A model with simultaneous first and second order phase transitions

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We introduce a two dimensional nonlinear XY model with a second order phase transition driven by spin waves, together with a first order phase transition in the bond variables between two “bond ordered phases”, one with local ferromagnetic order and another with local anti-ferromagnetic order. We also prove that at the transition temperature the bond-ordered phases coexist with a disordered phase as predicted by Domany, Schick and Swendsen. This last result generalizes the result of Shlosman and van Enter. We argue that these phenomena are quite general and should occur for a large class of potentials.

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I. INTRODUCTION AND MAIN RESULT

A usual feature in the Statistical Mechanics is the coexistence of several phases at low temperature. Typically, the number of coexisting pure phases decreases with increasing temperature up to some critical temperature \( \beta_c \) at which a single disordered phase appears. This \( q \)-state Potts model for sufficiently large \( q \) behaves slightly differently since it has \( q \) ordered phases below the transition temperature, but at the transition it has \( q + 1 \) phases, including a disordered phase. Thus, the Potts model demonstrates that order and disorder can coexist.

There is a continued interest in exploring the variety of ordering phenomena occurring in models of classical continuous \( \phi^4 \)-models. In the present work, one of our motivations was to look for the coexistence of ordered and disordered phases in such models (as opposed to the previously studied Potts model, which is a discrete spin model).

An interesting situation of coexisting order and disorder was found to occur in a strongly non-linear XY model. For that model it was recently proved rigorously by Shlosman and van Enter in Ref. 5 that there is some temperature at which a first order phase transition occurs between a (ferromagnetic) bond ordered phase, which means that the nearest neighbors are close, and a bond disordered phase, which means that the nearest neighbors are uncorrelated. This behavior resembles the Potts model with a magnetic field, which shows a unique ordered phase at low temperature, and two coexisting phases at the transition. The main difference is that the XY models has a continuous symmetry (\( O(2) \)), as opposed to Potts model where the symmetry is discrete. This continuous symmetry cannot be spontaneously broken by the Mermin-Wagner Theorem, which implies any long-range order is not accompanied by a non-vanishing magnetization.

In this paper we introduce a new family of \( O(2) \)-models defined on the two-dimensional square lattice, some of which exhibit a second order phase transition at sufficiently low temperature that coexists with a first order phase transition. Our family of models depends on five parameters: three positive integers, \( p, m, \) and \( n \), and two non-negative coupling constants, \( J, \) and \( K \):

\[
H = 2J \sum_{[i,j]} \left[ \cos \frac{m}{2}(\phi_i - \phi_j) \right]^{2p} + K \sum_{[i,k]} \cos \frac{n}{2}(\phi_i - \phi_k)
\]

where \( \phi_i \in [0,2\pi) \), and \([..]\] denotes nearest neighbors and \([..,..]\] denotes diagonal neighbors. The model considered in Refs 5 and 6 is the special case \( K = 0 \) and \( m = 1 \). As we will only consider \( K > 0 \), we can fix \( K \) by rescaling the temperature; we pick \( K = 1/4 \).

We prove that, for suitable values of the parameters, these models have both a first and a second order phase transition. Our main result is the following theorem, in which we demonstrate the occurrence of both phase transitions by means of estimates on on nearest neighbor and long range correlations. The correlation functions with specified boundary conditions (b.c.) are denoted by \( \langle \cdot \rangle^{b.c} \). We consider three types of boundary conditions: 1) \( f \), for ferromagnetic, indicating parallel nearest neighbor spins, 2) \( a \), for antiferromagnetic, which favors antiparallel nearest neighbor spins, and 3) \( d \), for disordered, denoting the third phase, which appears at the transition temperature. The precise meaning of the various boundary conditions is clarified later.

