

Self-avoiding trails with nearest-neighbour interactions on the square lattice

A Bedini¹, A L Owczarek¹ and T Prellberg²

¹ Department of Mathematics and Statistics, The University of Melbourne, Parkville, Vic 3010, Australia

² School of Mathematical Sciences, Queen Mary University of London, Mile End Road, London E1 4NS, UK

E-mail: abedini@ms.unimelb.edu.au, owczarek@unimelb.edu.au and t.prellberg@qmul.ac.uk

Received 27 October 2012, in final form 11 January 2013

Published 8 February 2013

Online at stacks.iop.org/JPhysA/46/085001

Abstract

Self-avoiding walks and self-avoiding trails, two models of a polymer coil in dilute solution, have been shown to be governed by the same universality class. On the other hand, self-avoiding walks interacting via nearest-neighbour contacts (ISAW) and self-avoiding trails interacting via multiply visited sites (ISAT) are two models of the coil-globule, or collapse transition of a polymer in dilute solution. On the square lattice it has been established numerically that the collapse transition of each model lies in a different universality class. The models differ in two substantial ways. They differ in the types of subsets of random walk configurations utilized (site self-avoidance versus bond self-avoidance) and in the type of attractive interaction. It is therefore of some interest to consider self-avoiding trails interacting via nearest-neighbour attraction (INNSAT) in order to ascertain the source of the difference in the collapse universality class. Using the flatPERM algorithm, we have performed computer simulations of this model. We present numerical evidence that the singularity in the free energy of INNSAT at the collapse transition has a similar exponent to that of the ISAW model rather than the ISAT model. This would indicate that the type of interaction used in ISAW and ISAT is the source of the difference in the universality class.

PACS numbers: 05.40.-a, 05.50.+q, 05.10.Ln

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

1. Introduction

The collapse transition of a polymer in a dilute solution has been a focus of study in lattice statistical mechanics for decades [1, 2]. Any lattice model of a collapsing polymer has two

key ingredients: an excluded volume effect expressing the impenetrability of monomers, and a short-range attractive force, which mimics the complex monomer–solvent interaction. When the effects of the excluded volume and the short-range attraction balance each other, the polymer undergoes a collapse transition which separates two distinct phases: a swollen and a collapsed phase.

The canonical lattice model of the configurations of a polymer in solution has been the model of self-avoiding walks (SAW) where a random walk on a lattice is not allowed to visit a lattice site more than once. SAW display the desired excluded volume effect and are swollen in size relative to unrestricted random walks at the same length. A common way to introduce a short-range interaction is to assign a negative energy to each non-consecutive pair of monomers lying on neighbouring lattice sites, modelling an effective attractive force. This is the interacting self-avoiding walk (ISAW) model, which is the standard lattice model of polymer collapse using SAW.

The properties of lattice polymers are also related to those of magnetic systems near their critical point [3]. More precisely, lattice polymers are related to magnets with $O(n)$ symmetry in the formal limit of zero components ($n \rightarrow 0$). This relation is of great importance, since it allows the application of the methods of statistical field theory to the study of polymer models, and the collapse transition can be understood as the tri-critical point of such systems [1, 4, 5].

The study of the critical properties of lattice polymers, and thus of $O(n)$ models when we let $n \rightarrow 0$, in two dimensions has been ongoing over decades theoretically and numerically. Nienhuis in 1982 [6] was able to compute the critical exponents of free SAW by considering a model of non-intersecting loops on the hexagonal lattice, and in 1987 Duplantier and Saleur [7] were able to model the bond interaction introducing vacancies on the same lattice, obtaining a full set of critical exponents for the polymer collapse transition in the ISAW model. Their conjectured values for the exponents have been subsequently confirmed numerically by Prellberg and Owczarek in 1994 [8]. We will refer to (the universality class of) this critical point as the ' θ -point'.

Introducing attractive interactions between bonds opens the doors to more complex possibilities. In the quest for a solvable $O(n)$ model on the square lattice, Blöte and Nienhuis in 1989 [9] considered a lattice model, which includes energies for site-collisions and straight segments. For this model five critical branches are exactly known [9–12]. One of these branches (named 'branch 0' in [9]) is similar to the θ -point previously found by Duplantier and Saleur [7] (for this branch Batchelor [13] obtained the exponents $\nu = 4/7$, $\gamma = 6/7$), and two branches correspond to dense and dilute (SAW) polymers. 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 new tri-critical point (with exponents $\nu = 12/23$, $\gamma = 53/46$) is another candidate for describing a collapsing polymer.

A different model of a collapsing model can be constructed starting from self-avoiding trails (SATs). A SAT is a lattice walk configuration where the excluded volume is obtained by preventing the walk from visiting the same bond, rather than the same site, more than once. This is a slightly weaker restriction, and SAW configurations are a proper subset of SAT configurations. The interacting version of self-avoiding trails (ISAT), customarily obtained by giving an energy to multiple visited sites, also presents a collapse transition.

