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Numerical simulation of a lattice polymer model at its integrable point

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Abstract

We revisit an integrable lattice model of polymer collapse using numerical simulations. This model was first studied by Blöte and Nienhuis (1989 *J. Phys. A: Math. Gen.* **22** 1415) and it describes polymers with some attraction, providing thus a model for the polymer collapse transition. At a particular set of Boltzmann weights the model is integrable and the exponents $\nu = 12/23 \approx 0.522$ and $\gamma = 53/46 \approx 1.152$ have been computed via identification of the scaling dimensions $x_t = 1/12$ and $x_h = -5/48$. We directly investigate the polymer scaling exponents via Monte Carlo simulations using the pruned-enriched Rosenbluth method algorithm. By simulating this polymer model for walks up to length 4096 we find $\nu = 0.576(6)$ and $\gamma = 1.045(5)$, which are clearly different from the predicted values. Our estimate for the exponent ν is compatible with the known θ-point value of $4/7$ and in agreement with very recent numerical evaluation by Foster and Pinettes (2012 *J. Phys. A: Math. Theor.* **45** 505003).

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(Some figures may appear in colour only in the online journal)

1. Introduction

The study of the critical properties of lattice polymers, and thus of $O(n)$ models when we let $n \to 0$, in two dimensions has been ongoing over decades theoretically and numerically. Nienhuis, in 1982 [2], considered a model of non-intersecting loops on the hexagonal lattice which allowed him to compute the critical exponents for free self-avoiding walks (SAWs) ($\nu = 3/4$, $\gamma = 43/32$), which model dilute polymers, and for dense polymers ($\nu = 1/2$, $\gamma = 19/16$). In 1987 Duplantier and Saleur [3] were able to model bond interactions

introducing vacancies on the same lattice, obtaining a full set of critical exponents for the polymer collapse transition in the interacting self-avoiding walk (ISAW) model. This collapse transition, a tri-critical point, goes under the name of 'θ-point' and has critical exponents $\nu = 4/7$ and $\gamma = 8/7$. There was debate at the time over the surface exponents which was resolved by Vanderzande *et al* [4] and Stella *et al* [5] on the hexagonal lattice and on the square lattice by Foster *et al* [6].

In the quest for a solvable $O(n)$ model on the square lattice, Blöte and Nienhuis in 1989 [7] considered a lattice model (related to the Izergin–Korepin vertex model) which includes weights for site-collisions and straight segments (stiffness). For this model five critical branches are exactly known [7–10]. In one of these branches (named 'branch 0' in [7]) straight segments are completely suppressed and it can be shown that in this case the model maps to the ISAW model on the Manhattan lattice for which the conjectured exponents are $\nu = 4/7$, $\gamma = 6/7$ [11–13]. Two other branches correspond to dense and dilute polymers as obtained by Nienhuis in [2], and the two remaining branches are, respectively, associated with a combination of Ising-like and $O(n)$ critical behaviour and with a new tri-critical point. This other tri-critical point, which we shall refer as the Blöte–Nienhuis (BN)-point, is another candidate for describing a collapsing polymer and has exponents $\nu = 12/23$ and $\gamma = 53/46$ [10]. The configurations associated with this particular $O(n)$ model, which we shall call vertex-interacting self-avoiding walks (VISAWs), are forbidden to cross and therefore are a subset of self-avoiding trails (SAT). The Boltzmann weights corresponding to BN-point are known exactly and can be expressed as algebraic numbers.

Foster and Pinettes [14] have studied the semi-flexible VISAW at this special BN-point, and have also studied the VISAW model without stiffness, using the corner transfer matrix renormalization group method. Some agreement and some discrepancy with the scaling dimensions proposed [7–10] was found in [14] and a first order nature to the transition was conjectured. Very recently Foster and Pinettes [1] have used transfer matrices and the density matrix renormalization group method (DMRG) to consider the bulk and surface exponents of these models. They have found values of the exponent ν much closer to 4/7 than 12/23. In this paper we study by means of Monte Carlo simulation the semi-flexible VISAW polymer model precisely at the BN-point. We find estimates for the exponents, and hence the scaling dimensions, that are in harmony with those found by Foster and Pinettes [1] and at variance with those predicted by Warnaar *et al* [10].

