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

According to the predictions of the Renormalisation Group (RG), "universality" holds. This means that in great generality the nature of the phase transition between high-temperature and low-temperature phases, and more in particular the corresponding critical exponents, will depend only on dimension, symmetry and the range (short-range or long-range) of the interaction. The classical Landau mean field theory similarly predicts that the nature of the sponataneously 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, 27, 42, 43].

In some cases, such as for the nearest-neighbour q-state Potts models, one might think that it is the nature of the broken (permutation) symmetry which seems to govern whether there is a first-order (at high q) or a second-order (at low q) transition. However, this is not really the case in general. Indeed, as Onsager [18] already knew, there seems to be no general method to predict whether a transition is first-order or second-order. For example, an essentially short-range (large but more or less finite-range) 2-dimensional 3-state Potts model with a first-order transition (as opposed to the nearest-neighbor second-order transition) was found in [5].

In this contribution, based on [15, 16], we will present another class of models, which are invariant under rotation symmetries, but in having first-order transitions, differ from the "universal", naively expected, second-order behaviour.

For short-range ferromagnetic, d-dimensional, rotation-invariant n-vector models standard lore [1] predicts the following (universal) behaviour:

1) If $d = 2$, there is at any temperature a unique Gibbs measure; for $n = 2$ (classical XY spins, in field theoretical language the "nonlinear sigma model") at zero external field there is no spontaneous magnetization, but there is 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.

2) If $d = 3$ or higher, there is a second-order transition between a magnetised 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. In an external field there is always a unique Gibbs measure.

Here 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 [14, 21, 22, 40, 39]. We will here mostly consider spin models, living on a finite-dimensional lattice $\mathbb{Z}^d$. The spins will take values in a circle ($n = 2$) or be n-component unit vectors on an n-sphere.

We will use small Greek letters $\sigma, \eta, \ldots$ to denote spin configurations in finite or infinite sets of sites. The nearest-neighbour Hamiltonians in a finite volume Λ, usually a d-dimensional torus, will be given by

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

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

$$\mu^{\Lambda}(d\sigma) = \frac{1}{Z^{\Lambda}} \exp[-H^{\Lambda}(\sigma)] \mu_0^{\Lambda}(d\sigma) \tag{2}$$

Here μ_0 denotes the rotation-invariant product measure. The choice of the function U of the inner product between the spins at neighbouring sites – which take values on the interval $[-1, 1]$ – will determine our model. For our proofs we will always need that the interactions

are *Reflection Positive*, which restricts us to interactions living on the unit cube, or interactions which are long-range of a particular form [21, 35], and we are restricted to studying the infinite-volume limits of the above periodic-boundary-condition measures.
The choice

$$U(x) = -x \tag{3}$$

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

$$W(\theta) = U(cos(\theta)) = -cos(\theta) \tag{4}$$

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 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 [13] as an example of the phenomenon we display, although their arguments – which we here prove to be correct – were later contested [25, 23]. The original choice of [13] was

$$W(\theta) = -(\frac{1}{2}(1 + cos\theta))^{p} \tag{5}$$

for p large enough.

We concentrate mostly on a mathematically slightly simpler but essentially similar choice of model, which was introduced by [3]:

$$W(\theta) = -1[-\varepsilon, +\varepsilon](\theta) \tag{6}$$

where the parameter ε will be chosen small.

Both these potentials have the form of a deep (depth $= 1$) and narrow (width $= O(\frac{1}{\sqrt{p}})$, 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 therein.

First we notice that by the Mermin-Wagner theorem [32, 12, 24, 33], 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 [38], where a discrete, chiral, symmetry was shown to be broken).

Our first result about the square-well model says that:

Theorem
For ε 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 ε (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, such as was developed by Dyson, Fröhlich, Israel, Lieb, Simon [35]. One obtains a Peierls-type contour estimate by comparing any contour probability with and estimating the probability of a "universal contour", in which in our case at distance 2 one finds alternating diagonals of "good" ordered and "good" disordered sites (see [37]).

