PHASE TRANSITIONS IN THE TWO-DIMENSIONAL O(3) MODEL

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We use Monte Carlo, transfer-matrix and finite-size scaling methods to investigate two-dimensional O(n) models with n > 2, in particular the case n = 3 which includes the classical Heisenberg model. Depending on the type of interaction and the lattice structure, two different types of phase transitions are present. One type resembles the hard-hexagon transition and occurs in the loop representation of the honeycomb O(n) model. The other type is a first-order transition which occurs for spin-spin interactions that are strongly nonlinear in the neighbor-spin products. When the nonlinearity is decreased, the first-order line ends in a critical point. The existence of the first-order line is in agreement with mean-field theory as well as with high- and low-temperature approximations.

1. Introduction

The O(n) spin model represents a system of interacting n-dimensional vectors \( \vec{s} \equiv (s_1, s_2, \ldots, s_n) \) on a lattice. The O(n) symmetry implies that the Hamiltonian is invariant under rotations in the space of the spin vectors. We consider the case of O(n) symmetric pair interactions

\[
\mathcal{H}/k_B T = - \sum_{<i,j>} h(\vec{s}_i, \vec{s}_j)
\]  

(1)

where the sum is on all pairs of nearest neighbors, and \( h \) is an arbitrary function with implicit temperature dependence. The ‘linear’ case, i.e. \( h(x) = Kx \) where \( K \) is the coupling constant, includes the classical XY model (n = 2) and the classical Heisenberg model (n = 3). For reasonable choices of the function \( h \), in particular monotonically increasing functions, it is plausible that the model belongs to the same universality class as the linear model.
The question whether or not two-dimensional O\((n)\) models with \(n > 2\), and in particular with \(n = 3\), undergo a phase transition at a sufficiently low temperature has received considerable attention;\(^{1-6}\) see also references therein. These papers contain conflicting answers. However, according to the prevailing interpretation, ordering transitions are absent in the O\((n)\) model with \(n > 2\). The main argument relies on the spin-wave result\(^1,3\) by Bloch that a spontaneously magnetized state cannot exist at a nonzero temperature. This does not qualify as a proof for the absence of a transition: the spin-wave argument applies as well to the XY \((n = 2)\) model where a phase transition\(^7\) is known to occur (but not to a spontaneously magnetized state). The latter transition is however linked to topological excitations (vortices) which lack relevance for \(n = 3\). This, together with an exact result of Kunz and Wu\(^4\) which excludes phase transitions in a part of the \(n > 2\) parameter space, forms the basis of the above-mentioned prevailing interpretation.

However, here we describe two sorts of transition for \(n > 2\). The first type, which occurs in the O\((n)\) loop model on the honeycomb lattice, is described in section 2. It is unphysical in the spin representation, because negative Boltzmann weights occur. It is thus consistent with the hypothesis that phase transitions are absent in two-dimensional spin models with \(n > 2\). However, in section 3 we describe a phase transition in a genuine Heisenberg-type O\((3)\) model. The phase transition does not lead to a long-range ordered state (in the sense of a nonzero spontaneous magnetization) and is therefore consistent with the spin-wave theory.

2. Phase Transition in the Loop Model

The ‘loop’ version of the O\((n)\) model is defined by the choice \(h(x) = \log(1 + ax)\), where the parameter \(a\) is an inverse-temperature-like parameter, and the normalization \(\vec{s}_i \cdot \vec{s}_i = n\). The model on the honeycomb lattice can be mapped\(^5\) onto a gas of nonintersecting loops running over the edges of the honeycomb lattice. Each edge covered by a loop carries a Boltzmann weight \(a\), and each loop a weight \(n\). The loop representation has enabled exact solutions along special lines in the \(n, a\) plane for \(n \leq 2\) \(^{8-11}\) and for \(n \geq 2\).\(^12\) From these solutions we know that for \(n \leq 2\) an ordering transition occurs at finite values of \(x\), and that for \(n > 2\) the loop model is in a long-range ordered state for \(x = \infty\). This state is not of the ‘ferromagnetic’ type, but chooses between 3 sublattices, and reminds of the hard-hexagon model.

In the absence of exact solutions in most of the \(n, x\) plane, we have applied Monte Carlo and transfer-matrix techniques.\(^13\) Surprisingly, a transition to the long-range ordered state was found at finite values \(x < \infty\). The hard-hexagon-like critical line spans the range \(2 < n < \infty\). The resulting phase diagram is shown in fig. 1. Also shown are the boundary of the ‘physical region’ of the spin model, where the energy \(h(\vec{s}_i, \vec{s}_j)\) is real for all \(\vec{s}_i, \vec{s}_j\) (curved line in the middle), and a region where a transition is rigorously excluded (above the curved line on the far right). The latter line is based on the work by Kunz and Wu;\(^4\) see also an erratum.\(^15\) We observe that the newly found critical line indeed avoids the excluded region. It is
Fig. 1. Phase diagram of the O($n$) model on the honeycomb lattice in the $n$-$a$ plane. The horizontal scale is chosen as $1 - 8/(n + 10)$ in order to show the whole range up to $n = \infty$. The vertical scale displays $W(n) = 1/[(n + 10)^{1/6}]$. The data points show our results for the newly found phase transition. The curve in the range $-2 < n \leq 2$ shows an exact solution. The region on the right hand side of curve ending at $n = W = 0$ is unphysical in the spin representation. Rigorous arguments exclude phase transitions in the region indicated at the upper right.

