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Collapse transition of self-avoiding trails on the square lattice

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Abstract

The collapse transition of an isolated polymer has been modelled by many different approaches, including lattice models based on self-avoiding walks and self-avoiding trails. In two dimensions, previous simulations of kinetic growth trails, which map to a particular temperature of interacting self-avoiding trails, showed markedly different behaviour for what was argued to be the collapse transition than that which has been verified for models based of self-avoiding walks. On the other hand, it has been argued that kinetic growth trails represent a special simulation that does not give the correct picture of the standard equilibrium model. In this work we simulate the standard equilibrium interacting self-avoiding trail model on the square lattice up to lengths over 2,000,000 steps and show that the results of the kinetic growth simulations are, in fact, entirely in accord with standard simulations of the temperature dependent model. In this way we verify that the collapse transition of interacting self-avoiding walks and trails are indeed in different universality classes in two dimensions.

Keywords: Interacting self-avoiding trails

1. Introduction

Over the past 25 years various lattice models of a single self-interacting polymer chain have been analysed in both two and three dimensions (and beyond). These include various types of self-interacting self-avoiding walk, self-interacting trails [1] (lattice paths that can intersect at a lattice vertex but not along a lattice edge) and self-interacting random (fully self-intersecting) walk models. The fundamental physical phase transition [2] that these models are compared to is that of the collapse of single polymer in a poor solvent as the temperature is lowered. The question that arises when considering the bulk of these studies is how robust is the universality class of the collapse transition. The standard theory [3–5] of the collapse transition is based on the $n \to 0$ limit of the magnetic tricritical $\phi^4 - \phi^6$ O(n) field theory and related Edwards model with two and three body forces [6,7], which predicts an upper critical dimension of three with subtle scaling behaviour in that dimension. As an analysis of these theories is not exact in two dimensions, lattice models form the basis of our knowledge. Analyses of both two- and three-dimensional self-interacting trails [8,9] indicate that they are

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in a different universality class to that of self-interacting self-avoiding walks in those respective dimensions. There is no clear understanding of why this is the case if true. A complication of this scenario occurs because the numerically most extensive work on trails [8,9], and that which draws the conclusion of separate universality classes, uses so-called "kinetic growth" simulations, or "smart kinetic trails", to study the collapse point of self-interacting trails. These simulations are of trails produced in such a way that one argues they form a distribution of self-interacting trails at one particular temperature. One then further argues from the numerical evidence that this temperature is precisely the collapse temperature. Now, it was claimed [10] that the collapse transition associated with "smart kinetic trails" is first-order. Clear evidence was produced in [10] to demonstrate that there was first order transition in three dimensions on the diamond lattice. On the other hand, no evidence of this could be found in two dimensions.

The explanation of this relates to the vanishing of renormalized three-body interactions in the smart kinetic trails. It was further suggested in Ref. [10] that studying the smart kinetic trails was misleading when considering the full equilibrium self-interacting trail model.

To try to see if these arguments hold in two dimensions we have simulated self-avoiding trails over a range of temperatures near the collapse point. The collapse temperature is indeed the point onto which the smart kinetic trails map, and we compare these with our earlier results concerning two-dimensional trail collapse based on the smart kinetic trail simulations.

2. The model

The model of self-interacting trails (ISAT) on the square lattice is defined as follows. Consider all different bond-avoiding paths φ_N of length N that can be formed on the square lattice with one end fixed at a particular site (the set Ω_N). Associate an energy $-\varepsilon$ with each doubly-visited site. For each configuration φ_N count the number $m(\varphi_N)$ of doubly-visited sites of the lattice and give that configuration a Boltzmann weight ω^m, where $\omega = \exp(\beta\varepsilon)$. The partition function of the ISAT model is then given by

$$Z_N(\omega) = \sum_{\varphi_N \in \Omega_N} \omega^{m(\varphi_N)}. \tag{2.1}$$

The reduced and normalized internal energy

$$U_N = \frac{1}{N}\langle m \rangle \tag{2.2}$$

and reduced and normalized specific heat

$$C_N = \frac{1}{N}(\langle m^2 \rangle - \langle m \rangle^2) \tag{2.3}$$

are defined in the usual way.

