the last 4 chapters of [16]. The fact that our models satisfy the property of reflection positivity follows immediately from the conditions described there.

Our systems are as follows. On each site of the lattice $\mathbb{Z}^d$ we have a three-component unit spin, described by spherical coordinates ϕ and θ; our models are then described by a nearest neighbour generalized XY interaction, i.e. the plane rotator interaction in the ϕ-variables combined with a product of p-powers of single-site terms in the θ-variables [28]. For a finite $\Lambda \subset \mathbb{Z}^d$ the (dimensionless) Hamiltonian reads:

$$H^{\Lambda}(\phi,\theta) := -\sum_{\langle i,j\rangle\subset\Lambda} [\sin(\theta_i)\sin(\theta_j)]^p \cos(\phi_i - \phi_j) \tag{1}$$

The integer exponent $p > 0$ is a parameter in our model, and a large value of p means that spins can only interact noticeably when they are in a narrow *ditch* around the equator $\theta = \pi/2$, whose width is of order $O(1/\sqrt{p})$. This narrow and deep ditch plays a similar role as the narrow-well potentials of [12, 13, 4].

We present our proof for the *two-dimensional* model where the ditch has a *square*, instead of a polynomial, shape. Extensions to polynomial shapes then can be done as in [12, 13, 4]. Indeed, our proof can be seen to be almost a corollary of these papers, to which we refer for further details.

So, we consider the *square-ditch* approximation of the generalized XY model (1) with Hamiltonians

$$H_{\varepsilon}^{\Lambda}(\phi,\theta) := -\sum_{\langle i,j\rangle\subset\Lambda} n(\theta_i)n(\theta_j)\ \cos(\phi_i - \phi_j)\ ,\ \ n(\theta) := 1_{\varepsilon}(\theta)\ , \tag{2}$$

where $1_{\varepsilon}(x)$ denotes the characteristic function of the interval $[\pi/2 - \varepsilon, \pi/2 + \varepsilon]$.

The square-ditch approximation (2) implies that two spins can interact only when they both are in the ditch; in other words, one can interpret (2) as the Hamiltonian of annealed site-diluted plane rotator model with lattice-gas occupation numbers $n = 0, 1$, as discussed in [6, 7], and as is also suggested by the notation.

Notice that the (*a priori*) one-site distribution of those numbers is induced by the uniform probability θ-measure on the interval $[0, \pi]$. Therefore, ε is related to the chemical potential ν that governs the lattice-gas overall particle density. By the standard definition of the lattice-gas chemical potential we obtain:

$$\nu = \beta^{-1} \ln \frac{2\varepsilon}{\pi - 2\varepsilon}\ , \tag{3}$$

where $\beta^{-1} = \Theta$ denotes the (dimensionless) temperature of the system. Hence at fixed temperature the chemical potential becomes negative and large in magnitude when ε is close to zero, which corresponds to a small lattice-gas density; whereas for $\varepsilon \to \pi/2$, i.e. for $\nu \to +\infty$, one obtains a non-diluted plane rotator model (2) with $n(\theta) = 1$ for all θ.

For the proof we consider in a two-dimensional lattice a square Λ, of a linear size N which is a multiple of 4, with *periodic* boundary conditions. Associated to Hamiltonians $H_{\varepsilon}^{\Lambda}(\phi,\theta)$ are Gibbs measures

$$\mu^{\Lambda}(d\phi, d\theta) = \frac{1}{Z^{\Lambda}} \exp[-\beta H_{\varepsilon}^{\Lambda}(\phi,\theta)]\mu_0^{\Lambda}(d\phi, d\theta)\ ,$$

which are *reflection positive* (RP). Here μ_0 denotes the rotation-invariant product measure, and β is the dimensionless inverse temperature.

RP is the key property for the *chessboard estimates*. They allow us then, following e.g. [13], to obtain *contour* estimates. First we can establish the estimate on the partition function

$$Z^\Lambda \geq 1$$

and furthermore, by integrating over intervals $|\theta| \leq \varepsilon$ and $|\phi| \leq \pi/20$, we see that also

$$Z^\Lambda \geq (C_1\,\varepsilon \exp(2C_2\beta))^{|\Lambda|}$$

with constants C_1 and $C_2 = \cos(\pi/20)$ (which is close to 1) which are independent of ε.

