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Semi-flexible interacting self-avoiding trails on the square lattice

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ABSTRACT

Self-avoiding walks self-interacting via nearest neighbours (ISAW) and self-avoiding trails interacting via multiply-visited sites (ISAT) are two models of the polymer collapse transition of a polymer in a dilute solution. On the square lattice it has been established numerically that the collapse transition of each model lies in a different universality class.

It has been shown that by adding stiffness to the ISAW model a second low temperature phase eventuates and a more complicated phase diagram ensues with three types of transition that meet at a multi-critical point. For large enough stiffness the collapse transition becomes first order. Interestingly, a phase diagram of a similar structure has been seen to occur in an extended ISAT model on the triangular lattice without stiffness. It is therefore of interest to see the effect of adding stiffness to the ISAT model.

We have studied by computer simulation a generalised model of self-interacting self-avoiding trails on the square lattice with a stiffness parameter added. Intriguingly, we find that stiffness does not change the order of the collapse transition for ISAT on the square lattice for a very wide range of stiffness weights. While at the lengths considered there are clear bimodal distributions for very large stiffness, our numerical evidence strongly suggests that these are simply finite-size effects associated with a crossover to a first-order phase transition at infinite stiffness.

1. Introduction

The collapse transition of a polymer in a dilute solution has been a continuing focus of study in lattice statistical mechanics for decades [1,2]. This transition describes the change in the scaling of the polymer with length that occurs as the temperature is lowered. At high temperatures the radius of gyration of a polymer scales in a way swollen relative to a random walk: this is known as the excluded volume effect. At low temperatures a polymer condenses into a dense, usually disordered, globule, with a much smaller radius of gyration. The interest in this phase transition has occurred both because of the motivation of physical systems but also because of the study of integrable cases [3,4] of lattice models, that have proved especially fruitful in two dimensions. While the canonical lattice model of the configurations of a polymer in solution has been the self-avoiding walk (SAW), where a random walk on a lattice is not allowed to visit a lattice site more than once, an alternative has been to use bond-avoiding walks, or a self-avoiding trail. A self-avoiding trail (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. These were used initially to model polymers with loops [5] but have subsequently occurred in integrable loop models in two dimensions [4]. A model of collapsing polymers can be constructed starting from self-avoiding

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trails, known as interacting self-avoiding trails (ISAT). Here energies are associated with multiply-visited sites and by favouring configurations with many such sites a collapse transition can be initiated.

Owczarek and Prellberg studied numerically the ISAT collapse on the square lattice by two different approaches [6,7] and in either case found a strong continuous transition with specific heat exponent $\alpha = 0.81(3)$. Recently, on the triangular lattice Doukas et al. [8] found that by changing the weighting of doubly and triply visited sites a first-order transition can ensure or alternatively, depending on the ratio of these weightings, a weaker second-order transition that mimics the collapse found in the canonical interacting self-avoiding walk (ISAW) model (also know as the θ-point). They also found that the low temperature phase could become fully dense rather than globular.

Correspondingly, there is also a modification of the ISAW model that displays two phase transitions for a range of parameters, namely the *semi-flexible* ISAW model [9–11]. Here two energies are included: the nearest-neighbour site interaction of the ISAW model and also a stiffness energy associated with consecutive parallel bonds of the walk (equivalently, a bending energy for bends in the walk). This has been studied on the cubic lattice by Bastolla and Grassberger [9]. They showed that when there is a strong energetic preference for straight segments, this model undergoes a single first-order transition from the excluded-volume high-temperature state to a fully dense state. On the other hand, if there is only a weak preference for straight segments, the polymer undergoes two phase transitions. On lowering the temperature the polymer undergoes a θ-point transition to the liquid globule followed by a first-order transition to the fully dense phase at a lower temperature. Recent work by Krawczyk et al. [12] concerning the ISAW model on the square lattice in the presence of a stiffness parameter showed that the introduction of stiffness can change the universality class of the collapse transition in two dimensions. For large stiffness the transition becomes first order and the collapsed phase moves from being globular to fully dense. It is also interesting to note that in the case of directed polymers the situation is slightly different with the collapse transition becoming first order for any positive stiffness [13].

Recently, Foster [14] introduced and studied a generalised ISAT model on the square lattice which incorporates stiffness. Using transfer matrices and the phenomenological renormalisation group, that study predicted that the ISAT universality class is unaffected by a range of values of stiffness. However, the results suggested the appearance of a first-order transition for sufficiently large stiffness.

In this work we use Monte Carlo simulation to explore ISAT in the presence of stiffness and the predictions of Foster [14]. We also explore the low temperature phase of the model and find that there is only one low temperature phase and that it is fully dense for the range of stiffness studied.

2. ISAT

The model of interacting trails on the square lattice is defined as follows. Consider the ensemble $\mathcal{T}_n$ of self-avoiding trails (SAT) 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 $-\varepsilon_t$ with each doubly visited site, and denote their number by $m(\psi_n)$. The probability of ψ_n is then given by

$$\frac{e^{\beta\varepsilon_t m(\psi_n)}}{Z_n^{ISAT}(T)}, \tag{2.1}$$

where we define the Boltzmann weight $\omega_t = \exp(\beta\varepsilon_t)$ and β is the inverse temperature $1/k_BT$. The partition function of the ISAT model is given by

$$Z_n^{ISAT}(T) = \sum_{\psi_n \in \mathcal{T}_n} \omega_t^{m(\psi_n)}. \tag{2.2}$$

The finite-length reduced free energy is

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

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

$$\kappa(T) = \lim_{n\to\infty} \kappa_n(T). \tag{2.4}$$

It is expected that there is a collapse phase transition at a temperature T_c characterised by a non-analyticity in $\kappa(T)$.

The collapse transition can be characterised via a change in the scaling of the size of the polymer with temperature. It is expected that some measure of the size, such as the radius of gyration or the mean squared distance of a monomer from the end points, $R_n^2(T)$, scales at fixed temperature as

$$R_n^2(T) \sim An^{2\nu} \tag{2.5}$$

with some exponent ν. At high temperatures the polymer is swollen and in two dimensions it is accepted that $\nu = 3/4$ [3]. At low temperatures the polymer becomes dense in space, though not necessarily space filling, and the exponent is $\nu = 1/2$. However, for the ISAT model the collapsed phase has been seen to be space filling [15]. If the collapse transition is second