It is known that SAW and SAT share the same statistics in their high-temperature phase, but theoretical prediction and numerical evidence [14, 15] strongly suggest that the collapse transition of the ISAT model is in a different universality class to that of ISAW, although there is no clear understanding of why this would be the case. An interesting possible explanation of the ISAT collapse has been provided by Foster [16] in terms of the tri-critical point with exponents $\nu = 12/23$, $\gamma = 53/46$ derived from the $O(n)$ model.

Although they both aim to describe the same physical system, the ISAW and ISAT models differ in both their geometrical properties and their interaction. Their different critical behaviour could be due to either one of these two differences.

To investigate this further, we considered a mixed model where trails interact in the same way as SAW, that is, by a nearest-neighbour interaction. We shall call this hybrid model interacting nearest neighbour self-avoiding trails, or INNSAT. In the next section we review the ISAW and ISAT models describing the different behaviour that they have been shown to demonstrate. In section 3 we formally introduce the model and the quantities of interest. We then describe our results in section 4 and summarize our conclusions in the final section.

2. ISAW and ISAT

2.1. Interacting self-avoiding walks (ISAW)

Let us recall briefly the definition and main properties of the ISAW model. Consider the ensemble \mathcal{S}_n of SAW of length n , that is, of all lattice paths of n steps that can be formed on the square lattice such that they never visit the same site more than once. Given a SAW $\varphi_n \in \mathcal{S}_n$, we define a *contact* whenever there is a pair of sites that are neighbours on the lattice but not consecutive on the walk. We associate an energy $-\varepsilon_c$ with each contact. Denoting by $m_c(\varphi_n)$ the number of contacts in φ_n , the probability of φ_n is given by

$$\frac{e^{\beta\varepsilon_c m_c(\varphi_n)}}{Z_n(T)}, \quad (2.1)$$

and the partition function $Z_n(T)$ is defined in the usual way as

$$Z_n(T) = \sum_{\varphi_n \in \mathcal{S}_n} e^{\beta\varepsilon_c m_c(\varphi_n)}, \quad (2.2)$$

where β is the inverse temperature $1/k_B T$ (k_B is Boltzmann's constant). We define a Boltzmann weight (fugacity) $\omega_c = \exp(\beta\varepsilon_c)$. The finite-length-reduced free energy is

$$\kappa_n(T) = \frac{1}{n} \log Z_n(T) \quad (2.3)$$

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

$$\kappa(T) = \lim_{n \rightarrow \infty} \kappa_n(T). \quad (2.4)$$

As mentioned above, it is expected that there is a collapse phase transition at a temperature T_θ , which is known as the θ -point, characterized by a non-analyticity in $\kappa(T)$.

The temperature T_θ also separates regions of different finite-length scaling behaviour for fixed temperatures. Considering this finite-length scaling, for high temperatures ($T > T_\theta$) the excluded volume interaction is the dominant effect, and the behaviour is universally the same as for the non-interacting SAW problem: for large n , the mean squared end-to-end distance (or equivalently the radius of gyration) R_n^2 and partition function Z_n are expected to scale as

$$R_n^2 \sim A n^{2\nu} \quad \text{with } \nu > 1/2 \quad \text{and} \quad (2.5)$$

$$Z_n \sim D \mu^n n^{\gamma-1}, \quad (2.6)$$

respectively, where $\log \mu = \kappa(T)$ and the exponents ν and γ are expected to be universal. In two dimensions it is well established [6] that $\nu = 3/4$ and $\gamma = 43/32$ for $T > T_\theta$. The constants A and D are temperature dependent.

Fixing the temperature precisely at the θ -point, $T = T_\theta$, Duplantier and Saleur [7] found $\nu = 4/7$ and $\gamma = 8/7$ in two dimensions.

For low temperatures ($T < T_\theta$) it is accepted that the partition function is dominated by configurations that are internally dense, though not necessarily fully dense. The partition function should then scale differently from that at high temperatures, since a collapsed polymer should have a well-defined surface (and associated surface free energy) [17]. One expects in d dimensions large- n asymptotics of the form

$$R_n^2 \sim An^{2/d} \tag{2.7}$$

and

$$Z_n \sim D\mu^n \mu_s^{n^{d-1}/d} n^{\nu'-1}, \tag{2.8}$$

with $\mu_s < 1$. The constants A and D are temperature dependent. It is expected that the internal density smoothly goes to zero as the temperature is raised to the θ -point.