It was argued in Refs. [11,12] that the smart kinetic growth trails simulates at a specific Boltzmann weight $\omega = \omega_c \equiv 3$ and it was later argued [8] that ω_c is indeed the collapse value of the Boltzmann weight.

Let us assume that the phase transition occurring at ω_c is critical and furthermore that the specific heat diverges at the transition (all previous work supports this second proposition). Now we define the exponent α from the divergence of the thermodynamic limit specific heat as usual as

$$c(\omega) = \lim_{N\to\infty} C_N \sim |\omega_c - \omega|^{-\alpha}. \tag{2.4}$$

Let us return to finite N scaling and consider the peak in the specific heat near ω_c. Let the peak be located at $\omega_{c,N}$ and define the width of the transition $\Delta\omega$ by the difference in the omega values at the half-heights (that is, the values of ω that give values of C_N as $C_N(\omega_{c,N})/2$). The crossover exponent is defined by

$$\Delta\omega \sim \frac{a}{N^{\phi}}, \tag{2.5}$$

where a is a constant, and, in turn, gives us a scaling variable $(\omega - \omega_c)N^{\phi}$ on which to scale for data collapse. The standard scaling theory [13] predicts that the crossover exponent ϕ is related to the specific heat exponent

α via the scaling relation

$$2 - \alpha = 1/\phi \tag{2.6}$$

and that the shift of the peak from its thermodynamic limit value is also governed by ϕ, that is

$$|\omega_c - \omega_{c,N}| \sim \frac{b}{N^{\phi}}, \tag{2.7}$$

where b is a constant. Moreover, the peak value of the finite size specific heat should then behave as Ref. [13]

$$C_N(\omega_{c,N}) \sim dN^{\alpha\phi}, \tag{2.8}$$

where d is a constant. Using all of the above one can obtain local estimates of the exponents α and ϕ from this form, and these can be independently verified by studying the width and the shift of the transition via the specific heat peak.

A further independent test is to study the internal energy as it is predicted to scale as

$$U_N(\omega_{c,N}) \sim U_\infty(\omega_c) - eN^{(\alpha-1)\phi}, \tag{2.9}$$

where U_∞ is the thermodynamic limit internal energy and e is a constant. Usually this would be more difficult to analyse as $U_\infty(\omega_c)$ is unknown but for this model we can argue that $U_\infty = 0.4$ as follows from a kinetic growth argument.

Consider an N-step loop which occupies M lattice sites. The number of contacts is given by the number m of doubly visited sites, and we have $m = N - M$. Any site of this loop could have been the starting point, and in order for a site to be visited twice, the loop must not have been closed at the first return visit. The probability of not closing upon the first return is $2/3$, so that for large loops $m/M \to 2/3$, from whence it follows that $m/N \to 2/5$.

In our previous work [8] we estimated

$$\phi = 0.88^{+0.07}_{-0.05} \tag{2.10}$$

and so $\alpha \approx 0.86$. This is equivalent to the value of $\alpha\phi \approx 0.76$ for the exponent describing the divergence of the specific heat peak. We note that the established values for self-interacting self-avoiding walks in two dimensions [14], that is, $\phi = 3/7$ and $\alpha = -1/3$, imply that the specific heat does not diverge! On the other hand, if there was a first order transition $\alpha = \phi = 1$.

3. Results

We have used the now standard PERM algorithm [15] to simulate ISAT at various fixed temperatures around $\omega_c = 3$ for trail lengths from $2^{15} = 32768$ (denoted as 32 K) in factors of 4 up to $2^{21} = 2097152$ (denoted as 2048 K). We chose the range of temperatures by first simulating at $\omega = 3$ and then reweighting the obtained histogram to give an estimate of the location of the specific heat peak $\omega_{c,N}$. We then repeated the simulation at $\omega_{c,N}$. The multi-histogram method [16] was then used to give data throughout the transition region. The simulations at $\omega = 3$ gave almost identical results to those additionally using the peak data. The quantities of interest such as $\Delta\omega$ and $\omega_{c,N}$ were re-estimated.