2. Semi-flexible VISAW

The semi-flexible VISAW model can be defined as follows. SATs, or simply trails, are lattice paths that can be formed such that they never visit the same bond more than once. Such paths can generally visit the same site of the lattice either by a *collision*, where the trail touches itself, or via a *crossing*, where two straight segments of the path cross over one another. Consider the *subset* of bond-avoiding lattice paths (trails) on the square lattice, $\mathcal{V}_n$, where *no* crossings are allowed. Given such a restricted trail $\psi_n \in \mathcal{V}_n$, we associate an energy $-\varepsilon_t$ every time the path visits the same site more than once, which it can only do by *colliding* with itself; see figure 1. Additionally, we define a straight segment of the trail by two consecutive parallel edges, and we associate an energy $-\varepsilon_s$ to each straight segment of the trail, modelling the stiffness of the polymer chain.

For each configuration $\psi_n \in \mathcal{V}_n$ we count the number $m(\psi_n)$ of doubly-visited sites and $s(\psi_n)$ of straight segments; see figure 1. Hence we associate with each configuration a

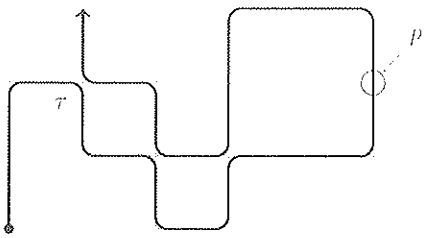

Figure 1. An example of a semi-flexible VISAW configuration with three ($m = 3$) collisions associated with a Boltzmann weight τ and five ($s = 5$) straight segments, each associated with a Boltzmann weight p.

Boltzmann weight $\tau^{m(\psi_n)} p^{s(\psi_n)}$ where $\tau = \exp(\beta\varepsilon_t)$, $p = \exp(\beta\varepsilon_s)$, and β is the inverse temperature $1/k_B T$. The partition function of the model is given by

$$Z_n(\tau, p) = \sum_{\psi_n \in \mathcal{V}_n} \tau^{m(\psi_n)} p^{s(\psi_n)}. \tag{2.1}$$

The finite-length reduced free energy is

$$\kappa_n(T) = \frac{1}{n} \log Z_n \tag{2.2}$$

and the thermodynamic limit is obtained by taking the limit of large n, i.e.,

$$\kappa(T) = \lim_{n\to\infty} \kappa_n(T). \tag{2.3}$$

It is expected that there is a collapse phase transition at a temperature T_c characterized by a non-analyticity in $\kappa(T)$. Equivalently, one can think of varying τ at fixed p so that there is a collapse at some value of $\tau = \tau_c(p)$.

The probability of a configuration ψ_n is then

$$p(\psi_n; \tau, p) = \frac{\tau^{m(\psi_n)} p^{s(\psi_n)}}{Z_n(\tau, p)}, \tag{2.4}$$

and the average of any quantity Q over the ensemble set of path $\mathcal{V}_n$ is given generically by

$$\langle Q \rangle_n(\tau, p) = \sum_{\psi_n \in \mathcal{V}_n} Q(\psi_n)\, p(\psi_n; \tau, p). \tag{2.5}$$

In this paper we are interested in the following quantities. We calculate three measures of the size of the polymer, $\langle R_e^2 \rangle_n$, $\langle R_m^2 \rangle_n$ and $\langle R_g^2 \rangle_n$, defined as follows. We specify any n-step path ψ_n on a lattice by a sequence $\mathbf{r}_0, \mathbf{r}_1, \ldots, \mathbf{r}_n$ of vector positions of the vertices of that path. Firstly, we are interested in the average-square end-to-end distance

$$\langle R_e^2 \rangle_n = \langle \mathbf{r}_n \cdot \mathbf{r}_n \rangle, \tag{2.6}$$

secondly, the ensemble average of the mean-square distance of a monomer from the endpoints

$$\langle R_m^2 \rangle_n = \frac{1}{n+1} \sum_{i=0}^{n} \langle \mathbf{r}_i \cdot \mathbf{r}_i \rangle, \tag{2.7}$$

and defining the average centre-of-mass as

$$\langle R_c^2 \rangle_n = \frac{1}{(n+1)^2} \sum_{i=0}^{n} \sum_{j=0}^{n} \langle \mathbf{r}_i \cdot \mathbf{r}_j \rangle, \tag{2.8}$$

we, thirdly, are interested in the average radius-of-gyration

$$\langle R_g^2 \rangle_n = \langle R_m^2 \rangle_n - \langle R_c^2 \rangle_n. \tag{2.9}$$

In the above formulae we use $\mathbf{r}_0 \equiv \mathbf{0}$.