**Theorem.** For sufficiently large \( p, m = 1, \) and \( n = 2 \), the models with Hamiltonian 1 have the following properties:

1) There exists an inverse temperature \( \beta_1 \), and functions \( b^{b.c}(\beta,p) < 1 \), and \( h^{b.c}(\beta,p) < 1 \), such that:

a) for \( \beta > \beta_1 \), there is a first ordered phase transition between the bond ferromagnetic phase and the bond anti-
ferromagnetic phase:

\[ \langle \cos(\phi_i - \phi_j) \rangle^f > 1 - \epsilon^f(\beta, p) \]  
\[ \langle \cos(\phi_i - \phi_j) \rangle^a < -1 + \epsilon^a(\beta, p) \]

for nearest neighbor pairs \([i, j]\).

b) at \(\beta\), there is a first order phase transition between the bond ordered ferromagnetic phase, the bond antiferromagnetic phase and the disordered phase:

\[ \langle \cos(\phi_i - \phi_j) \rangle^f > 1 - \eta^f(p) \]  
\[ \langle \cos(\phi_i - \phi_j) \rangle^a < -1 + \eta^a(p) \]  
\[ \langle |\cos(\phi_i - \phi_j)\rangle^d \rangle < \eta^d(p) \]

II) At sufficiently low temperature there is a second order phase transition to phase with power law decay of the two point correlation:

\[ \frac{C}{(1 + N)^{2\beta'}} \leq \langle \cos(\phi_0 - \phi_N) \rangle \leq \frac{1}{N^{\beta'(2J_1 + J_2)}} \]  

where \(\beta' > \frac{1}{2}\) and \(\beta'(\beta) \to \infty\) when \(\beta \to \infty\), and \(N\) denotes any site at distance \(N\) from the origin.

We interpret our result as follows: two phases coexist at low temperature, one with a local ferromagnetic order, and one with a local anti-ferromagnetic order, but in large distance spin waves destroy both the long range ferromagnetic order and the long range anti-ferromagnetic order leading to a second order phase transition at some lower temperature. The situation has to be opposed to the rotator model in two dimensions, which exhibits a second order phase transition at low temperature, but no first order phase transition. Notice that the Lebowitz inequalities, which were used in Ref. 9, to prove the uniqueness of the correlation functions in the two dimensional rotator model are not valid in our model.

In the next section we describe the different phases of our model more precisely and introduce associated restricted ensembles used for the proof of the theorem. The proof itself is given in a separate section.

II. THE BOND-ORDERED PHASES. RESTRICTED ENSEMBLES

We want to prove that below a temperature \(\beta_t^{-1}\) two two order phases coexist: one in which ferromagnetically ordered bonds dominate and another in which antiferromagnetically ordered bonds dominate. We also want to show that at the first-order transition temperature, \(\beta_t\), three phases coexist: the two ordered phases plus a disordered phase. We will give the complete proof of this last statement, from which it will be then be clear how to prove the first. First, we give some definitions and describe the ground states of the model.

For the purpose of describing the ground states, a plaquette is called ferromagnetic if \(\phi_i = \phi_j\) for each nearest neighbor bond, \([i, j]\), of the plaquette, and antiferromagnetic if \(\phi_i - \phi_j = \pi\) for each bond. We will extend these definitions to finite temperature a couple of paragraphs further down.

The Hamiltonian \(H^{(p,1,2)}\) has two families of ground states, each parametrized by an angle:

- the ferromagnetic ground states, in which all plaquettes are ferromagnetic;
- the antiferromagnetic ground states, which have only antiferromagnetic plaquettes.

It is not hard to see that these are the only ground states and it is easy to specify boundary conditions that select one of them.

Next, we define families of configurations that are close to one the ground state configurations and that will carry most of the weight of the equilibrium states for an appropriate range of temperatures. Restricted ensembles and the corresponding partition functions can then be defined by summing over all configurations in each of these families. For each bond \(b = [i, j]\) three characteristic functions:

\[ \chi^f[\phi_i - \phi_j] = \begin{cases} 1 & |\phi_i - \phi_j| < \epsilon \\ 0 & \text{else} \end{cases} \]  
\[ \chi^a[\phi_i - \phi_j] = \begin{cases} 1 & |\phi_i - \phi_j - \pi| < \epsilon \\ 0 & \text{else} \end{cases} \]  
\[ \chi^d[\phi_i - \phi_j] = 1 - \chi^f[\phi_i - \phi_j] - \chi^a[\phi_i - \phi_j] \]

Here again, and in the sequel, \(f\) stands for ferromagnetic, \(a\) for antiferromagnetic, and \(d\) for disordered.

