Collapse of a polymer in two dimensions

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Abstract

We numerically investigate the influence of self-attraction on the critical behaviour of a polymer in two dimensions, by means of an analysis of finite-size results of transfer-matrix calculations. The transfer matrix is constructed on the basis of the $O(n)$ loop model in the limit $n \to 0$. It yields finite-size results for the magnetic correlation length of systems with a cylindrical geometry. A comparison with the predictions of finite-size scaling enables us to obtain information about the phase diagram as a function of the chemical potential of the loop segments and the strength of the attractive potential. Results for the magnetic scaling dimension can be interpreted in terms of known universality classes. In particular, when the attractive potential is increased, we observe the crossover between polymer critical behaviour of the self-avoiding walk type to behaviour described earlier for the theta point.

1 Introduction

A useful formulation of the polymer problem can be given in terms of the $O(n)$ loop model on a lattice, in the limit $n \to 0$. In this formulation, loops have a weight $n$ so that the number of loops is minimized as $n \to 0$. In the simplest case, only one other parameter plays a role: a weight factor $a$ may be assigned to each loop segment, in order to control the density of the loop configurations. A loop segment is the part of a loop that covers precisely one lattice edge. Loops do not intersect. For small $a$ the vacuum state – without any loops – is stable; in contrast, for large $a$, most of the lattice edges are covered by a loop. The critical point separating the vacuum state and the dense phase has already been explored in detail; it is found to belong to the same universality class as the SAW (self-avoiding walk).
Exact results for the $O(n)$ loop model on the honeycomb lattice have been obtained [1–4] that reveal two branches of critical points (two points for each $n$ in the range between 0 and 2). One of these branches is interpreted as a critical point separating the disordered and long-range phases; the other branch is supposed to describe the ordered phase. This branch has algebraically decaying correlations for general $n$; in this sense it still qualifies as a critical branch.

This picture applies to the case where the loop segments do not interact. A natural extension of the noninteracting loop model is to adjust the vertex weights in a way representing attractive forces between loop segments. Such interactions, if they are of a sufficient strength, will influence the character of the phase transition between the vacuum and the dense phase. In the case of strong attractive forces, the critical state, which is relatively dilute, becomes unstable, so that the phase transition becomes first-order.

The higher order critical point, separating the first-order transition from the continuous one, describes a polymer on the verge of collapse, and is called the theta point. An exactly known critical point of an $n = 0$ loop model with vacancies on the honeycomb lattice, described by Duplantier and Saleur [5], belongs to the universality class of this theta transition.

The formulation of the square $O(n)$ loop model given in Ref. [6] contains three adjustable parameters. One of these applies to the weight of vertices visited twice by a loop. There, both loop parts make $90^\circ$ bends such that they collide but do not intersect. Thus, by varying this vertex weight one can tune the attractive forces.

For this three-parameter model, there are several branches of exactly known critical points [6–9]. Two of these have the same universal properties as those mentioned above for the honeycomb lattice. Two other branches are associated with a combination of Ising-like and $O(n)$ critical behaviour. The fifth branch, which was dubbed ‘branch 0’, is related with the dense phase of the $O(n+1)$ model [6] and contains an integrable critical point [6,10] similar to the above-mentioned theta point [5]. In particular, the $O(n = 0)$ point has been shown to be equivalent to interacting walks on the Manhattan lattice at the theta point [11], with a set of exponents in agreement with those proposed for the theta transition [5], if one associates the magnetic dimension $x_m = \eta/2 = 0$ [5] with the critical dimension $x_{\text{int},1}$ which was discussed in Ref. [6].

Thus, the subset of the parameter space contains a considerable variety of critical points for which exact information is available [6–12]. Nevertheless, it covers only a small part of the parameter space. Therefore, it is of interest to explore the critical surface by numerical means. In particular, here we investigate the influence of attractive forces between the loop segments in the square $O(n)$ loop model, in the hope to observe the crossover between the
normal $O(n = 0)$ or SAW-like critical point and the proposed theta point.