2.1. Scaling

The partition function at, and above, the collapse temperature is believed to scale as

$$Z_n \sim D\mu^n n^{\gamma-1} \tag{2.10}$$

where μ is known as the connective 'constant' and is related to the thermodynamic free energy via

$$\mu = e^{\kappa(T)}. \tag{2.11}$$

The constant D is also temperature dependent but γ is expected to be universal, depending only on the temperature in as much as its value is above, or at, the collapse temperature. In two dimensions it is well established [2] that for $T > T_c$ (equivalently $\tau < \tau_c(p)$) we have $\gamma = 43/32$.

The collapse transition can also be characterized via a change in the scaling of the size of the polymer with temperature. The three measures of the size of the polymer defined above are expected to scale as

$$R_n^2 \sim C_R n^{2\nu}, \tag{2.12}$$

where the amplitude C_R is non-universal and temperature dependent, while ν is expected to be universal, depending only on the temperature in as much as its value is above, at, or below, the collapse point. In two dimensions it is also established [2] that $\nu = 3/4$ for $T > T_c$.

Duplantier and Saleur [3] identified a tri-critical point, known as the θ-point, which is expected to describe the collapse of a polymer in two dimensions. This point has thermal and magnetic scaling dimensions $x_t = 1/4$, $x_h = 0$ and consequently polymer exponents $\nu = 4/7$ and $\gamma = 8/7$. On the other hand, Warnaar *et al* [10] predicted $\nu = 12/23$ and $\gamma = 53/46$ for the semi-flexible VISAW model at its collapse point.

2.2. Amplitudes

One can also usefully define the finite-length amplitude ratios

$$A_n = \frac{\langle R_g^2 \rangle_n}{\langle R_e^2 \rangle_n} \quad \text{and} \quad B_n = \frac{\langle R_m^2 \rangle_n}{\langle R_e^2 \rangle_n}, \tag{2.13}$$

since these approach universal values [15]

$$A_n \to A_\infty = \frac{C_{R_g}}{C_{R_e}} \quad \text{and} \quad B_n \to B_\infty = \frac{C_{R_m}}{C_{R_e}} \tag{2.14}$$

in the limit $n \to \infty$. For collapsing polymers, the limiting values should depend only on dimension and whether the temperature is above or at the collapse transition point.

For free SAWs (which should include the VISAW model at high temperatures) it was predicted [16, 17] that

$$\lambda A_\infty - 2B_\infty + \tfrac{1}{2} = 0. \tag{2.15}$$

In the derivation [16] of this invariant the factor multiplying A_∞ was given by

$$\lambda = 2 + \frac{y_t}{y_h}, \tag{2.16}$$

where $y_t = 4/3$ and $y_h = 91/48$ are the thermal and magnetic renormalization group eigenvalues, respectively, of the dilute O(0) model. These eigenvalues are related to the conformal scaling dimensions via $y = 2 - x$. Hence

$$\lambda(x_t, x_h) = 2 + \frac{2 - x_t}{2 - x_h}. \tag{2.17}$$

The identity (2.15) implies that one can estimate this function of the scaling dimensions as

$$\lambda(x_t, x_h) = \frac{4B_\infty - 1}{2A_\infty}, \tag{2.18}$$

from estimates of A_∞ and B_∞. This was done for various collapse models in [18]. Hence, if we have a conjectured value of one of the scaling dimensions we can estimate the other from an estimate of λ.