To explore the singularity in the free energy at the collapse point further, it is useful to consider the (reduced) internal energy and the specific heat, which are defined as

$$u_n(T) = \frac{\langle m_c \rangle}{n} \quad \text{and} \quad c_n(T) = \frac{\langle m_c^2 \rangle - \langle m_c \rangle^2}{n}, \tag{2.9}$$

with limits

$$U(T) = \lim_{n \rightarrow \infty} u_n(T) \quad \text{and} \quad C(T) = \lim_{n \rightarrow \infty} c_n(T). \tag{2.10}$$

When $T \rightarrow T_\theta$, the singular part of the specific heat behaves as

$$C(T) \sim B|T_\theta - T|^{-\alpha}, \tag{2.11}$$

where $\alpha < 1$ for a second-order phase transition. If the transition is second order, the singular part of the thermodynamic limit internal energy behaves as

$$U(T) \sim B|T_\theta - T|^{1-\alpha} \tag{2.12}$$

when $T \rightarrow T_\theta$, and there is a jump in the internal energy at T_θ if the transition is first order (an effective value of $\alpha = 1$).

Tri-critical scaling [18] predicts that around the critical temperature, the finite-length scaling of the singular part of the specific-heat $c_n(T)$ obeys the following crossover scaling form:

$$c_n(T) \sim n^{\alpha\phi} \mathcal{C}((T - T_\theta)n^\phi), \tag{2.13}$$

when $T \rightarrow T_\theta$ and $n \rightarrow \infty$, and that the exponents α and ϕ are related via

$$2 - \alpha = \frac{1}{\phi}. \tag{2.14}$$

If one considers the peak of the finite-length specific heat it will behave as

$$c_n^{\text{peak}} \sim n^{\alpha\phi} \mathcal{C}(x^{\text{max}}), \tag{2.15}$$

where x^{max} is the location of the maximum of the function $\mathcal{C}(x)$.

The work of Duplantier and Saleur (1987) predicts the exponents for the θ -point collapse as

$$\phi = \phi_\theta = 3/7 \tag{2.16}$$

and

$$\alpha = \alpha_\theta = -1/3. \tag{2.17}$$

It is important to observe that this implies that the specific heat does not diverge at the transition since the exponent

$$\alpha_0 \phi_0 = -1/7 \approx -0.14 \tag{2.18}$$

is negative. However, the peak values of the third derivative of the free energy with respect to temperature will diverge with positive exponent

$$(1 + \alpha_0) \phi_0 = 2/7 \approx 0.28. \tag{2.19}$$

2.2. Interacting self-avoiding trails (ISAT)

The model of interacting trails on the square lattice is defined as follows. Consider the ensemble \mathcal{T}_n of SATs of length n , that is, of all lattice paths of n steps that can be formed on the square lattice such that they never visit the same bond more than once. Given a SAT $\psi_n \in \mathcal{T}_n$, we associate an energy $-\varepsilon_l$ with each doubly visited site. Denoting by $m_l(\psi_n)$ the number of doubly visited sites in ψ_n , the probability of ψ_n is given by

$$\frac{e^{\beta \varepsilon_l m_l(\psi_n)}}{Z_n^{\text{ISAT}}(T)}, \tag{2.20}$$

where we define the Boltzmann weight $\omega_l = \exp(\beta \varepsilon_l)$ and the partition function of the ISAT model is given by

$$Z_n^{\text{ISAT}}(T) = \sum_{\psi_n \in \mathcal{T}_n} \omega_l^{m_l(\psi_n)}. \tag{2.21}$$

Previous work [14, 15] on the square lattice has shown that there is a collapse transition at a temperature $T = T_c$ with a strongly divergent specific heat, and the exponents have been estimated as

$$\phi_{it} = 0.84(3) \quad \text{and} \quad \alpha_{it} = 0.81(3), \tag{2.22}$$

arising from a scaling of the peak value of the specific heat diverging with the exponent

$$\phi_{it} \alpha_{it} = 0.68(5). \tag{2.23}$$

This result is a clear difference to the ISAW θ -point described above where the singularity in the specific heat is *convergent*. Additionally, at $T = T_c$ the finite-length scaling of the end-to-end distance was found to be consistent [14] with the form

$$R_n^2(T) \sim An(\ln n)^2 \tag{2.24}$$

as $n \rightarrow \infty$. Again, this is quite different to the exponent $\nu = 4/7$ for the ISAW.

Another important difference is that it has been recently observed [19, 20] that the low temperature phase is maximally dense on the triangular and square lattices. On the square lattice this implies that if one considers the proportion of the sites on the trail that are at lattice sites which are not doubly occupied via