In Section 2 we briefly introduce the $O(n)$ loop model, and the transfer matrix used for the numerical calculations. Section 3 contains an analysis and a discussion of the numerical work. For this purpose, it also summarizes the finite-size scaling formulas and an element of the theory of conformal invariance used in the analysis.

2 The model and its transfer matrix

The loop representation of the $O(n)$ model yields an expression for the partition function in terms of a sum over all graphs consisting of closed loops, covering a subset of the lattice edges [13,1]. The simplest case, with only two parameters, the loop weight $n$ and the weight factor $a$ per bond, has been investigated for the $O(n)$ loop model on the honeycomb lattice. In addition to exact results, conclusions based on a numerical investigation are available. Finite-size scaling of transfer-matrix results can be applied in parts of the parameter space where no exact information is known. These results [14] have confirmed the interpretation of the two critical branches as mentioned above.

In this work, we apply a similar method to the square lattice. The square $O(n)$ loop model is now formulated in terms of loop weights $n$, bond weights $a$, and an additional weight factor $p$ associated with each straight vertex, and an additional weight factor $q$ associated with each ‘collision’. Thus, the vertex weights are $w_0 = 1$ for an empty vertex (not visited by a loop), $w_1 = a$ for a vertex visited once by a loop making a $90^\circ$ bend, $w_2 = ap$ for a vertex visited once by a straight loop part, and $w_3 = a^2q$ for a vertex visited twice (see Fig. 1). Using these weights, the partition function becomes

$$Z = \sum_\mathcal{G} w_1^{N_1} w_2^{N_2} w_3^{N_3} n^{N_i},$$

where the sum is over all loop configurations $\mathcal{G}$. The graph $\mathcal{G}$ consists of $N_i$ nonintersecting loops, with $N_i$ ($i = 1, 2, 3$) the total number of vertices of the type indicated by index $i$.

A transfer matrix can be constructed for this loop model; a detailed description is given in Ref. [6]. The transfer matrix can be seen as an operation that builds up a cylinder on which the lattice $O(n)$ model is wrapped, by adding one circular row, and thus increasing the length of the cylinder by one unit. The presence of the open end of the cylinder allows non-empty bond configurations even for $n = 0$, where closed loops are actually excluded. The transfer matrix indices are a numerical coding of ‘connectivities’: the way in which the
Fig. 1. Vertex weights for the O(n) loop model on the square lattice. In the present work we choose \( p = 0 \), so that 180° vertices are excluded.

dangling bonds, or loop segments, are connected at the end of the cylinder. The allowed connectivities are ‘well nested’: no four occupied edges can be crosswise connected. This property is a consequence of the absence of intersections, and greatly restricts the number of connectivities. A sparse-matrix decomposition [6] allowed us to obtain transfer-matrix eigenvalues for systems up to linear size \( L = 12 \) using only modest computational resources.

These transfer matrix eigenvalues are meaningful because they determine the free energy and the length scales determining the decay of the correlation functions along the cylinder. In the general case, the free energy per unit of area \( f \) of a model on an infinitely long cylinder with finite size \( L \) is determined by

\[
f(L) = L^{-1} \ln \Lambda_L^{(0)},
\]

where \( \Lambda_L^{(0)} \) is the largest eigenvalue of the transfer matrix. In the paramagnetic phase of the O\((n = 0)\) loop model, as well as on the critical line separating the ordered phase, \( \Lambda_L^{(0)} = 1 \). The corresponding eigenvector is dominated by the vacuum. This eigenvalue 1 persists in the ordered phase, but there it is no longer the largest eigenvalue. For reasons of continuity, we maintain the notation \( \Lambda_L^{(0)} = 1 \).

