Phase Transition in the $n > 2$ Honeycomb O(n) Model

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We determine the phase diagram of the O(n) loop model on the honeycomb lattice, in particular, in the range $n > 2$, by means of a transfer-matrix method. We find that, contrary to the prevailing expectation, there is a line of critical points in the range between $n = 2$ and ∞. This phase transition, which belongs to the three-state Potts universality class, is unphysical in terms of the O(n) spin model, but falls inside the physical region of the n-component corner-cubic model. It can also be interpreted in terms of the ordering of a system of soft particles with hexagonal symmetry.

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The O(n) model can be defined in terms of vector spins $\vec{s} = (s_1, s_2, \ldots, s_n)$ on a lattice [1]. This definition includes the Ising, the XY, and the Heisenberg models for $n = 1$, 2, and 3, respectively. The isotropic nature of the model imposes the rotationally invariant form $w(\vec{s} \cdot \vec{t})$ on the Boltzmann weight of an interacting pair $(\vec{s}, \vec{t})$ of neighbor spins. On the basis of universality, one expects that the nature of a phase transition does not depend on the microscopic lattice structure or the choice of the function w. Thus one may choose $w(\vec{s} \cdot \vec{t}) = 1 + x\vec{s} \cdot \vec{t}$, and place the spins on the honeycomb lattice, while still maintaining the expectation that the results characterize O(n) universality classes in two dimensions. The resulting partition integral of the O(n) spin model is

$$Z_{\text{spin}} = \int \prod_k d\,\vec{s}_k \prod_{\langle ij \rangle} (1 + x\vec{s}_i \cdot \vec{s}_j), \tag{1}$$

where the indices i, j, and k represent lattice sites, the second product is over all nearest-neighbor pairs, and the spins are normalized such that $\vec{s}_i \cdot \vec{s}_i = n$. Thus the Boltzmann weight w is positive in the region $|x| < 1/n$. For the honeycomb lattice this special choice enables a mapping on the O(n) loop model [2], with a partition sum

$$Z_{\text{loop}} = \sum_{\text{all } \mathcal{G}} x^{N_b} n^{N_l}, \tag{2}$$

where the graph $\mathcal{G}$ covers N_b bonds of the lattice, and consists of N_l closed, nonintersecting loops.

Another equivalence of the honeycomb O(n) model applies to the n-component corner-cubic model on the triangular lattice [2]. The components of each spin can here independently take discrete values ± 1. The spins are thus pointing towards the corners of an n-dimensional hypercube. The interactions between neighboring spins are chosen such that at most one component can be different. Within the freedom left by this restriction, each nearest-neighbor pair receives a Boltzmann weight of 1 if the spins are equal, and a weight of x if they are different. Thus the partition sum is

$$Z_{\text{ccub}} = \left[\prod_k \prod_{l=1}^{n} \sum_{\sigma_{kl}=\pm 1} \right] \prod_{\langle ij \rangle} (\delta_{\vec{\sigma}_i \cdot \vec{\sigma}_j, n} + x\,\delta_{\vec{\sigma}_i \cdot \vec{\sigma}_j, n-2}), \tag{3}$$

where the vector spins $\vec{\sigma}$ are labeled with their lattice site. The product on k runs over all sites, and $\langle ij \rangle$ denotes all nearest-neighbor pairs of the triangular lattice. Interfaces separating unequal spins define the loop gas on the dual, i.e., the honeycomb lattice, as described by (2).

These three models are described by only two parameters: x and n. In the language of the O(n) loop model, n is the loop weight, and x is the weight of a vertex visited by a loop. In both spin models, n is the spin dimensionality, and x a temperaturelike parameter. Its correspondence with the O(n) spin temperature follows from the interpretation of w as the Boltzmann factor.

The absence of loop intersections in the loop model facilitates its analysis, in part via mappings on other models such as the kagomé 6-vertex (ice-rule) model and the Coulomb gas. Indeed, progress has been made involving exact [2–7] and numerical [8,9] analyses of this loop model.