On the other hand, let us call a site *ordered*, if the spin on that site, as well as all its neighbours, are in the ditch, and *disordered*, if it is not in the ditch, and consider the same universal contour as in [30, 13], consisting of alternating diagonals at distance 2, which, in turn, consist of ordered and disordered sites (separated by sites which are neither); thus we find that the restricted partition function obtained by integrating all configurations compatible with the universal contour satisfies

$$Z^\Lambda_{univcont} \leq ((2\varepsilon)^{3/4} \exp(\beta))^{|\Lambda|}.$$

Then, just as in the proof of Theorem 1 of [12] we obtain

$$\frac{Z^\Lambda_{univcont}}{Z^\Lambda} \leq \varepsilon^{|\Lambda|/(4+C_3)}$$

with C_3 some constant determined by the choice of C_1 and C_2.

This implies by standard arguments that, when ε is chosen small enough, contours separating ordered and disordered sites are suppressed, uniformly on a temperature Θ interval; since at low temperatures most sites are ordered and at high temperatures most sites are disordered, there will be a temperature, where disordered and ordered phase(s) (or infinite-volume Gibbs measures) *coexist*.

We notice that by the Mermin-Wagner theorem [23, 10, 20, 26], in two dimensions all Gibbs measures are rotation-invariant, so that the spontaneous magnetisation is necessarily zero. Since the results of [28] imply that the generalized XY models (1) at low temperatures display a BKT phase, our present statement says that for these models with high-exponent-p-potentials the transition between this phase and the high-temperature one is first-order.

In the three-dimensional version of the model (1), however, the low-temperature phase is magnetized, but again the transition in temperature to the high-temperature regime is first-order.

Notice also that in general proofs involving contour arguments do not provide very sharp estimates about the optimal parameter values for which a first-order transition appears, therefore we will not pursue this road. Below we discuss what we expect to be the situation based on numerical data, that is, which is the value of the parameter p above which one might expect the first-order transition to appear.

Before ending this section, let us go back in some more detail to the lattice-gas interpretation of the square-ditch approximation (2).

The theorem just proven implies that, for $d = 2$, the XY lattice-gas model possesses a first-order transition on a suitable curve in the (Θ, ε)-plane. This answers an open question from [7] about the first-order phase transition in $d = 2$ diluted plane rotator model (2). On the whole our results complement those of [7, 19] and [28] for this model, since they concern different parts of the phase diagram in the (Θ, ν)- or in the (Θ, ε)-plane, as well as the mechanism of the phase transition.

For example, in [19] the existence of the low-temperature BKT phase in the diluted plane rotator model is proven for a relatively large *positive* ν, but without any conclusion on the mechanism connecting low-temperature and high-temperature behaviour. On the other hand, the Ginibre and the Wells inequalities applied to this model (in the same way as it was done for the generalized XY model in [28]) ensure the existence of a low-temperature BKT phase for *any bounded* ν, but again without conclusion on the mechanism of the transition.

Moreover, the same analysis leads also to the existence of a low-temperature BKT phase for generalized XY models with annealed site-dilution, for all ν, similarly to what happens for the plane rotator model.

In [7] the first-order phase transition with simultaneous jumps of magnetization and particle density was established in the $d > 2$ diluted plane rotator model in some domain of both types of ν (*positive* and *negative*) at very low temperatures.

In the present note we find (as a byproduct of our generalized-XY-model analysis) a first order-phase transition in the diluted plane rotator model (2) for *moderate negative* ν, since we consider in (3) sufficiently small ε as well as sufficiently small Θ. As mentioned before, this answers positively the question from [7] about the first-order phase transition in model (2), at least for those ν.

Based on [6], one knows that staggered states may be involved in the mechanism of a first order transition at positive chemical potentials, at intermediate temperatures; this will not happen in the regime of negative chemical potentials which is covered by our results.

3 Related results and extensions

Extensions of the above theorem to other pair interaction potentials are also possible.