For practical reasons, the set of connectivities is split into two disjoint subsets: the even subset, where all the dangling bonds are connected pairwise; and the odd subset where, in addition, a single, unpaired dangling bond occurs. The vacuum-dominated leading eigenvector naturally occurs in the even sector. The odd sector contains a line of covered bonds, running along the length direction of the cylinder. Such a line is not a part of a closed loop, and does not occur in the graphs \( \mathcal{G} \) of Eq. (1). Therefore, the odd sector does not contribute to the partition sum.

However, the odd connectivities are important for the calculation of the mag-
netic correlation length of the O(n) model. The graphs containing, in addition with closed loops, a single line of covered bonds connecting two points are precisely those describing the magnetic correlation function between O(n) spins located on those points. It is expressed as $Z'/Z$, where $Z$ is given by Eq. (1), and $Z'$ by the same equation but with $G$ replaced by $G'$ representing all graphs consisting of closed loops plus a single line connecting the two spins.

Thus, the inverse magnetic correlation length $\xi^{-1}(L)$ can be expressed in terms of $\Lambda_{L}^{(0)}$ and $\Lambda_{L}^{(1)}$ which denotes the largest eigenvalue in the odd sector:

$$\xi^{-1}(L) = \ln(\Lambda_{L}^{(0)}/\Lambda_{L}^{(1)}).$$

A convenient quantity in the finite-size analysis is the ‘scaled gap’ $x(u, L) = L/[2\pi\xi(u, L)]$ whose arguments include, besides the finite size $L$, also a temperature-like parameter $u$. For instance we may choose $u = a-a_c$ where $a_c$ denotes the critical value of the bond weight $a$. But $u$ may also be chosen to parametrize the distance to fixed points located on the critical surface. In the vicinity of a renormalization fixed point, finite-size scaling leads to the equation

$$x(u, L) = x_h + \frac{1}{2\pi} L^{y_u} u [d\xi^{-1}(u, 1)/du]_{u=0} + \ldots,$$

where $x_h$ is the magnetic scaling dimension [15] of the corresponding fixed point, and $y_u$ the renormalization exponent associated with $u$, governing the flow to or away from the fixed point. Thus, if $y_u < 0 (> 0)$, $x(u, L)$ converges to (diverges from) $x_h$ with increasing $L$. This allows us to analyse the behaviour of the finite-size results $x(u, L)$ in the light of the phase diagram.

3 Results

Before starting the actual transfer-matrix calculations at $n = 0$, we summarize the role of the three parameters. First, the bond weight $a$ (or $w_1$) is adjusted in order to find the critical point. Expressing the scaled gap in $a$, ignoring the irrelevant scaling fields, and using finite-size scaling of the correlation length, the critical point $a_c$ is determined by numerical data for two subsequent even finite sizes $L$ and $L + 2$:

$$x(a_c, L) = x(a_c, L + 2).$$

Only even sizes are used because, in general, the odd systems display different finite-size amplitudes [6]. Corrections to scaling introduce deviations from
Eq. (5) so that extrapolation of the finite-size estimates of $a_c$ was performed. For details, see e.g. Ref. [16].

The parameter $p$ is here important with regard to the Ising-like degrees of freedom that play a role in the square loop model [6]. In order to clarify this point, we introduce an Ising spin on each elementary face, such that two neighboring spins are equal only when a loop passes between them. Clearly when $p = 0$ a loop is adjacent to spins of one sign only, signalling a broken Ising symmetry. This means that an Ising-like ordering transition occurs when $p$ is lowered.

In the present work, we wish to focus on the collapsing polymer problem, while avoiding the interfering effects associated with Ising-like ordering. A possible way to circumvent these effects is to exclude type 2 vertices by putting $p = w_2 = 0$, so that the Ising degrees of freedom are already frozen even in the relatively dilute SAW-like critical state. An increasing polymer density does not further affect this Ising ordering.