The specification of the bond is ferromagnetic if \(\chi^f[.] = 1\), anti-ferromagnetic if \(\chi^a[.] = 1\), and disordered if \(\chi^d[.] = 1\). In the figures we will indicate a ferromagnetic bond by a thick line, an antiferromagnetic bond by a thin line, and a disordered bond by a zigzag line. The specification of the four bonds of a plaquette will be denoted by \(stuv\), where \(s, t, u, v \in \{f, a, d\}\), and where the bonds are ordered in clockwise fashion starting from the top horizontal bond. As before, a ferromagnetic plaquette is one with specification \(ffff\), an antiferromagnetic plaquette has \(aaaa\), etc. (See Figure II.)

FIG. 1: Three examples of plaquettes. Thick lines denote ferromagnetic bonds (nearly parallel spins), thin lines denote anti-ferromagnetic bonds (nearly antiparallel spins) and a zigzag line is used to denote all other cases, which we call disordered bonds. The first two plaquettes are the ferro and antferromagnetic ground state plaquettes and will be labeled \(ffff\) and \(aaaa\), respectively. The third plaquette is neither ferromagnetic, antiferromagnetic, nor disordered and is labeled by the sequence \(adaf\).
configuration there corresponds an antiferromagnetic one obtained by adding \( \pi \) to each spin on the sites of \( A \).

The restricted partition functions \( \Xi_V(f), \Xi_V(a), \) and \( \Xi_V(d) \), are the partition functions with the configuration sum restricted to \( R^f_v, R^a_v, \) and \( R^d_v \), respectively.

The one-to-one correspondence between \( R^f_v \) and \( R^a_v \), implies that \( \Xi^f_v = \Xi^a_v \).

A contour \( \Gamma \) is the set of configurations, which are equivalent to a precontour’s configuration \( \gamma \). A contour \( \Gamma \) is specified by: 1) a geometric support \( S(\Gamma) \), which is a connected set of plaquettes; 2) a family of equivalent configurations defined on \( S(\Gamma) \).

III. THE PROOF

Proof of I.a and I.b. The existence of a first order phase transition is a consequence of the three conditions:

a) both the probability of an ordered plaquette of an antiferromagnetic plaquette are small at high temperature,

b) the probability of a disordered plaquette is small at low temperature, c) the probability of the contours are small at every temperature. The proof of I.a) and I.b) will be achieved via chess-board estimates, which require that the Hamiltonian is reflection positive. We expand the Hamiltonian,

\[
H = J \sum_{i,j,m=1,2,\ldots,q} A_m \cos 2m(\varphi_i - \varphi_j) + \frac{1}{4} \sum_{[i,k] \in V} \cos(\varphi_i - \varphi_k)
\]

Here, the \( A_m \) are positive integers. Obviously the Hamiltonian is reflection positive with respect to the axis of the lattice. For simplicity we choose \( J = 1 \).

We prove directly part I.b), because I.a) follows by symmetry. Peierls bounds via chess-board estimates are obtained using universal contours, which are obtained from a plaquette configuration \( stuv \), by reflections through the axes of the lattice. See Figures 2 and 3 for examples of universal configurations \( U(stuv) \), which should be thought of as equivalence classes of configurations.