The following picture emerges from the works cited above. At high temperatures (small x) the O(n) spin system is paramagnetic: spin-spin correlations decay exponentially with distance. The loop model configuration is sparse. At lower temperatures the largest loop size increases, in parallel with the spin-spin correlation length. Both lengths diverge at the O(n) critical point, while the average loop size remains finite [10]. The location of this critical point and a number of critical exponents are exactly known for the honeycomb O(n) model [3,11,12] in the range $-2 \le n \le 2$. The specific-heat singularity is thus known to become progressively weaker with increasing n, until the specific-heat exponent reaches $\alpha = -\infty$ at $n = 2$: the essential singularity at the Kosterlitz-Thouless transition [13] of the XY model. Thus, the critical point at $n = 2$ can naturally be interpreted as the boundary case between the range $n < 2$ with an ordering transition, and

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the range $n > 2$ without such a transition. Indeed, this was the prevailing expectation, expressed, e.g., in [7], and in line with [2].

However, in this paper we show that a phase transition does occur for $n > 2$. The physical nature of this transition hinges on the tendency of the loops to take the form of elementary hexagons for large n. In the limit of large n and constant fugacity $x^6 n$ of such loops, the model reduces to the hard-hexagon model, as noted by Domany *et al.* [2]. Baxter's exact solution [4] shows that the latter model undergoes a phase transition which breaks the symmetry between the three sublattices, and belongs to the three-state Potts universality class.

Before showing that this hard-hexagon-like transition extends to finite values of n, we derive a rigorous bound on the locus of this transition. The mapping on the kagomé lattice 6-vertex model leads to vertex weights [3,7]

$$\{\omega_1, \omega_2, \omega_3, \omega_4, \omega_5, \omega_6\} = \{1, 1, v, v, cz, cz^{-1}\}, \quad (4)$$

where ω_i is the weight of the ith type of vertex as defined in [7] and

$$v = c = 2x\cosh 3\lambda, \qquad z = e^{2\lambda}, \qquad n = 2\cosh 6\lambda. \quad (5)$$

We take $n > 2$, $x > 0$, and $\lambda > 0$ so that $v, c > 0$, and consider the zeros of the partition sum in the complex z plane. The analysis can be carried out by using the Asano construction of small polynomials. The first step is to map the 6-vertex model onto an Ising problem for which the Asano construction can be performed [14]. To the four edges incident at a vertex one associates Ising spins with respective fugacities z_i, $i = 1, \ldots, 4$. The 6-vertex model partition function is then obtained by contracting small polynomials $M_c(z_1, z_2, z_3, z_4)$ associated with each of the vertices. From the explicit expression of M_c deduced in [14], one finds $M_c(z_1, z_2, z_3, z_4) \neq 0$ in the regime

$$|z_i|^2 < \sqrt{1 + a^2} - a, \quad (6)$$

where $a = (v + 1)/c$. Now the contraction of the polynomials involves the replacement of $z_i z_i' \to z$, where z_i and z_i' are the fugacities of the same Ising spin coming from two small polynomials. It then follows from a lemma due to Ruelle [15] that the 6-vertex model partition sum is free of zeros in the regime $|z| < \sqrt{1 + a^2} - a$. It is now a simple matter to specialize to the loop model (5), and deduce that (2) is free of zeroes in the regime $|x| < (\sinh 2\lambda - 1)/2\cosh 3\lambda$, or, explicitly,

$$|x| < \frac{1}{\sqrt{n + 2}}[F_+ - F_- - 1], \quad (7)$$

where $F_\pm = [(n \pm \sqrt{n^2 - 4})/16]^{1/3}$. The analyticity of the free energy now follows as a consequence of the Penrose-Lebowitz Lemma [16]. We remark that a similar result in [7] contains a misprint [17].