Thus, we scanned the parameter space using $w_1 = a$, $w_2 = 0$, and $w_3 = qa^2$ where the parameter $q$ governs the attraction between the loop segments. This choice of parameters includes the integrable theta point mentioned above, for which $a = 0.5$, $q = 2$.

Using finite size parameters $L = 2, 4, 6, 8$ and 10, Eq. (5) was solved for $q = 0, 1.0, 1.5, 1.8, 1.9, 2.0, 2.1, 2.2, 2.5, 3.0$ and 4.0. The extrapolated critical points are shown in Table 1.

The value $a_c = 0.63860(5)$ at $q = 0$ gives the connective constant $1/a_c \simeq 1.565\ldots$ for SAWs with a $90^\circ$ turn at every step, in good agreement with the estimate 1.5657(19) [17]. The scaled gaps at the intersections are plotted versus the system size $L$ in Fig. 2. These data are to be compared to Eq. (4) where we may interpret $t$ as a field parametrizing the critical line; the leading temperature field vanishes in effect for the solution of Eq. (5). The field along the critical line is expected to be irrelevant in the vicinity of the SAW-like fixed point; at a higher critical point, it is expected to be relevant. Indeed, for $q < 2$ we observe, for increasing $L$, a converging trend towards the exactly known value $x_h = 5/48 = 0.104166\ldots$ for the SAW model. This convergence reflects the stability of the SAW-like fixed point. For $q = 2$ the finite-size data converge well to $x_h = 1/4$, in agreement with the known value at the integrable point.

For $q > 2$ the phase transition becomes discontinuous as a function of the temperature-like parameter $a$, as is revealed by an intersection of the two largest eigenvalues $\Lambda_0 = 1$ and $\Lambda_2$ of the transfer matrix in the even sector. For the interpretation of the results shown in Fig. 2 it is important to note that we used $\Lambda_0 = 1$ in Eq. (3), even where other eigenvalues exceed 1; this occurs
Table 1

Numerical results for the critical value of the bond weight $a$ for $O(n = 0)$ loop models with different values of the loop-loop interaction parameter $q$ (see column 1). For $q \leq 1.5$ we assumed a correction term proportional to $L^{-9/4}$, for $q > 1.5$ one proportional to $L^{-1}$. The rightmost column shows the estimated value for the magnetic dimension $x_h$ where extrapolation was possible. The extrapolations for $q = 2$ are in a good agreement with the exact values $a_c = 1/2$ and $x_h = 1/4$.

| $q$  | $a_c$       | $x_h$     |
|------|-------------|-----------|
| 0.0  | 0.63860 (5) | 0.1045 (5)|
| 1.0  | 0.5769 (1)  | 0.104 (1) |
| 1.5  | 0.5399 (1)  | 0.11 (1)  |
| 1.8  | 0.5165 (1)  |           |
| 1.9  | 0.5084 (1)  |           |
| 2.0  | 0.5001 (1)  | 0.2500 (2)|
| 2.1  | 0.4917 (1)  |           |
| 2.2  | 0.4833 (2)  |           |
| 2.5  | 0.4575 (5)  |           |
| 3.0  | 0.421 (1)   |           |
| 4.0  | 0.368 (1)   |           |

for $q > 2$ even at the line of phase transitions. Using this analytic continuation we avoid irregularities caused by the intersections mentioned. The increasing trend of the data in Fig. 2 for $q > 2$ reflects the instability of the theta-like fixed point.

However, the lines connecting the finite-size results in Fig. 2 are running almost horizontally for $q \approx 2$; the finite-size dependence of the scaled gap is rather weak. This corresponds with a small value of the exponent $y_u$ in Eq. (4) when applied to the theta point. Indeed, from Coulomb gas arguments [5,19] one expects $y_u = 3/4$.