$$p_n = \frac{n - 2\langle m_l \rangle}{n}, \tag{2.25}$$

then it is expected that

$$p_n \rightarrow 0 \quad \text{as} \quad n \rightarrow \infty. \tag{2.26}$$

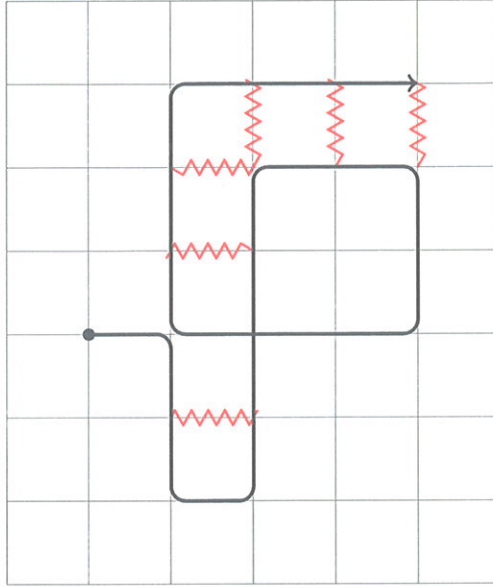


Figure 1. An example of INNSAT configuration with $m_c = 6$, that is, there are six nearest-neighbour contacts illustrated via zigzag (red) lines. The trail can visit a site of the lattice twice by ‘touching’ and by ‘crossing’ itself. The number of doubly visited sites is $m_t = 2$. Note that there is no contact between the second and the seventh visited site of the walk, even though these are non-consecutive nearest-neighbour sites, as both sites are visited consecutively by a different segment of the trail.

3. The INNSAT model

We define our interacting model of trails (INNSAT) as follows. Consider the set of bond-avoiding paths \mathcal{T}_n as defined in the previous section. When two sites are adjacent on the lattice but not consecutive along the walk, so as not to be joined by *any* step of the walk, we again refer to this pair of sites as a nearest-neighbour *contact* and we give it a weight $\omega_c = e^{\beta \varepsilon_c}$, analogously to the ISAW model. In figure 1 a trail of length $n = 21$ with $m_c = 6$ contacts is illustrated.

Denoting by $m_c(\psi_n)$ the number of contacts in ψ_n , the probability of ψ_n is given by

$$\frac{e^{\beta \varepsilon_c m_c(\psi_n)}}{Z_n^{\text{nt}}(T)}, \tag{3.1}$$

where the partition function is

$$Z_n^{\text{nt}}(T) = \sum_{\psi_n \in \mathcal{T}_n} \omega_c^{m_c(\psi_n)}. \tag{3.2}$$

The intensive reduced internal energy and specific heat are as for ISAW:

$$u_n(T) = \frac{\langle m_c \rangle}{n} \quad \text{and} \quad c_n(T) = \frac{\langle m_c^2 \rangle - \langle m_c \rangle^2}{n}. \tag{3.3}$$

We shall also consider the proportion of the sites on the trail that are at lattice sites which are not doubly occupied via

$$p_n = \frac{n - 2\langle m_t \rangle}{n}, \tag{3.4}$$

where m_t is the number of doubly visited sites as defined above.

We shall see there is a collapse transition at a single temperature, T_p , equivalently, fugacity ω_c^p . If the INNSAT model behaves in the same way as the ISAW model, we would not expect the specific heat to diverge at this collapse point, so we also need to introduce a quantity t_n proportional to the third derivative of the free energy as

$$t_n = \frac{\langle m_c^3 \rangle - 3\langle m_c \rangle \langle m_c^2 \rangle + 2\langle m_c \rangle^3}{n}. \quad (3.5)$$

This quantity should have a singular part that behaves as

$$t_n(T) \sim n^{(\alpha+1)\phi} \mathcal{T}((T - T_p)n^\phi), \quad (3.6)$$

around the collapse point, i.e. as $T \rightarrow T_p$ and $n \rightarrow \infty$. Hence, the peaks of this quantity t_n will scale with the exponent $(\alpha + 1)\phi$.

4. Numerical results

We have first simulated the INNSAT model using the flatPERM algorithm [21] up to the length $n = 1000$. With $S_n \simeq 2.7 \times 10^6$ iterations, we collected 2.6×10^{10} samples at the maximum length. Following [21], we also measured the number of samples adjusted by the number of their independent growth steps, obtaining $S_n^{\text{eff}} \simeq 1.6 \times 10^8$ ‘effective samples’.

FlatPERM outputs an estimate W_{n,m_c} of the total weight of the walks of length n at fixed values of m_c . From the total weight one can access physical quantities over a broad range of temperatures through a simple weighted average, e.g.

$$\langle \mathcal{O} \rangle_n(\omega) = \frac{\sum_{m_c} \mathcal{O}_{n,m_c} \omega^{m_c} W_{n,m_c}}{\sum_{m_c} \omega^{m_c} W_{n,m_c}}. \quad (4.1)$$

We have begun by analysing the scaling of the specific heat by calculating the location of its peak $\omega_n^p = \arg \max_{\omega} c_n(\omega)$ and thereby evaluating $c_n^p = c_n(\omega_n^p)$. We have also found the two peaks of $t_n(T)$ as a function of temperature: the peak values we denote as $t_n^{p,\pm}$.

