First-order transitions for n-vector models in two and more dimensions; rigorous proof.

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Abstract: We prove that various SO(n)-invariant n-vector models with interactions which have a deep and narrow enough minimum have a first-order transition in the temperature. The result holds in dimension two or more, and is independent on the nature of the low-temperature phase.

Recently Blöte, Guo and Hilhorst [2], extending earlier work by Domany, Schick and Swendsen [4] on 2-dimensional classical XY-models, performed a numerical study of 2-dimensional n-vector models with non-linear interactions. For sufficiently strong values of the non-linearity, they found the presence of a first-order transition in temperature. In [4] a heuristic explanation of this first-order behavior, based on a similarity with the high-q Potts model, was suggested, explaining the numerical results. A further confirmation of this transition was found by Caracciolo and Pellisetto [1], who considered the $n \to \infty$ (spherical limit) of the model, and found the same first-order transition.

On the other hand, various studies, mostly based on Renormalization-Group analyses or Kosterlitz-Thouless type arguments based on the picture of binding-unbinding of vortices, have contested this first-order behaviour (e.g. [5, 7, 6]).

Here we settle the issue by presenting a rigorous proof of the existence of this first-order transition.

It may seem somewhat surprising that two-dimensional n-vector models, whose magnetization by the Mermin-Wagner theorem [8] is always zero, can have such a phase transition. The reason is that the transition we are talking about here is manifested by the long-range order in higher-order correlation functions. Such transitions were discovered by one of us some time ago, see [11]. But the results of [11] were related to the fact that there the symmetry group was the (disconnected) group $O(2)$, and at the transition point the discrete symmetry $\mathbb{Z}_2$ is broken, while the connected part – $SO(2)$ – of the symmetry persists. The nature of the transition we study here, however, is not connected to any type of symmetry breaking, and as such is much closer to the high-q q-state Potts model, or the model studied in [3], where a first order transition between a low-energy and a high-entropy phase occurs. Thus we confirm the original intuition of [4].

For XY-spins in two dimensions there can be a low-temperature phase with slow polynomial decay of correlations, while the majority belief in the field, despite the work of Patrascioiu and Seiler [9], is that for $n > 2$, the n-vector models at low finite temperatures have exponentially decaying correlations, just as at high temperatures. Our result unfortunately does not say anything about this question.

Our proof is directly inspired by the existing proofs for low-energy–high-entropy phase transitions, and is indeed an adaptation of those. We employ the method of Reflection Positivity [10] (RP). For simplicity we write the proof for 2-dimensional XY-spins, the extension to the general case is immediate.

We remark that also the generalization to higher dimensions is immediate. Thus the low-temperature phase can be either magnetized, Kosterlitz-Thouless-like (not magnetized with slow correlation decay), or possibly non-magnetized with exponentially decaying correlations. As such our result contradicts strong "universality" claims, stating that universality classes of interactions exist, all elements of which have the same kind of phase transition between a high-temperature phase and a low-temperature phase, and which are only determined by the dimension of the system, the symmetry of the interaction and whether the interaction is short-range or long-range.

We will consider the Hamiltonian given by

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

To formulate our result we have to introduce for every n.n. bond $b = (i, j)$ the following bond observables:

$$P_b^< (\phi_i, \phi_j) = \begin{cases} 1 & \text{if } |\phi_i - \phi_j| < \varepsilon/2, \\ 0 & \text{if } |\phi_i - \phi_j| > \varepsilon/2, \end{cases} \tag{2}$$

which project on the ordered bond configurations, and $P_b^> (\phi_i, \phi_j) = 1 - P_b^< (\phi_i, \phi_j)$. Our main result is contained in the following

Theorem 1 *Suppose the parameter p is large enough. Then there exists a transition temperature $\beta_c = \beta_c (J, p)$, such that there are two different Gibbs states, $\langle \cdot \rangle^<$ and $\langle \cdot \rangle^>$, at $\beta = \beta_c$, corresponding to the Hamiltonian (1). For some specific choice of $\varepsilon = \varepsilon (p)$ in (2), we have for the "ordered" state $\langle \cdot \rangle^<$ that*

$$\langle P_b^< \rangle^< > \kappa (p) ,$$

while in the "disordered" phase $\langle \cdot \rangle^>$

$$\langle P_b^> \rangle^> > \kappa (p) ,$$

for each bond b, with $\kappa (p) \to 1$ as $p \to \infty$.