...completely embedded in the unphysical region of the spin model, but it is physical in the language of the O($n$) loop model.

3. The Strongly Nonlinear O(3) Model

We use Eq. (1) for the Heisenberg case $n = 3$ with a spin-spin interaction

$$h(\vec{s}_i \cdot \vec{s}_j) = 2K[(1 + \vec{s}_i \cdot \vec{s}_j)/2]^p$$

with spins normalized to length 1. The parameter $p$ determines the degree of non-linearity of the energy function $h$. This form is chosen as to avoid powers of negative numbers, and to limit the energy range to $2K$, as in the linear case.

3.1. Mean-field theory

Consider a spin $\vec{s}_i$, interacting with $z$ neighbors. Denote the average magnetization of the spin system as $m$, say along the $x$-axis. The local energy is

$$E_{\text{loc}} = -2zK[(1 + \vec{s}_i \cdot \vec{m})/2]^p = -2zK[(1 + xm)/2]^p$$

and the thermal average of the $x$-component of $\vec{s}_i$ satisfies

$$\langle x \rangle = \int_{-1}^{1} x e^{-E_{\text{loc}}} dx / \int_{-1}^{1} e^{-E_{\text{loc}}} dx$$

For large enough $K$, the self-consistency equation $\langle x \rangle = m$ has solutions at nonzero $m$. While $m$ is a decreasing function of $K$, this function depends qualitatively on
For small enough values of $p$, $m$ decreases continuously to 0 at the critical point $K = K_c$. We thus find $K_c$ by solving $\partial \langle x \rangle / \partial m = 1$ which leads to

$$K_c = \frac{2p^{-3}3}{p}$$

(5)

For larger values $p$, $\langle x \rangle$ increases faster than linear with $m$ for small $m$, but still levels off at large $m$. The nonzero solutions of $\langle x \rangle = m$ thus become duplicate, i.e., the transition turns first order for large $p$. These two distinct ranges of $p$ are separated by the tricritical point, which can be determined by solving for $K$ and $p$ in $\partial \langle x \rangle / \partial m = 1$ and $\partial^3 \langle x \rangle / \partial m^3 = 0$ at $m = 0$. The second equation expresses the absence of the lowest order of nonlinearity of $\langle x \rangle$ as a function of $m$. The tricritical coordinates are $p_{\text{tri}} = (-1 + \sqrt{33})/2$ and $K_{\text{tri}} = 2^{p_{\text{tri}}^{-3}3}/p_{\text{tri}}$.

For $p > p_{\text{tri}}$, the first-order transition point follows by equating the areas enclosed by the $\langle x \rangle$ vs. $m$ curve and the $\langle x \rangle = m$ line. Thus we have determined the first-order line numerically; the resulting phase diagram is shown in fig. 2.

![Fig. 2. Mean-field phase diagram of the nonlinear O(3) model on the square lattice, in the $K$ versus $p$ plane. The line of phase transitions consists of two parts: a continuous transition at small $p$, and a first-order part. The two parts are separated by a tricritical point (asterisk).](image)

3.2. High- and low-temperature approximations

Estimates of the location of a first-order transition (if any) can also be obtained from intersections of high- and low-temperature approximations of the free energy. Neglecting loop diagrams in the high-temperature expansion the lattice effectively reduces to the Bethe lattice, for which we obtain the free energy via a transfer-matrix-like approach. The partition function $Z_b$ ‘per bond’ between spins $\vec{s}$ and $\vec{t}$ equals

$$Z_b = \int \mathrm{d}\vec{s} \exp\{2K [(1 + \vec{s} \cdot \vec{t})/2]^p\}$$

(6)
which is independent of \( \hat{t} \). Expansion of the exponential function yields

\[
Z_b = 4\pi \sum_{k=0}^{\infty} \frac{(2k)^k}{(1 + pk)k!}
\]

(7)

where the prefactor accounts for the spin degrees of freedom and the sum for the spin-spin interaction. The partition function of a Bethe lattice with \( N \) spins, each interacting with \( z \) neighbors, and \( zN/2 \) bonds follows as

\[
Z_{BL} = (4\pi)^N \left( \sum_{k=0}^{\infty} \frac{(2k)^k}{(1 + pk)k!} \right)^{zN/2}
\]

(8)