Also in the vicinity of the stable SAW-like fixed point, the finite-size dependence of the data shown in Fig. 2 is rather weak. This stands in a strong contrast with the rapid convergence observed [18] for $O(n = 0)$ loop models with $p = 1$, which can be interpreted [16] in terms of an irrelevant exponent $y_i = -2$. The present slow trends near the SAW-like fixed points may be explained by an irrelevant exponent $-11/12$, in analogy with the case of ‘trails’ where loops are allowed to intersect [16]. In the Coulomb gas representation, loop intersections and collisions correspond with the same diagrams.
Fig. 2. Finite-size dependence of the scaled gap of O(n) models. These data are taken at values of the bond weight \( a \) solving the scaling equation for the correlation length for two subsequent system sizes. The lines connecting the data points are for visual aid only. Starting from below, the lines apply to \( q = 0, 1.0, 1.5, 1.8, 1.9, 2.0 \) (dashed line), 2.1, 2.2, 2.5, 3.0 and 4.0 respectively.

We have performed extrapolations on the basis of the numerical solutions of Eq. (5). According to finite-size scaling, the solutions \( a(q, L) \) obtained from finite sizes \( L \) and \( L - 2 \) behave as \( a(q, L) = a(q) + bL^{y_u - y_t} + \cdots \) where \( y_t \) is the leading temperature exponent; \( y_t = 4/3 \) at the SAW-like fixed point, and \( y_t = 7/4 \) at the theta point. For the second temperature-like exponent we may expect \( y_u = -11/12 \) and \( y_u = 3/4 \) respectively. On the basis of our limited range of finite sizes, it was not possible to well determine \( y_u \) independently for all \( q \). Only in the case \( q = 0 \) we could confirm that \( y_u - y_t \approx -2.2 \) as expected. For \( q = 2.1 \) and 2.2 we find results for \( y_u - y_t \) consistent with \(-1\) but the data show that further corrections are important. Thus we assumed \( y_u - y_t = -9/4 \) for \( q \leq 1.5 \) and \( y_u - y_t = -1 \) for \( q > 1.5 \), and extrapolated the finite-size estimates of the critical points accordingly. The results are shown in Table 1. More details of the fitting procedure can be found in Ref. [16].

Since the solutions of Eq. (5) converge to the critical point, the scaled gaps converge to the corresponding magnetic scaling dimension. For those cases where the finite-size convergence was sufficiently fast, extrapolated results are included in Table 1. The results for \( q = 0, 1 \) and 1.5 are in a good agreement with the expected O\((n = 0)\) magnetic dimension \( x_h = 5/48 = 0.104166\ldots \). Thus, the fact that the Ising degree of freedom is frozen does not seem to alter the universal properties. For \( q = 2 \) our result for the magnetic dimension
agrees well with \( x_h = 1/4 \) as found earlier for this integrable point of the square \( O(n = 0) \) model \([6,10]\). For larger values of \( q \) the finite-size data assume a monotonically increasing trend with \( L \), in accordance with earlier observations at first-order transitions, for instance that of the Potts model with a large number of states \([20]\).

The phase diagram of the model, summarizing our findings, is shown in Fig. 3. The vacuum state occurs near the origin, and a dense phase at large values of \( w_1 \) and \( w_3 \). These phases are separated by a line of phase transitions of which the upper part is first order, and the right hand part is critical, with the theta point separating both parts.

![Phase diagram of the O(n = 0) model for \( w_2 = 0 \). The line of phase transitions has a first-order part (solid line) and a continuous part (broken line). This line is an interpolation between the numerical results (open circles), the exactly known theta point at \( w_1 = 1/2 \) (black circle) and the exactly known point at \( w_1 = 0 \) (black square).](image)

In conclusion, our data confirm that the introduction of sufficiently strong attractive forces in the critical \( O(n = 0) \) model leads to the collapse of a polymer in two dimensions. The critical exponents at the point of collapse are in agreement with the predictions of Duplantier and Saleur \([5]\) provided we avoid the onset of Ising-like ordering which is known to lead to a different universality class \([6]\).
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