Before analysing the model (1), we present an even simpler toy model, which already displays the mechanism, and which is even closer to the Potts model. The single spin space is the circle, S^1, the free measure is the Lebesgue measure, normalized such that S^1 has measure one, so $S^1 = \left[-\frac{1}{2}, \frac{1}{2}\right]$. (One can take here any sphere $\mathbb{S}^n$ instead.) The toy Hamiltonian is

$$H = -J \sum_{i,j \in \mathbb{Z}^2} U (\phi_i, \phi_j) \tag{3}$$

The nearest neighbour interaction $U(\phi_1, \phi_2) = U(|\phi_1 - \phi_2|)$ is given by

$$U(\phi) = \begin{cases} -1 & \text{if } |\phi| \leq \frac{\varepsilon}{2}, \\ 0 & \text{otherwise.} \end{cases}$$

Here ε plays a similar role to $\frac{1}{q}$ in the q-state Potts model. The Hamiltonian is RP under reflections in coordinate planes. For the case $\mathbb{Z}^2$ one has also RP under reflections in lines at 45 degrees, passing through the lattice sites. That case is the easiest.

One has to show that:

- $\langle P_b^{>} \rangle_\beta$ is small for large β; (the ordered, typical low-temperature phase bonds)
- $\langle P_b^{<} \rangle_\beta$ is small for small β; (the disordered, typical high-temperature phase bonds)
- $\langle P_{b'}^{<} P_{b''}^{>} \rangle_\beta$ is small for all β,

provided ε is small enough. Here $\langle \cdot \rangle_\beta$ is the state with periodic b.c. in the box Λ of size L, and b', b'' are two orthogonal bonds sharing the same site. The estimates have to be uniform in L, for L large. The first two are straightforward application of RP and the chess-board estimate. So let us get the last one. By the chess-board estimate,

$$\langle P_{b'}^{<} P_{b''}^{>} \rangle_\beta \leq \left\langle P^{\#} \right\rangle_\beta^{1/|\Lambda|}, \tag{4}$$

where the observable $P^{\#}$ is the indicator

$$P^{\#} = \prod_{b \in E_{01}} P_b^{<} \prod_{b \in E_{23}} P_b^{>}.$$

Here E_{01}, E_{23} is the partition of all the bonds in Λ into two halves; E_{01} consists of all bonds $(x, x + e_1)$ and $(x, x + e_2)$, for which $x^1 + x^2 = 0$ or $1 \bmod 4$, while E_{23} is the other half; e_1 and e_2 are the two coordinate vectors.

To proceed with the estimate (4) we need the estimate on the partition function. We have

$$Z_\Lambda(\beta, \varepsilon) \geq \left(\frac{\varepsilon}{2}\right)^{|\Lambda|} e^{2\beta|\Lambda|} + (1 - 4\varepsilon)^{|\Lambda|/2}. \tag{5}$$

(The first summand is obtained by integrating over all configurations ϕ, such that $|\phi_x| \leq \frac{\varepsilon}{4}$ for all $x \in \Lambda$. For the second one we take all configurations ϕ which are arbitrary on the even sublattice and which satisfy $|\phi_x - \phi_y| > \varepsilon/2$ for every pair of n.n.; for every y on the odd sublattice that leaves the spins to be free in a set of measure $\geq 1 - 4\varepsilon$.) Solving

$$\left(\frac{\varepsilon}{2}\right)^{|\Lambda|} e^{2\beta_0|\Lambda|} = (1-4\varepsilon)^{|\Lambda|/2}$$

for β_0 we find

$$e^{4\beta_0} = (1-4\varepsilon)\left(\frac{\varepsilon}{2}\right)^{-2}, \tag{6}$$

so for $\beta \geq \beta_0$ the first term in (5) dominates, while for $\beta \leq \beta_0$ the second term dominates. Similarly, the partition function $Z^{\#}_{\Lambda}(\beta, \varepsilon)$, taken over all configurations ϕ with $P^{\#}(\phi) = 1$ satisfies

$$Z^{\#}_{\Lambda}(\beta, \varepsilon) \leq e^{\beta|\Lambda|} \varepsilon^{\frac{3}{4}|\Lambda| + O\left(\sqrt{|\Lambda|}\right)}. \tag{7}$$

If $\beta \geq \beta_0$, we write, using (6):

$$\langle P^{<}_{b'} P^{>}_{b''} \rangle_\beta \leq \frac{e^\beta \varepsilon^{\frac{3}{4}}}{\frac{\varepsilon}{2} e^{2\beta}} = 2\frac{1}{\varepsilon^{\frac{1}{4}} e^\beta} \leq 2\frac{1}{\left[\varepsilon\,(1-4\varepsilon)\left(\frac{\varepsilon}{2}\right)^{-2}\right]^{\frac{1}{4}}} \leq C\varepsilon^{1/4}.$$

If $\beta \leq \beta_0$, we similarly have

$$\langle P^{<}_{b'} P^{>}_{b''} \rangle_\beta \leq \frac{e^\beta \varepsilon^{\frac{3}{4}}}{(1-4\varepsilon)^{1/2}} \leq \frac{\left[(1-4\varepsilon)\left(\frac{\varepsilon}{2}\right)^{-2} \varepsilon^3\right]^{\frac{1}{4}}}{(1-4\varepsilon)^{1/2}} \leq C'\varepsilon^{1/4}.$$

So we are done.