Following [11, 26], we employ free-energy contours, rather than the more usual energy contours. Such a contour consists of a appropriately connected set of "bad" sites. A site is defined to be "good" if the bonds ending at it are either all ordered or all disordered, "bad" otherwise. The free energy of a bad site will turn out to be approximately $\frac{3}{4}$ that of a good site, once ε is small enough.

To estimate the universal contour, one has to integrate over all configurations such that the prescribed arrangement of ordered and disordered bonds, which has a positive density (one half) of bad sites, occurs. The proof follows a similar intuition as the proof of [26] for the large-q Potts model. This similarity with the Potts problem was already remarked upon in [13]. The correspondence is that ε, (and the same holds for $\frac{1}{\sqrt{p}}$), correponds to $\frac{1}{q}$. To perform the estimate we observe that the total partition function of an N-by-N square satisfies

$$Z_N \geq max[1, (\frac{1}{2\pi}\varepsilon\ exp2\beta)^{N^2}]. \tag{7}$$

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 $Z_{univcont}$ which is the integral over all configurations compatible with the universal contour satisfies

$$Z_{univcont} \leq (2\varepsilon)^{\frac{1}{4}N^2} exp\beta(\frac{1}{2}N^2)expO(N). \tag{8}$$

These estimates are valid on a temperature interval. We conclude that somewhere on this interval there is a first-order transition in temperature at some β_t, between an ordered and a disordered Gibbs measure, as was first numerically found in [13]. The value of β_t is approximately given by $2\beta_t = -ln\varepsilon$.

The non-square-well model can be treated in a very similar way (see [15, 16] and also [6]). 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 in [8, 7]. In this case the low-temperature phase, as well as the high-temperature phase, presumably has exponential decay of the spin-spin correlations. For the $n \to \infty$ spherical limit see also [9, 10].

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 and a disordered 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 ([36]) potential is $U(x) = -\sum_n 2^{-n} 1_{\varepsilon_n}(x)$ with $\varepsilon_n (= \varepsilon_{n-1}^3) = \varepsilon^{3^{n-1}}$, with the first ε 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 [29, 30], 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. [27, 28, 34]) in $d = 3$, whereas the occurrence of a transition in the limit $n \to \infty$ in $d = 2$ has been a matter of controversy [42, 43]. Additional numerical references are mentioned in [16]. Further models of this type, with a larger number of sharp minima, combined with a term causing a chiral symmetry breaking as in [38], are considered in [31].

5) Similarly as for the Potts gauge model of [26], we can prove the existence of a first-order transition in various nonlinear lattice gauge models with continuous symmetries. In some of such models too first-order transitions were concluded on the base of numerical data (see e.g. [17, 2, 41]). In [16] 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.

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 sperical limit –, or the dimension d –the mean-field limit – [4] of the lattice 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 [6]).

The method of Reflection Positivity we use 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, whereas for Pirogov-Sinai methods the phases need to be pure and will typically have some kind of exponential decay of correlations. On the other hand, with RP methods we cannot obtain results for interface or surface 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 tricitical point.

Although our proofs require a fairly large nonlinearity (that is, a large value of p, or a small value of ε), 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 are occurring, especially for the liquid-crystal models, for much smaller values of p,n, and/or d.

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References

[1] The rigorous results about ferromagnetic 2-component models are described for example in Random Walks, Critical Phenomena and Triviality in Quantum Field Theory by R. Fernández, J. Fröhlich and A. D. Sokal, Springer, 1992. A more recent result on the Kosterlitz-Thouless transition [20] of the 2-dimensional XY model can be found in L. Chayes, *Comm. Math. Phys.* 197, 623–640, 1998. The description of critical (2nd-order transition) points and the behaviour of their exponents as is expected in the physics literature can be found for example in various contributions to Phase Transitions and Critical Phenomena, Vol 6, Eds C. Domb and M. S. Green, Academic Press, 1976.

[2] G. Arnold, B. Bunk,T. Lippert and K.Schilling. Compact QED under scrutiny: it's first order. arXiv:hep-lat/0210010, 2002.