Our numerical analysis is based on the calculation of $Z_{\rm loop}$ for $L \times \infty$ honeycomb lattices on a cylinder, with $L = 3, 6, \ldots,$ and 15, by a transfer-matrix method [5,18]. The axis of the cylinder is parallel to one of the lattice edge directions. The transfer matrix $\mathbf{T}$ acts in the vector space whose basis vectors are assigned to "connectivities," i.e., the ways in which the loop segments on the dangling bonds at the end of the cylinder are interconnected. Its largest eigenvalue $\Lambda_{0,L}$ determines the free energy f_L density by

$$f_L = \frac{2}{L\sqrt{3}} \ln(\Lambda_{0,L}). \quad (8)$$

The prefactor accounts for the area occupied by one row of elementary hexagons as appended due to the action of $\mathbf{T}$, using the small diameter of the elementary faces as the length unit. Further eigenvalues $\Lambda_{i,L}$ of $\mathbf{T}$ are associated with correlation lengths $\xi_{i,L}$ describing the exponential decay of various types of correlations in the length direction of the cylinder:

$$\xi_{i,L}^{-1} = (2/\sqrt{3})\ln(\Lambda_{0,L}/\Lambda_{i,L}). \quad (9)$$

Here we consider three types of correlations ($i = 1$, 2, and 3) and their associated eigenvalues $\Lambda_{i,L}$ of $\mathbf{T}$ (the eigenvalues are not necessarily sorted in magnitude). It is helpful that the associated eigenstates classify according to the symmetries of the lattice, i.e., rotations and inversions about the axis of the cylinder.

(1) The O(n) spin-spin correlation function. In the loop model it is represented by a modified partition sum, such that the two correlated sites are connected by a single loop segment. The pertinent eigenvalue $\Lambda_{1,L}$ resides in the "odd sector" of $\mathbf{T}$ which has an unpaired loop segment running in the length direction of the cylinder [9]. The correlation length ξ_1 is usually denoted ξ_h, the magnetic correlation length.

(2) The energy-energy correlation function. The associated eigenvalue is denoted $\Lambda_{2,L}$, and ξ_2 may be denoted ξ_t because it pertains to correlations between temperature-like fluctuations. The corresponding eigenvector resides in the even sector [9] (no unpaired loop segment) of $\mathbf{T}$ and is invariant under lattice symmetries. The largest eigenvalue with these properties is $\Lambda_{0,L}$; the second largest one is $\Lambda_{2,L}$.

(3) The color-color correlation function. The associated eigenvalue is named $\Lambda_{3,L}$, and its eigenvector can be characterized with the help of the operator $\mathbf{R}$ that rotates the lattice by one unit about the axis of the cylinder. Because $\mathbf{R}^L$ is the unit operator, the eigenvalues of $\mathbf{R}$ are $\exp(2\pi i k/L)$, $k = 1, 2, \ldots, L$. To explore the possibility of a symmetry breaking between three differently "colored" sublattices of the honeycomb model, we have computed common eigenvectors $\vec{V}_3$ of $\mathbf{T}$ and $\mathbf{R}$ with the appropriate symmetry, behaving as $\mathbf{R} \cdot \vec{V}_3 = \exp(2\pi i/3)\vec{V}_3$. Thus L is a multiple of 3. The largest eigenvalue obtained is called $\Lambda_{3,L}$, and the associated correlation length ξ_3 or ξ_c. It applies to the color-color, or Potts magnetic correlation function.

The numerical results for the eigenvalues of $\mathbf{T}$ reflect the divergences of the correlation lengths at the critical point, whose location can thus be found by means of phenomenological renormalization [19]. Moreover, the theory of conformal invariance provides information on the universality class. At criticality the free energy displays the following finite-size dependence [20–22]:

$$f_L \simeq f_\infty + \frac{\pi c}{6L^2}, \tag{10}$$

where c is the conformal anomaly [23], while the correlation lengths satisfy [24]

$$L\xi_{i,L}^{-1} \simeq 2\pi X_i \tag{11}$$

which yields estimates of the scaling dimension X_i of the observable with correlation length $\xi_{i,L}$.