The probability of a plaquette configuration \( stuv \) is given via the following formula, which follows from successive applications of the Schwartz inequality.

\[
\langle stuv \rangle \geq \left[ \frac{\Xi_V[U(stuv)]}{\Xi_V} \right]^{\frac{1}{4}}
\]

First we need to prove a lower bound for \( \Xi_V \), which is similar to the one used in Ref. 2.

\[
\Xi_V \geq \left[ \frac{1}{C \sqrt{p}} \right]|V| \exp \beta [\frac{5}{2} - O(\frac{1}{C^2})] + \left[ 1 - \frac{4C}{\sqrt{p}} \right]^{|V|}
\]

We briefly recall the argument leading to (12).
The first term is obtained by integrating over all the configurations such that $|\varphi_i| \leq \frac{1}{C\sqrt{p}}$ for all $i \in V$, the second one by integrating over all the configurations over one Néel sublattice which satisfy $|\varphi_i - \varphi_j| > \frac{1}{C\sqrt{p}}$ for all nearest neighbors.

Secondly we derive an upper bound for the quantities $\Xi_V[U(stuv)]$ for the different restricted ensembles $P(D)$. The proofs of the conditions a) and b) are straightforward, so we focus on the proof of c), which is to prove that the probabilities of the various plaquettes occurring in contours are small at every temperature. Let $\beta_0$ be defined by:

$$e^{\beta_0} = \left[pC^2(1 - \frac{4C}{\sqrt{p}})\right]^{\frac{1}{2} + O\left(\frac{1}{C^2}\right)} \quad (13)$$

We have to estimate the probability of the contours with different specifications.

- **Two opposite bonds with $\chi^f = 1$ and two opposite bonds with $\chi^a = 1$**, i.e., a plaquette with specification $aaf$. The universal contour $U(aaf)$ is built from ferromagnetic vertical and horizontal bonds with even coordinates, and from anti-ferromagnetic vertical and horizontal bonds with odd coordinates as shown in Figure 2. We get the upper bound for $\Xi_V[U(aaf)]$ by noticing that the energies of the diagonal potentials are zero:

$$\Xi_V[U(aaf)] \leq \left[\frac{1}{C\sqrt{p}}\right]^{V} \exp[\beta|V|[2 + O\left(\frac{1}{C^2}\right)]]$$

a) We get for $\beta > \beta_0$:

$$\left\langle \Xi_U \right\rangle \leq \left[\frac{1}{C\sqrt{p}}\right]^{V} \exp\beta|V|[2 + O\left(\frac{1}{C^2}\right)] \quad (14)$$

b) For $\beta < \beta_0$ we obtain:

$$\left\langle \Xi_U \right\rangle \leq \left[\frac{1}{C\sqrt{p}}\right]^{V} \left[1 + 4C\sqrt{p}\right]^{\frac{1}{2}}$$

In both cases the expectations can be made small for $p$ large enough compared to $C$. It is obvious that the upper bounds for the expressions of $\left\langle \Xi_U \right\rangle$ computed at low and at high temperature have the same dependence on $C$ and $p$. This holds in general and therefore we will compute only one case for the other specifications.

- **One disordered bond and three ordered bonds**. The nature of the ordered bonds, $f$ or $a$, produces only minor
changes. Therefore, let us focus on one instances, say the universal contour $U(adaa)$ which is constructed from ordered horizontal bonds and even vertical bonds, and from disordered vertical odd bonds, as shown in Figure 3. For the upper bound for $\Xi_V[U(adaa)]$, we notice that the energy of the odd vertical bonds is zero:

$$\Xi_V[U(adaa)] \leq \left[ \frac{1}{C\sqrt{p}} \right]^{\frac{|V|}{2}} \exp \beta |V| \left[ 2 + O\left( \frac{1}{C^2} \right) \right],$$

which leads to the upper bound:

$$\langle \Xi \rangle \leq \left[ \frac{1}{C\sqrt{p}} \right]^{\frac{|A|}{2}} \exp \beta |V| \left[ 1 + 4C \sqrt{\frac{1}{p}} \right]$$  \hspace{1cm} (15)