For the non-linear models, we employ the fact that for small difference angles $\cos(\phi_i - \phi_j)$ is approximately $1 - O((\phi_i - \phi_j)^2)$ and furthermore that $\lim_{p\to\infty}(1 - \frac{1}{p})^p = e^{-1}$. This suggests to choose $\epsilon(p) = \frac{1}{\sqrt{p}}$. Because the separation between ordered and disordered bonds is somewhat arbitrary, to obtain an inequality similar to (5), we make a slightly different choice. We consider a bond (i,j) disordered if $|\phi_i - \phi_j| \geq \frac{C}{\sqrt{p}}$ for some large C. So first we choose a sufficiently large constant C. For the estimate of the ordered partition function we only integrate over the much smaller intervals of "strongly ordered" configurations: $|\phi_i| \leq \frac{C^{-1}}{\sqrt{p}}$ to obtain a lower bound:

$$Z_\Lambda(\beta, p) \geq \left(\frac{1}{2C\sqrt{p}}\right)^{|\Lambda|} e^{[2\beta(1-O(\frac{1}{C}))]|\Lambda|} + \left(1 - \frac{4C}{\sqrt{p}}\right)^{|\Lambda|/2}. \tag{8}$$

This makes use of the fact that the "strongly ordered" bonds all have energy almost equal to $-J$, whereas the disordered partition function is bounded by that of the toy model, but with ε replaced by $\frac{C}{\sqrt{p}}$.

For the estimate which shows that ordered and disordered bonds tend not to neighbor each other, we obtain:

$$Z_\Lambda^{\#}(\beta, p) \leq e^{\beta|\Lambda|}(\frac{C}{\sqrt{p}})^{(\frac{3}{4}+O(e^{-C}))|\Lambda|+O\left(\sqrt{|\Lambda|}\right)}. \tag{9}$$

The rest of the argument is essentially unchanged. We first chose C big enough (such that $\frac{1}{C}$ is small wrt to 1), and we can still choose p big enough such that p is large wrt to C^2, which finishes the argument.

References

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[7] H.J.F. Knops, First-order transition in the XY model, *Phys. Rev. B* 30, 470–472, 1984.

[8] The Mermin-Wagner theorem, which excludes the breaking of a continous symmetry in two dimensions, at finite temperatures, was first proved in: N.D. Mermin and H. Wagner "Absence of ferromagnetism or antiferromagnetism in one- or two-dimensional isotropic Heisenberg Models" *Phys. Rev. Lett.* 17, 1133–136, 1966. Since then various more precise and more general versions have been proved; for a recent result see e.g. D. Ioffe, S. B. Shlosman and Y. Velenik, "2D Models of Statistical Physics with Continous Symmetry: The Case of Singular Interactions", *Comm Math. Phys.*, 226, 433-454, 2002. The fact that the zero magnetization which is enforced by the Mermin-Wagner theorem is compatible with various types of phase transitions was noted for example by Kosterlitz and Thouless and also in [11].

[9] A. Patrascioiu and E. Seiler, in a series of papers (see e.g. "Is the 2D O(3) nonlinear σ-model asymptotically free?" *Phys.Lett. B*, 430, 314 1998) have claimed that a Kosterlitz-Thouless phase occurs at low temperatures in n-vector models also with $n \geq 3$. This claim is not widely believed, but the question is still open.

[10] Reflection Positivity is a by now fairly standard technique which was introduced into statistical mechanics from field theory, to prove the existence of various types of phase transitions, in a series of papers by F. J. Dyson, J. Fröhlich, R. B. Israel, E. H. Lieb, B. Simon and T. Spencer. The application to Potts models was performed by R.Kotecký and S.B. Shlosman, *Comm.Math.Phys.* 83, 493–515 , 1982. The method is reviewed for example in the last four chapters of H.-O. Georgii's book **Gibbs measures and Phase Transitions**, de Gruyter, 1988 or in S. B. Shlosman, The method of reflection positivity in the theory of first-order phase transitions, *Russ. Math.Surveys*, 41, 83–134, 1986. Our proof directly follows this last source.

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