It is clear that the specific heat peak is growing rather weakly as the length increases. As the specific heat might converge, we obtain finite size estimates of the specific heat exponent by considering

$$\log_2 \left[\frac{c_n^p - c_{n/2}^p}{c_{n/2}^p - c_{n/4}^p} \right] \quad (4.2)$$

which should converge to $\alpha\phi$ as $n \rightarrow \infty$. Assuming corrections to scaling of $n^{-3/7}$ as for ISAW, we find

$$\alpha_{\text{fit}}\phi_{\text{fit}} = -0.15(5), \quad (4.3)$$

as shown on the left-hand side of figure 2. This is consistent with a value of $-1/7 \approx -0.14$ for the θ -point universality class.

Furthermore, when we analyse t_n , which is proportional to the third derivative of the free energy, we find further consistent values of exponents. This derivative has two peaks $t_n^{p,\pm}$, and we obtain finite size estimates of the specific heat exponent from each of the peaks by considering

$$\log_2 \left[\frac{t_n^{p,\pm}}{t_{n/2}^{p,\pm}} \right] \quad (4.4)$$

which should converge to $(1 + \alpha)\phi$ as $n \rightarrow \infty$. From the plot on the right-hand side of figure 2 we estimate

$$(\alpha_{\text{fit}} + 1)\phi_{\text{fit}} = 0.26(5). \quad (4.5)$$

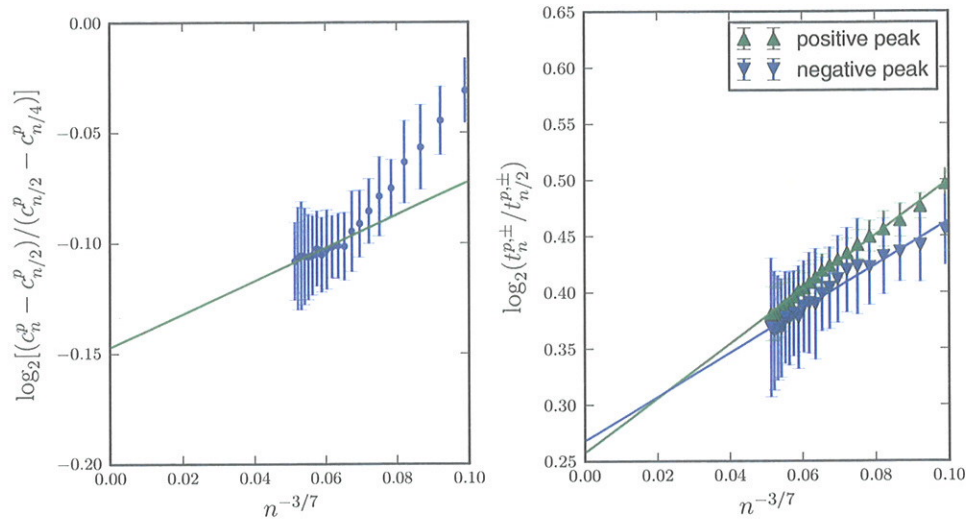


Figure 2. Left: a plot of (4.2) designed to estimate the exponent $\alpha\phi$ from the specific heat. Right: a plot of (4.4) designed to estimate the exponent $(1 + \alpha)\phi$ from the derivative of the specific heat. The upper (green) points are values from the negative peak of t_n while the lower (blue) points are from the positive peak of t_n .

There is still considerable curvature in the right-hand plot which would indicate a slightly larger value when higher order corrections to scaling are taken in account. Once again we conclude that the θ value of $2/7 \approx 0.28$ is consistent with our data.

We therefore conjecture that

$$\phi_{nt} = \phi_\theta \neq \phi_{it} \quad \text{and} \quad \alpha_{nt} = \alpha_\theta \neq \alpha_{it} . \tag{4.6}$$

Using the locations of the peaks of the specific heat and its derivative and assuming finite-size correction of the order of $n^{-3/7}$, we have estimated the location of the collapse point as indicated in figure 3. The magnitude of the difference between the three peak positions at finite length indicates the large corrections to scaling present in this problem at length 1000. We estimate

$$\omega^p = 1.78(1). \tag{4.7}$$

We next analysed the scaling of the end-to-end distance of the polymer. To obtain an estimate for the exponent ν we considered a finite-size effective exponent

$$\nu_n^{\text{est}}(\omega) = \frac{1}{2} \log_2 \left[\frac{\langle R^2 \rangle_n(\omega)}{\langle R^2 \rangle_{n/2}(\omega)} \right]. \tag{4.8}$$

Using the data obtained from our flatPERM simulations, we plotted this quantity against temperature for various values of the length n , as shown in figure 4. We find that the graphs for different values of n intersect around a particular value of the temperature. The location of this intersection point is a good estimator of the infinite-length critical temperature ω^p and of the exponent ν at the transition. We find a region of crossing points in ω between 1.78 and 1.80 with corresponding estimates of ν between 0.57 and 0.55. While the obtained exponent estimate range is a little below the θ point value of $4/7 \approx 0.571$, we expect that our estimate is affected by strong corrections to scaling. For comparison, we simulated the ISAW model and performed an identical analysis, shown in figure 5. The ISAW estimate of $\nu \approx 0.56$ at the