As already reported in [8], the transfer-matrix results for the magnetic correlation length $\xi_{h,L}$ indicate that there are no divergences when $n \gg 2$. Ferromagnetic critical points are therefore absent. However, the magnetic correlation length is insensitive to an ordering of the loops in a hard-hexagon-like fashion, because the loop sizes remain finite. The latter type of transition thus remains possible.

A finite-size analysis of ξ_t revealed its presence for several values of n. Plots of the scaled gap $X_{t,L} \equiv L/(2\pi\xi_{t,L})$ as a function of x revealed minima approaching the three-state Potts temperature dimension $X_t = 4/5$.

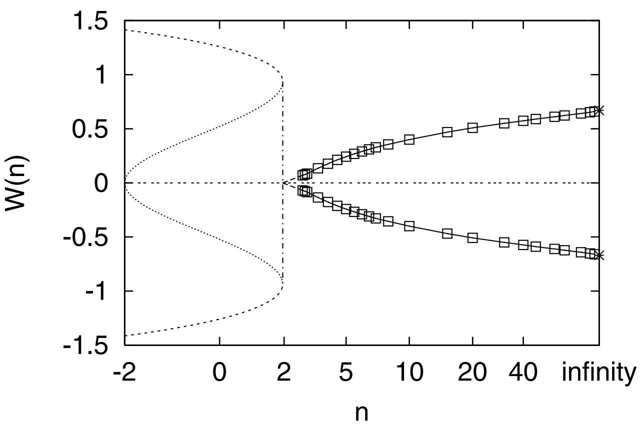

FIG. 1. Phase diagram of the O(n) model on the honeycomb lattice as a function of n and the relative weight x^{-1} of an empty vertex. Along the horizontal axis, we use a $1 - 8/(n + 10)$ scale. The vertical scale shows the scaled weight $W(n) = 1/[(n + 10)^{1/6}x]$. The model is exactly solvable on the curve shown for $n \leq 2$. Its outer branches (broken lines) describe the critical line [3] separating the disordered O(n) phase at large $|W(n)|$ from the low-temperature phase at small $|W(n)|$. The vertical line at $n = 2$ shows the critical state of the XY model. The line $W(n) = 0$ represents the fully packed loop model where empty vertices are forbidden. This line is critical for $n \leq 2$; its universal properties can be interpreted as a combination of low-temperature O(n) and solid-on-solid critical behavior [9]. An exact solution [26] shows that the line is no longer critical for $n > 2$. The data points ($\square$) show our results for the phase transition at $n > 2$. The curve connecting these points serves only as a guide to the eye. It also connects to the critical hard-hexagon model ($\times$) and the multicritical point $n = 2, W = 0$. The forbidden regime of (7) lies outside the scale shown.

The estimated critical points agree well with an analysis of the intersections of $X_{c,L} \equiv L/(2\pi\xi_{c,L})$ versus x curves for subsequent values of L. These intersections tend towards the expected value $X_c = 2/15$ for the three-state Potts universality class. Furthermore, our estimates of c are close to $4/5$ as expected for this classification.