3. Integrable Blöte–Nienhuis Point

The special multi-critical point of the $O(n)$ model that maps to the semi-flexible VISAW and allows for the calculation of the scaling dimensions via the Bethe Ansatz is given by special values of the parameters in the grand canonical partition function

$$G(K; \tau, p) = \sum_{n=0}^{\infty} K^n Z_n(\tau, p). \tag{3.1}$$

The location of this point is reported exactly in [7]

$$\begin{aligned} w &= K_{bn}^2 \tau_{bn} = \{2 - [1 - 2\sin(\theta/2)][1 + 2\sin(\theta/2)]^2\}^{-1} \\ K_{bn} &= -4w\sin(\theta/2)\cos(\pi/4 - \theta/4) \\ p_{bn}K_{bn} &= w[1 + 2\sin(\theta/2)] \\ \theta &= -\pi/4 \qquad \text{(branch 3 in [7]).} \end{aligned}$$

Alternatively, this can be expressed in explicit algebraic numbers or evaluated numerically as $K_{bn} = 0.446\,933\ldots$, $p_{bn} = 0.275\,899\ldots$, and $\tau_{bn} = 2.630\,986\ldots$.

From the value of K_{bn} we can give the conjectured value of the connective constant μ (2.11) in the canonical model (2.1) at fixed Boltzmann weights $(\tau, p) = (\tau_{bn}, p_{bn})$ as

$$\begin{aligned} \mu(\tau_{bn}, p_{bn}) = \frac{1}{K_{bn}} &= \left(\frac{\sqrt{2}}{2} + \frac{\sqrt{2}}{2}\sqrt{2 - \sqrt{2}} + \sqrt{2 - \sqrt{2}}\right)\sqrt{2 - \sqrt{2 - \sqrt{2}}} \\ &= 2.237\,469\,94\ldots. \end{aligned} \tag{3.2}$$

The set of scaling dimensions evaluated in [10] at this (multi-)critical point are

$$x_\ell = \frac{\ell^2}{16} - \frac{1}{6} \qquad \text{for } \ell \in \mathbb{N}. \tag{3.3}$$

The thermal x_t and magnetic x_h scaling dimensions were identified [10] as

$$x_h = x_{-1} = -\tfrac{5}{48} = -0.104\,16\ldots \qquad \text{and} \qquad x_t = x_2 = \tfrac{1}{12} = 0.083\,33\ldots. \tag{3.4}$$

It can be seen that these scaling dimensions are not those of unweighted SAWs: this is compatible with the hypothesis that they are those of a collapse multi-critical point.

The exponents ν and γ were then calculated [10] in the standard way as

$$\nu = \frac{1}{2 - x_t} = \frac{12}{23} = 0.521\,74\ldots \tag{3.5}$$

$$\gamma = 2\nu(1 - x_h) = \frac{53}{46} = 1.152\,17\ldots. \tag{3.6}$$

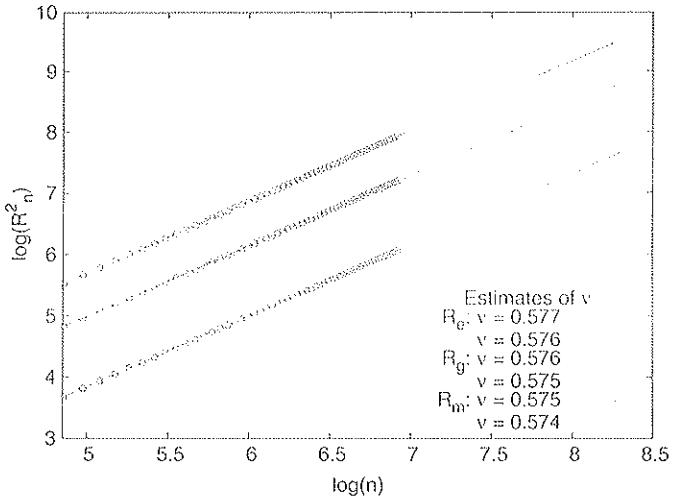

Figure 2. A double-logarithmic plot of three different measures R^2_n of the polymer size, the mean-square end-to-end distance $\langle R^2_e \rangle_n$ (top), the square of the radius of gyration $\langle R^2_g \rangle_n$ (bottom), and the mean-square distance of a monomer to its end points $\langle R^2_m \rangle_n$ (middle) versus the length n of the path. The data from different simulations up to lengths 1024 (blue circles), 2048 (green triangles), and 4096 (red line) clearly overlap. The exponent estimates for ν shown are derived from fitting straight lines through lengths 1024 to 2048 and 2048 to 4096, respectively.