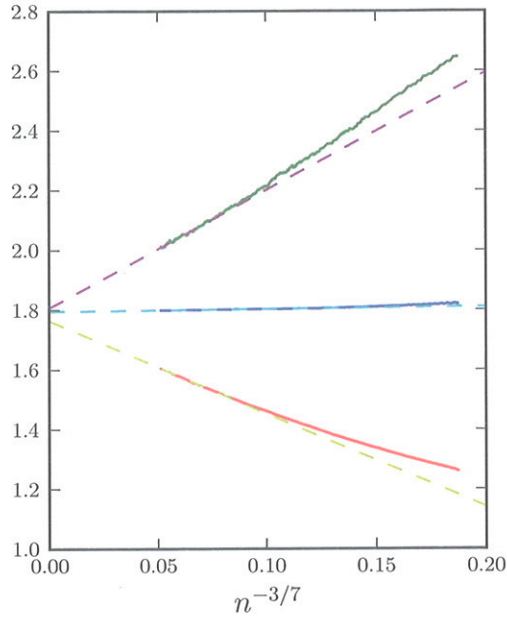


Figure 3. A plot of the locations of the two peaks of $t_n(T)$ and of $c_n(T)$ against $n^{-3/7}$. Extrapolation for $n \rightarrow \infty$ provides an estimate for the thermodynamic transition temperature ω^p . The upper (green) curve is the location of negative $t_n^{p,-}$ peak, the lower (red) curve is the location of positive $t_n^{p,+}$ peak while the middle (blue) curve is the location of the peak c_n^p of the specific heat.

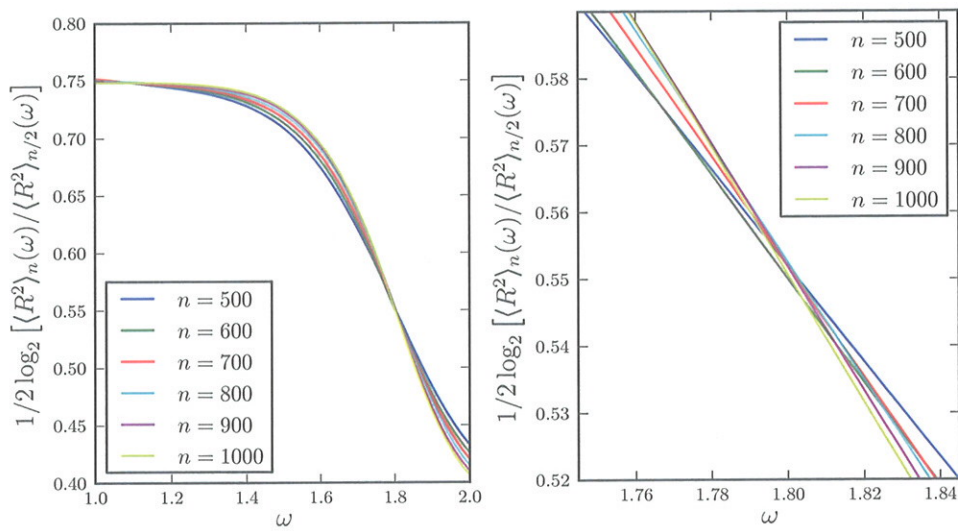


Figure 4. Estimates of the exponent ν for INNSAT from finite-size estimates (4.8) as a function of temperature (left) and a zoom (right) on the crossing region. There are crossing points in the region of ω between 1.78 and 1.80 giving corresponding estimates of ν between 0.57 and 0.55.