The results for the critical points are shown in Fig. 1. The horizontal scale is chosen such as to include the whole range up to $n = \infty$. The vertical scale displays $W(n) = (n + 10)^{-1/6}x^{-1}$. The n-dependent factor keeps the vertical coordinate finite for $n \to \infty$. In this limit the hard-hexagon critical point [4] occurs at $x^6 n = (11 + 5\sqrt{5})/2$. For large n the critical points estimates converge well with increasing system size L, and the corresponding values of X_t, X_c, and c (see Table I) agree well with the three-state Potts universality class. For smaller n, the extrapolations become less accurate, as expected near the XY-type critical state at $n = 2$ [8,9]. Nevertheless the results suggest that the critical line connects to the point $n = 2$, $x^{-1} = 0$. This agrees with the conclusion of Kondev and Henley [25], based on Baxter's exact solution of a three-coloring problem [26], that hard-hexagon-like order exists on the line $x^{-1} = 0$ for $n > 2$. Furthermore we note that the critical line indeed avoids the regime excluded by (7), which reads $|W(n)| > B_n$, $n > 10\sqrt{2}$, with B_n decreasing monotonically from $B_{10\sqrt{2}} = \infty$, to $B_\infty = 2$. The newly found phase transition is physical ($x \geq 0$) from the point of view of the loop and the corner-cubic models, but it lies far inside the unphysical region ($|x| > 1/n$) of the O(n) spin model (1) where negative weights occur. This discards its

TABLE I. Numerical results for critical points x_c and scaling dimensions X_t, and X_c, and the conformal anomaly c for several values of n. The results for x_c and X_t are extrapolated from the minima of the scaled gaps $X_{t,L}$; those for X_c and c are extrapolated at the estimated critical points. Estimated numerical uncertainties in the last decimal place are shown in parentheses. With the exception of the smallest values of n, the results agree well with three-state Potts universality: $c = X_t = 4/5$ and $X_c = 2/15$.

n	x_c	X_t	X_c	c
4	3.63 (2)	0.76 (5)	0.1 (1)	1.5 (3)
5	2.63 (1)	0.79 (3)	0.10 (4)	1.1 (3)
6	2.17 (1)	0.82 (3)	0.16 (3)	0.9 (2)
7	1.91 (1)	0.83 (3)	0.16 (3)	0.8 (2)
8	1.74 (1)	0.82 (2)	0.14 (2)	0.8 (1)
10	1.52 (1)	0.80 (1)	0.14 (1)	0.80 (5)
15	1.248 (1)	0.79 (1)	0.13 (1)	0.80 (3)
20	1.117 (1)	0.79 (1)	0.133 (3)	0.78 (2)
30	0.9821 (2)	0.79 (1)	0.134 (5)	0.79 (2)
40	0.9075 (1)	0.80 (1)	0.130 (4)	0.79 (1)
50	0.8581 (1)	0.80 (1)	0.134 (2)	0.79 (1)
75	0.7811 (1)	0.80 (1)	0.132 (2)	0.79 (1)
100	0.7342 (1)	0.80 (1)	0.132 (2)	0.79 (1)
200	0.63933 (2)	0.800 (3)	0.134 (1)	0.79 (1)
400	0.56193 (1)	0.802 (2)	0.134 (1)	0.79 (1)
800	0.49650 (1)	0.801 (1)	0.134 (1)	0.79 (1)

interpretation in terms of spin ordering. It is unrelated to the ordering phenomena in the O(3) spin model reported by Patrascioiu and Seiler [27] which are of a ferromagnetic nature, i.e., do not break the sublattice symmetry.

As noted in [9], the loops cover an even number of edges, so that the sign of x is redundant and the phase diagram is symmetric with respect to the line $x^{-1} = 0$. Since line $x^{-1} = 0$ is a locus of higher symmetry, the possibility of a different universal behavior arises. Indeed, at $n = 2$, $x^{-1} = 0$ we find different exponents, namely, $X_t = 1.46$ (1) (see [9]) and $X_c = 0.65$ (2), close to exact results which are $3/2$ and $2/3$, respectively [25].

In the limit $n \longrightarrow \infty$, n/x^6 constant, the loops occupy elementary hexagons, and behave as hard particles. However, for finite n larger loops are possible. If more space than one elementary face is available, a loop may grow to occupy that space. In this sense the finite-n model behaves as a system of soft particles with hexagonal symmetry. While large-n ordering phenomena may also occur on other lattices, their universality naturally depends on the lattice type and the vertex weights [28].

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