For \( z = 4 \), the high-temperature approximation of the free energy is thus

\[
\frac{F_{HT}}{NkT} = -\log(4\pi) - 2 \log \left( \sum_{k=0}^{\infty} \frac{(2k)^k}{(1 + pk)k!} \right)
\]

(9)

We use a low temperature approximation for spins almost aligned along the \( z \) axis:

\[
\hat{s}_i = \left( s^x_i, s^y_i, \sqrt{1 - s^x_i^2 - s^y_i^2} \right)
\]

where the \( x \) and \( y \) components are small. Small deviations between neighbors \( i \) and \( j \) increase the energy per bond

\[
E_{ij}/kT + 2K = \frac{1}{2}pK[(s^x_i - s^x_j)^2 + (s^y_i - s^y_j)^2]
\]

(10)

i.e. the Gaussian model applies to this quadratic form. After a Fourier transformation it is straightforward to obtain the partition function; the free energy follows as

\[
\frac{F_{LT}}{NkT} = -4K - \log Z^2_G \frac{N}{N} = -4K - \log(4\pi) + \log(8pK) + \frac{1}{N} \sum_{k} \log[(\sin \frac{1}{2}k_x)^2 + (\sin \frac{1}{2}k_y)^2]
\]

(11)

For large \( N \) the sum satisfies \( \frac{1}{N} \sum_{k} \log[(\sin \frac{1}{2}k_x)^2 + (\sin \frac{1}{2}k_y)^2] \simeq -0.2200507 \ldots \).

The low- and high-temperature approximations of the free energy are found to intersect, and thus predict the approximate location of a possible first-order transition line. These intersections were found numerically, and shown in fig. 3.

3.3. Monte-Carlo results

The model defined by Eqs. (1) and (2) was investigated by a conventional Monte Carlo algorithm with local spin updates. Randomly chosen orientations for the spin vectors were accepted or rejected with Metropolis-type probabilities. The autocorrelation times are found to increase considerably at low temperatures, especially for system sizes \( L \) exceeding about 100. The efficiency of the algorithm decreases even further at high values of \( p \) where the acceptance ratio becomes small.

Nevertheless we could resolve the phase diagram. No signs of a phase transition were found for \( p = 1 \), i.e. the linear Heisenberg model. But for larger \( p \), pronounced
maxima in the heat capacity appear, and for \( p \geq 16 \), we find numerical evidence for a divergence of the heat capacity. For \( p > 18 \), the simulations reveal a jump in the energy as a function of \( K \), and a clear hysteresis effect. The first-order character becomes even stronger at larger \( p \). The transition for \( p > 20 \) was found by Monte Carlo runs starting from a spin configuration of which one half was fully aligned, and the other half filled with randomly chosen spins. For \( p < 20 \) we determined the location \( K_{\text{max}}(p, L) \) of the heat capacity maximum \( c_{\text{max}}(p, L) \) as a function of \( K \) for system sizes up to \( L = 48 \), and extrapolated to \( L = \infty \). The heat capacity does not seem to diverge for \( p < 16 \). For \( p = 16 \) we observe a divergence approximately as \( L^{7/4} \), which indicates the presence of an Isinglike critical point. For \( p > 16 \) the divergence agrees with first-order behavior \( c_{\text{max}}(p, L) \propto L^2 \). The Monte Carlo data are included in fig. 3.

4. Discussion

We have provided evidence for two types of phase transitions in \( O(n) \) models with \( n > 2 \). The first type is unphysical in the spin language, and depends essentially on the underlying lattice structure. The second type is, however, found in a pure spin system, in a conspicuous disagreement with expectations formulated in the literature. We review the evidence presented above.

In low-dimensional models, mean-field theory tends to predict continuous phase transitions where they do not exist. The example found in section 3.1 should thus not be taken too seriously. The predicted first-order transition is more credible, because the strength of the predicted discontinuity increases at large \( p \), and the role of fluctuations may thus be reduced. Another defect of mean-field theory is
that it is based on an order parameter $m$ that is actually zero.$^{1,3}$ However, the long-wavelength spin waves, which are responsible for the suppression of $m$, hardly affect correlations at distances of a few lattice units. The mean-field result can thus still be regarded as suggestive of a first-order transition at large $p$.

Likewise, the result of the high- and low-temperature approximations is less than compelling. Nevertheless, here also the predicted energy jump increases with $p$: the two free-energy branches are pushed far away, mimicking high- and low-temperature configurations with only limited fluctuations. This lends some support to our approximation. The resulting first-order line is in a reasonable qualitative agreement with Monte Carlo results (fig. 3). It tends to become better at large $p$. The Monte Carlo runs provided a clear first-order picture: the numerical errors are very small in comparison to the differences with the two analytic approximations for the first-order line. The Monte Carlo results are clearly superior. Finally we mention that similar transitions may occur for larger values of $n$, and that Monte Carlo results of Domany et al.$^{14}$ for the analogous strongly nonlinear O(2) model showed that the Kosterlitz-Thouless transition is preempted by a first order one.

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