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Zipping transition in a model of two crosslinked polymers

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Abstract
We study a model of two self-avoiding walks that are allowed to cross. An attractive energy is associated with each crossing. We present a number of exact results on the free energy of this model and show the existence of a zipping temperature, below which the number of crossings becomes macroscopic. We give heuristic arguments which show that in $d = 2$ and $d = 3$ this zipping transition occurs at infinite temperature. Exact enumeration and Monte Carlo simulations on the square lattice strongly support this conjecture and lead to a precise value for the crossover exponent.

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1. Introduction

Polymers in a good solvent are usually modelled as self-avoiding walks [1, 2]. There exists by now an extensive literature on the critical and topological properties of single self-avoiding walks, which should describe the situation of an extremely diluted polymer solution.

On the other hand, much less is known on the properties of a collection of several self-avoiding walks, which can either cross each other or can be mutually avoiding. Such situations occur naturally when studying networks of crosslinked polymers [3].

The first simple step in studying the implications of crosslinking on polymer properties consists of investigating the behaviour of two polymers that are close to each other in space and that can interact through attractive or repulsive interactions. This leads to models for pairs of self-avoiding walks with mutual interactions. Several models of this type have been investigated recently. In some of these, the two polymers are considered to be *mutually avoiding* and are thought to represent the two strands of DNA [4]. One is then, in particular, interested in the denaturation transition where the two strands decouple. Models of this kind have also been discussed in the context of diblock copolymers [5, 6].

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accurate estimate of the crossover exponent was obtained: $\varphi = .516 \pm .005$, a value which is close to the prediction of the codimension additivity argument that gives $\varphi = 1/2$.

Models similar to ours have been studied recently in the literature. As a first example, we mention the diblock copolymer model introduced by Orlandini *et al* [5, 6]. That model differs from ours in the fact that the two SAWs are also mutually self-avoiding. In that case, numerical evidence shows convincingly that $\beta_z > 0$ for all lattices studied. Moreover, it could be shown exactly that in $d = 2$ the crossover exponent equals $9/16 = .5625$. Another model that is rather similar in spirit to the present one is the lattice version of the Poland and Sheraga model [28] of DNA, studied in [29]. In that model the two SAWs can only intersect at homologous sites, i.e. $\omega_i^{(1)} \neq \omega_j^{(2)}$, $i \neq j$. When $\omega_i^{(1)} = \omega_i^{(2)}$ an energy -1 is gained. This model is now known to have a first order zipping transition at a $\beta_z > 0$ [4, 30]. Finally, we mention that a model of two interacting *directed* polymers was solved exactly by Iglói [31]. Also in that model, the two polymers only zip at a finite temperature.

There is an interesting analogy between models of pairs of polymers such as those discussed above, and the behaviour of a SAW near a flat hyperplane. In that situation, one investigates a SAW that gains an energy -1 for each monomer that lies in the hyperplane. In the case that the SAW can cross the hyperplane, it is believed that for any finite temperature, the polymer is adsorbed to the hyperplane, meaning that a macroscopic number of monomers lies there [16]. On the other hand, if the SAW has to stay on one side of the hyperplane, adsorption only occurs below a strictly finite adsorption temperature. We can interpret our model as one for the adsorption of one polymer into another, and our results also suggest that in this case, where crossing is allowed, there is always adsorption of the two polymers into one another. On the other hand, in the model introduced in [5] the two SAWs cannot cross, and as discussed above, they only zip below a finite temperature.

Finally, we think it would be of interest to investigate the present model in higher dimensions. Also the implications of the current work for the problem of a SAW in a random environment (see introduction) deserve further examination.

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