4. Simulation results

We simulated the model (2.1) at the fixed values of $p = p_{bn}$ and $\tau = \tau_{bn}$ using the pruned-enriched Rosenbluth method (PERM) [19]. This method is based on the traditional Rosenbluth and Rosenbluth sampling method where biased samples of polymer configurations are generated along with a weight factor such that the weighted average over all polymer configurations will converge towards the correct Boltzmann average. PERM improves the efficiency of this algorithm by making multiple copies of partially grown chains that have a large statistical weight (enriching) and discarding configurations with small statistical weight (pruning). We ran three simulations with maximal length $N_{\max} = 1024$, 2048 and 4096, growing $S \simeq 10^7$ independent walks each and collecting from 8.7×10^7 to 1.5×10^8 samples at each maximal length. The number of samples adjusted by the number of their independent growth steps is between 2.1×10^5 and 4.8×10^5 'effective samples'.

In figure 2 we plot on a double-logarithmic scale the three different measures R^2_n of the polymer size. From various fits we consistently find estimates of ν near 4/7 rather than 12/23. Our best estimate is

$$\nu = 0.576(6). \tag{4.1}$$

This leads to an estimate of the thermal scaling dimension as

$$x_t = 0.26(2). \tag{4.2}$$

To obtain an estimate of γ we looked at the scaling of the canonical partition function (2.10). We first measured μ by a simple linear fit obtaining 2.2375(1), and observing that our value matches the value obtained from the BN-model, we then assumed $\mu = \mu_{bn}$. We hence plotted, in figure 3, on a double-logarithmic scale the normalized partition function Z_n/μ^n_{bn} versus the length n of the path.

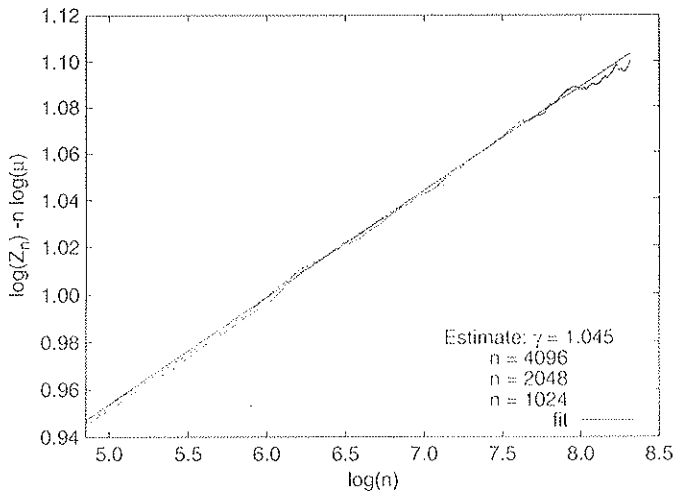

Figure 3. A double-logarithmic plot of the normalized partition function Z_n/μ^n versus the length n of the path. The difference between data from different simulations up to lengths 1024, 2048, and 4096 indicate the accuracy achieved. The exponent estimate for γ shown is derived from fitting straight lines through lengths 256 to 1024 to data from the best-converged simulation.

This allows us to estimate γ from straight line fits which we give as

$$\gamma = 1.045(5). \tag{4.3}$$

Interestingly, this value is different from both the θ-point value of $8/7 = 1.142\,28\ldots$ and the BN-point $53/46 = 1.1521\ldots$. Using $\gamma = 2\nu(1 - x_h)$ and our estimates of γ and ν in equations (4.3) and (4.1) gives us the estimate

$$x_h = 0.093(13). \tag{4.4}$$

We point out that this estimate is positive while the conjectured value above in equation (3.4) is not.