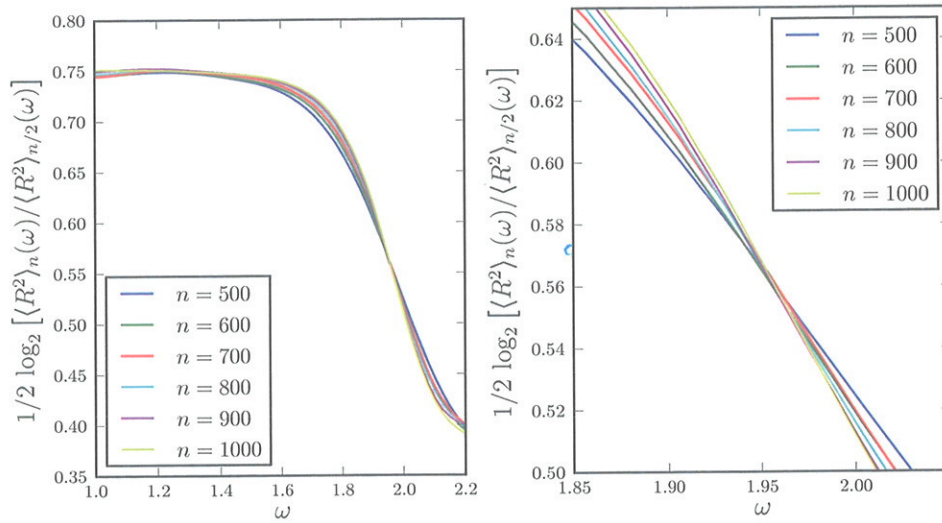


Figure 5. Estimates of the exponent ν for ISAW from finite-size estimates (4.8) as a function of temperature (left) and a zoom (right) on the crossing region. The crossing point is at $\omega \approx 1.96$ and $\nu \approx 0.56$. While the estimate for ν at the crossing point is closer to the value of $4/7$ than the one obtained for INNSAT, the difference provides evidence for the presence of fairly strong corrections to scaling.

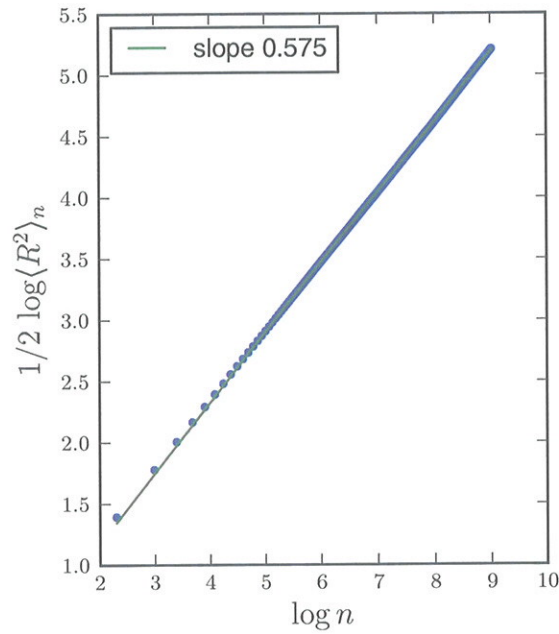


Figure 6. Estimate of the exponent ν from finite-size estimates (4.8) obtained from a thermal simulation at $\omega = 1.78$ up to the length $n = 8192$. This estimate is sensitive to the estimate of the critical fugacity. A lower critical estimate would lead to a higher exponent estimate.

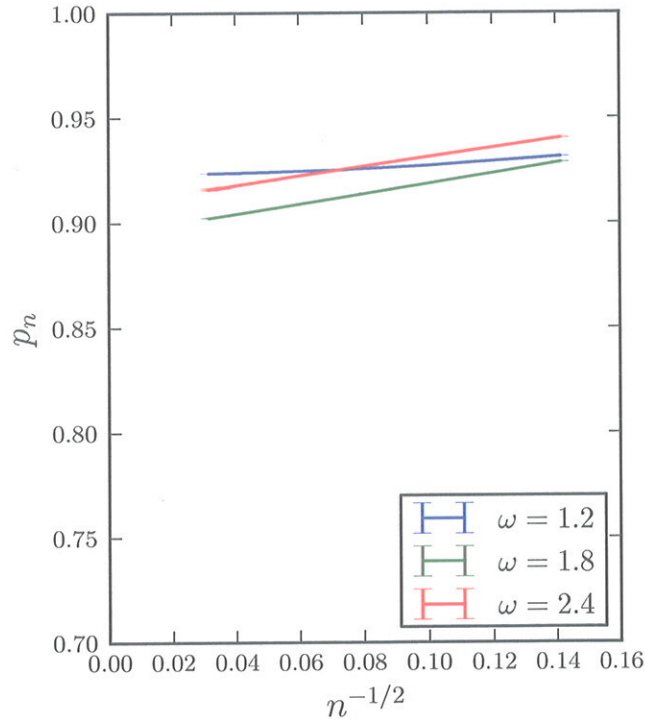


Figure 7. Plots of p_n , the proportion of steps visiting the same site once, at a high temperature, upper (blue) curve, and a low temperature, lower (green) curve against $n^{-1/2}$. The scale $n^{-1/2}$ chosen is the natural low temperature scale. In both cases the asymptotic thermodynamic value is well away from zero. Errors are shown but are not visible at this scale.

collapse transition, while being closer to $4/7$, also indicates the presence of strong corrections to scaling.

Hence, we ran a thermal simulation at the estimated critical fugacity of 1.78 up to $n = 8192$. With $S = 5 \times 10^6$ iterations, we obtained $S_n \simeq 1.8 \times 10^7$ samples at the maximum length (corresponding to $S_n^{\text{eff}} \simeq 1.2 \times 10^5$ ‘effective samples’). Figure 6 shows a log–log plot of the radius with respect to the size of the walk along with a linear best fit with slope 0.575. Of course, using $\omega = 1.77$ or $\omega = 1.79$ gives estimates of ν that differ by 0.01 so the sensitivity to the location of the critical point dominates the error of our estimate.