We attempted to scale all the data using a consistent set of exponents. The best fit for the specific heat data was obtained for

$$\alpha\phi = 0.66\dot{6} \quad \text{so } \alpha = 0.80 \text{ and } \phi = 0.8\dot{3}, \tag{3.1}$$

while for the internal energy data the best fit used

$$\phi = 0.85 \quad \text{so } \alpha \approx 0.82 \text{ and } \alpha\phi = 0.7. \tag{3.2}$$

Clearly there is an error of at least 0.025 in these estimates and the statistical spread confirmed an error of about 0.03. We have used the scaling relation (2.6) for consistency. The first figures show the scaling of various quantities using those exponent assumptions. In Fig. 1 the scaled difference of the internal energy to its thermodynamic value $(U_\infty - U_N)N^{(1-\alpha)\phi}$ and scaled specific heat $C_N N^{-\alpha\phi}$ are plotted against the scaling

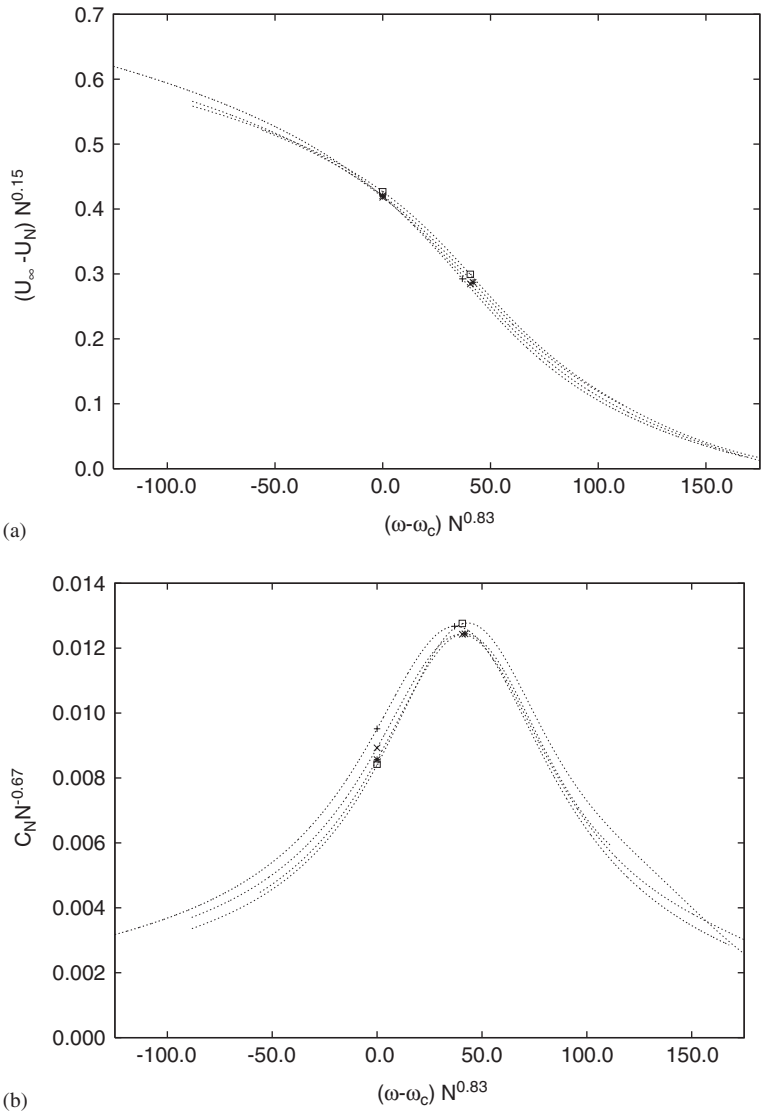

Fig. 1. Scaled internal energy gap $(U_\infty - U_N)N^{(1-\alpha)\phi}$ and specific heat $C_N N^{-\alpha\phi}$ versus scaled $(\omega - \omega_c)N^\phi$ for lengths 32, 128, 512, and 2048 K, comparing the individual data points with the results from the multi-histogram method.

variable $(\omega - \omega_c)N^\phi$. These demonstrate consistency in three ways: between the specific heat, the internal energy and the horizontal scaling variable all at once.

We have estimated the crossover exponent independently via both the shift $(\omega_{c,N} - \omega_c)$ and the width $\Delta\omega$ of the transition. Fig. 2 shows plots of the appropriate scaling combinations for these two quantities against N using the estimate $\phi = 0.84$ (in between our previous estimates), being the best value using these plots.