To obtain an independent estimate of x_h we attempted to estimate the universal quantity λ described above. In figure 4 we plot the finite-size amplitude ratio combination $\lambda_n = (4B_n - 1)/(2A_n)$ versus $n^{-4/7}$, which is the natural scale given the results above for the size measures. We find an estimate of this universal value as

$$\lambda = 2.93(3). \tag{4.5}$$

Unfortunately, the error estimate here is relatively larger than that estimated from the partition function analysis and we estimated $x_h = 0.12(4)$, which encompasses our more precise estimate in (4.4).

For the sake of completeness we have also found estimates of the universal amplitude ratios A and B by fitting against a correction of $n^{-4/7}$, which provide consistent straight fit extrapolations

$$A = 0.1534(10) \quad \text{and} \quad B = 0.475(5). \tag{4.6}$$

These values of A and B are different from the values for any of the three collapse models considered in [18].

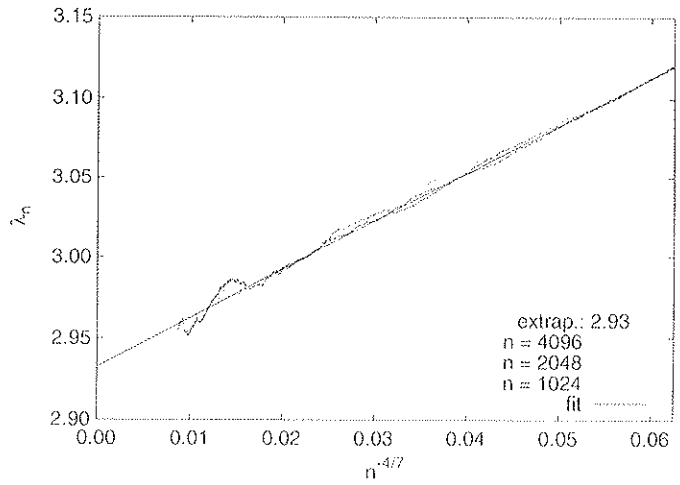

Figure 4. A plot of the finite-size amplitude ratio combination λ_n versus $n^{-4/7}$, together with a straight-line fit. The difference between data from different simulations up to lengths 1024, 2048, and 4096 indicate the accuracy achieved. The extrapolated value for λ shown is derived from fitting straight lines through lengths 256 to 1024 to data from the best-converged simulation.

5. Conclusions

We have simulated the special point, known as the BN (Blöte–Nienhuis) point, of the semi-flexible VISAW model of polymer collapse, which is associated with an integrable branch of the $O(n)$ loop model [7]. The exponent estimates we find, $\nu = 0.576(6)$ and $\gamma = 1.045(5)$, are not in accord with those previously found from the $O(n)$ loop model. Our estimate of ν is compatible with the value accepted for the θ-point, which is $4/7 = 0.5714\ldots$, and in good agreement with the results of Foster and Pinettes [1] who have used transfer matrices and DMRG. However, our estimate of γ is not comparable to any known value. We have found estimates of γ via two different methods: one method we used involved the direct estimation of the exponent from the partition function, and the other used results from conformal field theory and universal amplitude ratios of different size measures of the polymer; our estimates from these two methods broadly agree.

Our results seem to suggest that the BN point is θ like, at least with respect to its size scaling exponent with $\nu = 4/7$. This may seem at odds with our recent claim [20] that the VISAWs, which do not weight straight segments and have $p = 1$ in the notation of this paper, have a collapse transition in the same universality class as the interacting self-avoiding trails (ISAT) [21]. This was based, however, upon analysis of the specific heat. Of course, the two claims are not in direct contradiction but they lie uncomfortably together. In particular, it leaves open the question whether the conclusion that the ISAT universality class extends down to, and importantly includes, the VISAW line, where the weight for crossings segments (τ_x in [20]) vanishes. On the other hand, if both claims are true, there must be a change of universality class on varying p. It should be emphasized however that an estimate of the exponent ν for collapsing VISAWs is not available at the moment, since the lack of knowledge of the exact location of the transition for $p = 1$ makes obtaining good estimates a significantly harder task.

Clearly, something subtle is occurring in this system if our numerical analysis is accurate. Of course, large corrections to scaling may be at work here. In any case, further theoretical work is needed to tease out this issue.

Acknowledgments

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