Correspondingly, if we assume that the INNSAT is in the ISAW universality class we can use the value of $\nu = 4/7$ to better estimate the critical fugacity in the INNSAT model as

$$\omega^p = 1.783(5). \tag{4.9}$$

4.1. Low-temperature phase

There is strong evidence that the low-temperature phase of the ISAW model is a globular phase that is not fully dense, while for interacting trails the low-temperature phase is maximally dense. As discussed above, the trail fills the lattice asymptotically in a maximally dense phase, and the portion of steps not involved with doubly-visited sites should tend to zero as $n \rightarrow \infty$. Following the analysis in [19] we measured the proportion p_n of steps visiting the same site

twice, and we plotted p_n against $n^{-1/2}$ at two different temperatures respectively above and below the critical temperature, as shown in figure 7. We find that in both low-temperature and high-temperature phases only a small portion of the visited sites is visited again. The quantity p_n stays close to 1 and, in particular, does not tend to zero in either region. This phenomenon can be understood by noting that the nearest-neighbour interaction makes it energetically favourable for the walk to bounce away from an already visited site rather than to visit it again.

This result implies that the low temperature phase is not fully dense, just as for the ISAW low temperature phase. This provides a consistent picture that the collapse transition in the INNSAT model is between high and low temperature phases similar to the ISAW, making the conclusion that the thermodynamic transition between them is similar to the θ -point a natural one.

5. Conclusions

We have considered a lattice model of polymer collapse in two dimensions which uses the interaction type, nearest-neighbour contacts, of the canonical lattice model (ISAW) but the configuration space of an alternative model (ISAT), being bond-avoiding walks, also known as self-avoiding trails. We find that the critical behaviour of the free energy, and its derivatives of our model (INNSAT) seem to align with the θ -point universality class of the ISAW model rather than with that of the ISAT model, which has a rather strongly divergent specific heat not seen in either the ISAW or INNSAT models. The end-to-end distance scaling is broadly consistent with this conclusion, though estimates tend to be a little low. However, using the assumption that the INNSAT and ISAW models lie in the same universality class leads to a precise estimate of the critical fugacity as 1.783(5). Given the different universality classes for ISAT and INNSAT it may also be of interest to consider a model based upon self-avoiding trail configurations with both types of interactions.

Acknowledgments

Financial support from the Australian Research Council via its support for the Centre of Excellence for Mathematics and Statistics of Complex Systems and through its Discovery Program is gratefully acknowledged by the authors. ALO thanks the School of Mathematical Sciences, Queen Mary, University of London for hospitality.

References

- [1] de Gennes P-G 1975 *J. Phys. Lett.* 36 L55
- [2] de Gennes P-G 1979 *Scaling Concepts in Polymer Physics* (Ithaca, NY: Cornell University Press)
- [3] de Gennes P-G 1972 *Phys. Lett. A* 38 339
- [4] Stephen M J 1975 *Phys. Lett. A* 53 363
- [5] Duplantier B 1982 *J. Phys.* 43 991
- [6] Nienhuis B 1982 *Phys. Rev. Lett.* 49 1062
- [7] Duplantier B and Saleur H 1987 *Phys. Rev. Lett.* 59 539
- [8] Prellberg T and Owczarek A L 1994 *J. Phys. A: Math. Gen.* 27 1811
- [9] Blöte H W J and Nienhuis B 1989 *J. Phys. A: Math. Gen.* 22 1415
- [10] Batchelor M T, Nienhuis B and Warnaar S 1989 *Phys. Rev. Lett.* 62 2425
- [11] Nienhuis B 1990 *Int. J. Mod. Phys. B* 4 929
- [12] Warnaar S O, Batchelor M T and Nienhuis B 1992 *J. Phys. A: Math. Gen.* 25 3077
- [13] Batchelor M T 1993 *J. Phys. A: Math. Gen.* 26 3733
- [14] Owczarek A L and Prellberg T 1995 *J. Stat. Phys.* 79 951
- [15] Owczarek A L and Prellberg T 2007 *Physica A* 373 433

- [16] Foster D P 2009 *J. Phys. A: Math. Theor.* 42 372002
- [17] Owczarek A L, Prellberg T and Brak R 1993 *Phys. Rev. Lett.* 70 951
- [18] Brak R, Owczarek A L and Prellberg T 1993 *J. Phys. A: Math. Gen.* 26 4565
- [19] Doukas J, Owczarek A L and Prellberg T 2010 *Phys. Rev. E* 82 031103
- [20] Bedini A, Owczarek A L and Prellberg T 2013 Weighting of topologically different interactions in a model of two-dimensional polymer collapse *Phys. Rev. E* at press (arXiv:org/abs/1210.7196)
- [21] Prellberg T and Krawczyk J 2004 *Phys. Rev. Lett.* 92 120602