Finally, in Fig. 3 we demonstrate the convergence of the scaling by plotting scaling combinations that should be constant in the absence of corrections-to-scaling. These give us confidence in the results from the other figures.

We therefore conclude that our new simulations away from the "smart kinetic growth point" are in agreement with the exponent estimates of the smart kinetic growth simulations with perhaps slightly smaller values of ϕ and α as previous central estimates. We now estimate

$$\alpha = 0.81(3) \quad \text{and} \quad \phi = 0.84(3). \tag{3.3}$$

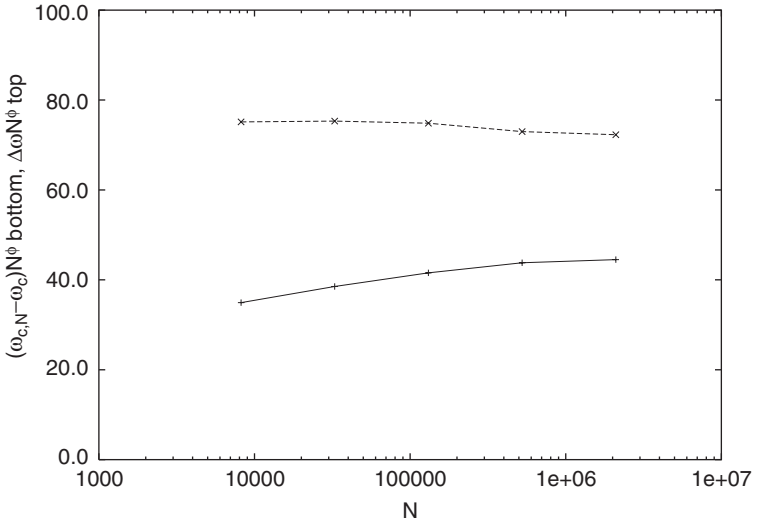

Fig. 2. Scaling of the transition: shift and width of the collapse region. Shown are the scaling combinations $N^\phi(\omega_{c,N} - \omega_c)$ and $N^\phi\Delta\omega$ versus N. We have that $\omega_c = 3$ and have used the estimate of $\phi = 0.84$.

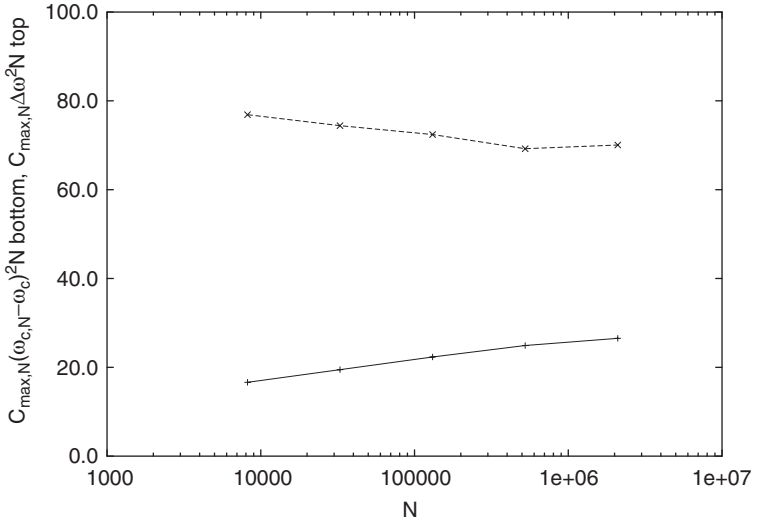

Fig. 3. Scaling of the transition: height of the specific heat peak. Shown are the scaling combinations $C_N(\omega_{c,N} - \omega_c)^2N$ and $C_N\Delta\omega^2N$ versus N. We have that $\omega_c = 3$.

4. Conclusion

We have simulated self-interacting self-avoiding trails on the square lattice up to lengths of 2,097,152 for a range of temperatures around the collapse transition temperature. We conclude that the results are in good agreement with earlier simulations based on smart kinetic trails. They demonstrate a phase transition which is neither of the type displayed by self-interacting self-avoiding walks nor is it first order, although it is very strong, as predicted by an analysis of the smart kinetic growth trails.

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