- **Two opposite disordered bond and two opposite ordered bonds.** The universal contour $U(adad)$ is built from ordered horizontal bonds, and from disordered vertical odd bonds as shown in Figure 3. We get the upper bound for $\Xi_V[U(adad)]$ by noticing that the energy of the vertical bonds is zero:

$$\Xi_V[U(adad)] \leq \left[ \frac{1}{C\sqrt{p}} \right]^{\frac{|V|}{2}} \exp \beta |V| \left[ 3 + O\left( \frac{1}{C^2} \right) \right]$$  \hspace{1cm} (16)

We get the upper bound:

$$\langle \Xi \rangle \leq \left[ \frac{1}{C\sqrt{p}} \right]^{\frac{|A|}{2}} \exp \beta |V| \left[ 1 + 4C \sqrt{\frac{1}{p}} \right]$$  \hspace{1cm} (17)

- **Two adjacent disordered bonds and two adjacent ordered bonds.** The universal contour $U(aadd)$ is built from ordered horizontal even bonds and even vertical bonds, and from disordered vertical odd and the horizontal bonds as shown in Figure 3. We get the upper bound for $\Xi_V[U(aadd)]$ by noticing that the energy of the odd vertical and horizontal bonds are zero, and that there are entropy contributions from the vertices with odd coordinates:

$$\Xi_V[U(aadd)] \leq \left[ \frac{1}{C\sqrt{p}} \right]^{\frac{|V|}{2}} \exp \beta |V| \left[ 3 + O\left( \frac{1}{C^2} \right) \right]$$  \hspace{1cm} (18)

We get the upper bound:

$$\langle \Xi \rangle \leq \left[ \frac{1}{C\sqrt{p}} \right]^{\frac{|A|}{2}} \exp \beta |V| \left[ 1 + 4C \sqrt{\frac{1}{p}} \right]$$  \hspace{1cm} (19)

- **Three disordered bond and one ordered bonds.** The universal contour $U(dadd)$ is built from disordered horizontal bonds and even vertical bonds, and from ordered vertical odd bonds as shown in Figure 3. We get the upper bound for $\Xi_V[U(dadd)]$ by noticing that the energy of the horizontal and the odd vertical and bonds is zero, and that there are entropy contributions from the vertices with even ordinates:

$$\Xi_V[U(dadd)] \leq \left[ \frac{1}{C\sqrt{p}} \right]^{\frac{|V|}{2}} \exp \beta |V| \left[ 1 + O\left( \frac{1}{C^2} \right) \right]$$  \hspace{1cm} (20)

We get the upper bound:

$$\langle \Xi \rangle \leq \left[ \frac{1}{C\sqrt{p}} \right]^{\frac{|A|}{2}} \exp \beta |V| \left[ 1 + 4C \sqrt{\frac{1}{p}} \right]$$  \hspace{1cm} (21)

For $p \gg C \gg 1$, the probability of each specification of a contour’s plaquette can be made small enough. Finally we prove the Peierls condition: first we sum over all the specifications of the contours with a fixed support using the estimates (14), (15), (17), (19), and (21); next we use the Koenigsberg’s lemma to get an upper bound on the entropy for the contours. This concludes our proof of part I of the Theorem.

**Proof of II** The upper bound on the two points correlation function is proved via a spin wave argument, the lower bound is deduced from the deep result of Fröhlich and Spencer for the two dimensional classical XY model. We now provide the details.

**II.a The lower bound**

We use the Ginibre inequalities, which are valid for ferromagnetic Hamiltonians.

$$\langle \exp (m_1 \phi_i (\phi_j - \phi_k)) \rangle_{H_v} \geq \langle \exp (m_2 (\phi_k - \phi_i)) \rangle_{H_v} \langle \exp (m_2 (\phi_k - \phi_i)) \rangle_{H_v}$$  \hspace{1cm} (22)

We first start by removing all the terms contained in the Hamiltonian with the exception of the diagonal interactions, then we are left with two independent rotator models, one on each of the sublattices.