[3] K. Alexander and L. Chayes. Non-perturbative Criteria for Gibbsian Uniqueness *Comm. Math. Phys.* 189:447–464, 1997.

[4] M. Biskup and L. Chayes. Rigorous analysis of discontinuous phase transitions via mean-field bounds. *Comm. Math. Phys.* 238:53–93, 2003.

[5] M. Biskup, L. Chayes and N. Crawford. Mean-field Driven First-Order Phase Transitions in Systems with Long-range Interactions. Arxiv math-ph/0501067, 2005.

[6] M. Biskup and R. Kotecký. Forbidden Gap Argument for Phase Transitions Proved by Means of Chessboard Estimates. Arxiv math-ph/0505011, 2005.

[7] H. W. J. Blöte and W. N. Guo. Phase transitions in the two-dimensional O(3) model. *Int.J.Mod. Phys. B*,16:1891–1897, 2002.

[8] H. W. J. Blöte, W. N. Guo and H. J. Hilhorst. Phase transition in a Two-Dimensional Heisenberg Model. *Phys. Rev. Lett.*, 88:047203, 2002.

[9] S. Caracciolo and A. Pelissetto. Two-dimensional Heisenberg model with nonlinear interaction. *Phys. Rev. E*, 66: 016120, 2002.

[10] S. Caracciolo, M. Mognetti and A. Pelissetto. Two-dimensional Heisenberg model with Nonlinear Interactions: $\frac{1}{N}$-Corrections. *Nucl. Phys. B*, 707:458–492, 2005.

[11] R. L. Dobrushin and S. B. Shlosman. Phases corresponding to the local minima of the energy. *Selecta Math. Soviet.* 1, 317–338, 1981.

[12] R. L. Dobrushin and S. B. Shlosman. Absence of Breakdown of Continuous Symmetry in 2-dimensional Models of Statistical Physics. *Comm.Math.Phys.*, 42:31–40, 1975.

[13] E. Domany, M. Schick and R. H. Swendsen. First Order Transition in an XY model with Nearest-Neighbor Interactions. *Phys. Rev. Lett.* 52, 1535–1538, 1984.

[14] A. C. D. van Enter, R. Fernández, and A. D. Sokal. Regularity properties and pathologies of position-space renormalization-group transformations: Scope and limitations of Gibbsian theory. *J. Stat. Phys.*, 72:879–1167, 1993.

[15] A. C. D. van Enter and S. B. Shlosman. First-Order Transitions for n-Vector models in Two and More Dimensions: Rigorous Proof. *Phys. Rev. Lett.*, 89:285702, 2002.

[16] A. C. D. van Enter and S. B. Shlosman. Provable First-Order Transitions for Nonlinear Vector and Gauge Models with Continuous Symmetries. *Comm.Math.Phys.*, 255:21–32, 2005.

[17] D. Espriu and L .Tagliacozzo. Compact lattice U(1) and Seiberg-Witten duality. arXiv:hep-th/0301086, 2003.

[18] R. P. Feynman. From " Surely You're Joking, Mr Feynman. W.W.Norton, 1985." Then professor Onsager got up and said in a dour voice: Professor Feynman is new in our field and I think he needs to be educated. There is something he ought to know and we should tell him....Onsager said: We should tell Feynman that *nobody* has ever figured out the order of *any* transition correctly from first principles...

[19] J. Fröhlich and E. H. Lieb. Phase Transitions in Anisotropic Lattice Spin Systems. *Comm.Math.Phys.*,60:233–267, 1978.

[20] J. Fröhlich and T. Spencer. Massless Phases and Symmetry Restoration in Abelian Gauge Theories. *Comm.Math.Phys.*,83:411–468, 1983.

[21] H.-O. Georgii. *Gibbs Measures and Phase Transitions*. Walter de Gruyter (de Gruyter Studies in Mathematics, Vol. 9), Berlin–New York, 1988.