For example, the models studied in [12, 13, 14, 4] involve $n-$component spins for any ($n \geq 2$) and possess an $O(n)$ symmetry. Indeed, their interactions are functions of the *scalar product* between the two interacting spins, having the shape of a narrow well.

The spin interaction in [18], Sect. 2.4, is of the same type and may be viewed as a diluted version of the Patrascioiu-Seiler model with a *narrow-ditch interaction*. For discussion of its low-temperature phase see e.g. [1].

The proof scheme indicated above works for various *combinations* of *single-site* terms and *nearest neighbour* interaction terms, of which at least some need to have a narrow shape. The spins can be n-component spins, and the symmetry can be *green*either O(n) or O(2) or some symmetry in between. For example, we might have narrow-ditch single-site potentials (as mentioned above), or narrow-well single-site potentials as in [9], as well as narrow-well interactions ([12, 13, 14]) or narrow-ditch interactions (see [18], Sect. 2.4, and [2]). The interactions can have *one* well (or ditch) for ferromagnets, *two* (for liquid crystal models, possessing $RP^{(n-1)}$ symmetry), or more and could also include diagonal nearest neigbour terms (as in [22], inspired by the model [29]). The narrowness of such terms then either creates or reinforces the first-order behaviour.

Another kind of possible extensions is related to *quantum* versions of our models. This observation is inspired by the recent paper [2], which studies, in particular, a non-linear quantum XY model. The main ingredient for their arguments is the *quantum* RP property, which is a quite subtle matter, but the *ferromagnetic* quantum XY model does verify it. Since in (2) the interaction terms are multiplied by simple single-site classical random variables (the scalar occupation numbers), the square-ditch Hamiltonian also verifies the *quantum* RP property. Then according to [2] we can claim the existence of the first order phase transition in this quantum model, since we proved it for the classical model (2) and we know that its quantum analogue verifies the quantum RP property.

4 Numerical estimates of transition orders and temperatures

When $d = 3$, a Mean Field (MF) study of the ordering transition is at least qualitatively correct, and relatively feasible in computational terms; moreover, this treatment can be refined by using various cluster-variational techniques; we used here a Two-Site Cluster (TSC) approach, and both treatments follow Ref. [28]. Calculations were carried out for $5 \leq p \leq 12$, and then $p = 12, 16, 20$.

In both cases we found that, upon increasing p, the transition changes from second to first order; the two treatments exhibited different thresholds, i.e. a threshold of p between 5 and 6 for MF, and a threshold of p between 10 and 11 for TSC; results of both treatments are presented and compared in Tables (1) and (2), where first-order transitional properties, such as the energy jump, ΔU^*, and the order parameter at the transition, $\overline{M}$, are shown for $p \geq 11$, where both treatments predict a first-order transition.

As a side remark, we also notice that the results of [3] imply the existence of a first-order transition for any $p \geq 6$ in sufficently high dimension.

On the other hand, simulation results, obtained for $d = 3$ and to be reported elsewhere [5], show a second-order transition for $p = 8$, and suggest a first-order one for $p = 12, 16, 20$.

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Table 1: MF results for transitional properties of the generalized XY models in three dimensions, obtained with different values of the exponent p.

p	Θ_{MF}	type	ΔU^*	$\overline{M}$
5	1.1082	II		
6	1.0287	I		
7	0.9741	I		
8	0.9336	I		
9	0.9019	I		
10	0.8762	I		
11	0.8548	I	1.2336	0.7506
12	0.8366	I	1.3140	0.7687
16	0.7836	I	1.5355	0.7836
20	0.7486	I	1.6712	0.8387

Table 2: TSC results for transitional properties of the generalized XY models in three dimensions, obtained with different values of the exponent p.

p	Θ_{TSC}	type	ΔU^*	$\overline{M}$
5	1.1011	II		
6	1.0416	II		
7	0.9935	II		
8	0.9537	II		
9	0.9199	II		
10	0.8907	II		
11	0.8659	I	0.3242	0.3994
12	0.8461	I	0.5437	0.5098
16	0.7906	I	1.0097	0.6721
20	0.7549	I	1.2578	0.7374