First, suppose $i$ and $j$ are on the same sublattice. Then we use the remaining interactions on that sublattice. We are left with the Hamiltonian: $H_v^{(i)} = \sum_{(i,k) \in V} \cos ((\phi_k - \phi_i))$, and we have

$$\langle \exp (\phi_k (\phi_i - \phi_0)) \rangle_{H_v^{(i)}} \geq \langle \exp (\phi_0 (\phi_i - \phi_0)) \rangle_{H_v^{(i)}}$$

Next we apply the result of Fröhlich and Spencer, Theorem C, for the two dimensional rotator model to get a lower bound.

$$\langle \exp (\phi_0 (\phi_i - \phi_0)) \rangle_{H_v^{(i)}} \geq \frac{C}{(1 + N)^{\beta'}}$$  \hspace{1cm} (23)

where $\beta' = \frac{1}{\sqrt{p}}$ and $\beta' (\beta) \to \infty$ when $\beta \to \infty$.

If $i$ and $j$ belong to different sublattices, the same lower bound of (23) holds with a slightly smaller constant $C$, again by using the Ginibre inequality (22) with $i = l$ and $j = k$ replaced by a nearest neighbor of $j$.

**II.b The upper bound.** The upper bound for the two points correlation function is obtained by using a well known spin wave argument. We use a nice argument that we learned from H. Kuma. It starts by defining a sequence of squares (or hypercubes in higher dimensions) and label them $B_1, B_2, \ldots$, as shown in Figure 4. Each $B_l$ is centered at the origin and its boundaries can be taken to intersect nearest neighbor bonds. We define the shells $C_l = B_{l+1} \setminus B_l$, each shell $C_l$ contains a square $R_l$ of the lattice, the nearest vertices contained in $R_l$ are
FIG. 7: The nested square boxes $B_i$ used in the argument for the upper bound II.b. are shown in dashed lines. The solid bonds are the new strongly ferromagnetic interactions introduced in the proof.

labelled by a couple $[l, i(l)]$, where $i(l)$ denotes the coordinates along $R_l$. We want to identify the continuous spins contained in each shell $R_l$ by using Ginibre’s inequality. To do so, we add to the Hamiltonian $H_V$ the ferromagnetic interactions: $\sum_{l=1}^{L} \sum_{i(l)} J_l \cos(\varphi_{i(l)+1} - \varphi_{i(l)})$, where the $J_l$ are positive. The correlations are increasing by Ginibre’s inequality. Next we let $J_l = \infty$, the correlations are again increasing:

$$\langle \cos(\varphi_0 - \varphi_N) \rangle_V \leq \frac{1}{Z^p_{L}} \times \int_0^{2\pi} d\varphi_1 \cdots \int_0^{2\pi} d\varphi_{N+1} \prod_{j=1}^{j=N} \times \exp \left[ 4jJ \sum_{m=1,2,\ldots,q} A_m \cos 2m(\varphi_j - \varphi_{j+1}) + \frac{1}{2} \cos(\varphi_j - \varphi_{j+1}) \right] \times \exp \left\{ i(\varphi_j - \varphi_{j+1}) \right\}$$

Where $Z^p_{L}$ is the normalization factor. The LHS is the two points correlation function corresponding to a one dimensional model, each term of the product can be computed, we get the following upper bound:

$$\langle \cos(\varphi_0 - \varphi_N) \rangle_V \leq N^{-1/(2p\beta(2J+\frac{1}{2}))}$$

IV. CONCLUSION

The coexistence between second order and first order phase transitions at the same temperature should be a fairly general phenomena in two-dimensional models with a continuous symmetry. For example it occurs in several non linear two dimensional XY models defined by (1) for other values of the pair $m, n$. In a more general setting, we have to consider potentials with continuous symmetry, which are peaked and with large flat parts to produce entropy. The problem will be to characterize the criticality, which in our case uses, a generalization of the work of Aizenman could be an alternative. We expect that the same situation should hold for some quantum models.

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