[22] H.-O. Georgii, O. Häggström and C. Maes. The random geometry of equilibrium phases. Phase transitions and critical phenomena (C. Domb and J.L. Lebowitz, Eds.), Academic Press, London, to appear.

[23] J. E. van Himbergen. From Continuous to First-order Transition in a Simple XY Model. *Phys. Rev. Lett*,53:5–8, 1984.

[24] D. Ioffe, S. B. Shlosman and Y. Velenik. 2D Models of Statistical Physics with Continuous Symmetry: The Case of Singular Interactions. *Comm. Math. Phys.*, 226: 433–454, 2002.

[25] H. J. F. Knops. First-order Transition the XY model. *Phys. Rev. B*,30:470–472, 1984.

[26] R. Kotecký and S. B. Shlosman. First-order transitions in large entropy lattice models. *Comm.Math. Phys.*, 83:493–515, 1982.

[27] H. Kunz and G. Zumbach. First-order phase transitions in the two- and three-dimensional RP^{n-1} and CP^{n-1} models, in the large-n limit. *J.Phys. A, Math. Gen.*, 22:L1043–L1048, 1982.

[28] H. Kunz and G. Zumbach. Topological phase transitions in a two-dimensional nematic n-vector model: A numerical study. *Phys. Rev. B*, 46:662–673, 1992.

[29] G. Lasher. Monte Carlo Results for a Discrete-Lattice Model of Nematic Ordering *Phys. Rev. A*, 5:1350–1354, 1972.

[30] P. A. Lebwohl and G. Lasher. Nematic-Liquid-Crystal Order-A Monte Carlo Calculation. *Phys Rev A*, 6:426–429, 1972 and 7:2222, 1973.

[31] A. Messager and B. Nachtergaele. A Model with Simultaneous First and Second Order Phase Tranditions. Arxiv cond-mat/0501229, 2005.

[32] N. D. Mermin and H. Wagner. Absence of Ferromagnetism or Antiferromagnetism in One- or Two-Dimensional Heisenberg Models. *Phys. Rev. Lett.*, 17:1133–136, 1966.

[33] C.-E. Pfister. On the Symmetry of the Gibbs States in Two-dimensional Lattice Systems. *Comm. Math. Phys.*, 79:181–188, 1981.

[34] S. Romano. Computer simulation study of a nematogenic lattice-gas model with fourth rank interactions. *Int.J.Mod.Phys.* B16:2901–2915, 2002.

[35] The method of Reflection Positivity was developed by F. J. Dyson, J. Fröhlich, R. B. Israel, E. H. Lieb, B. Simon and T. S. Spencer in a series of papers. It is described in the last chapters of [21] or in [37]. The chessboard estimate method goes back to [19].

[36] Dr Seuss. The Cat in the Hat comes Back. Random House, NY, 1958.

[37] S. B. Shlosman. The method of reflection positivity in the mathematical theory of first-order phase transitions. *Russian Mathematical Surveys*, 41: 83–145, 1986.

[38] S. B. Shlosman. Phase Transitions for two-dimensional Models with Isotropic Short-range Interactions and Continuous Symmetries. *Comm.Math.Phys* 71: 207-212, 1980.

[39] B. Simon. The Statistical Mechanics of Lattice Gases, Vol 1. Princeton University Press, Princeton N.J., 1993.

[40] Ya. G. Sinai. Theory of Phase Transitions: Rigorous Results, Pergamon Press, Budapest, 1982.

[41] J. Smit. Introduction to quantum fields on a lattice. Cambridge Lecture Notes in Physics, 15, CUP, Cambridge, 2002. See in particular Chapters 4 and 5.

[42] A. D. Sokal and A. O. Starinets. Pathologies of the large-N limit for $RP^{N-1}, CP^{N-1}, QP^{N-1}$ and mixed isovector/isotensor sigma-models. *Nucl. Phys. B*, 601: 425–502, 2001.

[43] O. Tchernyshyov and S. L. Sondhi. Liquid-gas and other unusual thermal phase transitions in some large-N magnets. *Nucl.Phys. B*, 639:429–449, 2002.