Semiflexible crossing-avoiding trails on plane-filling fractals

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A R T I C L E   I N F O

A B S T R A C T

We have studied the statistics of semiflexible polymer chains modeled by crossing-avoiding trails (CAT) situated on the family of plane-filling (PF) fractals. The fractals are compact, that is, their fractal dimension d_f is equal to 2 for all members of the fractal family. By applying the exact and Monte Carlo real-space renormalization group method we have calculated the critical exponent ν, which governs the scaling behavior of the end-to-end distance of the polymer, as well as the entropic critical exponent γ, for a large set of fractals, and various values of polymer flexibility. Our results, obtained for CAT model on PF fractals, show that both critical exponents depend on the polymer flexibility, in such a way that less flexible polymer chains display enlarged values of ν, and diminished values of γ. We have compared the obtained results for CAT model with the known results for the self-avoiding walk and self-avoiding trail models and discussed the influence of excluded volume effect on the values of semiflexible polymer critical exponents, for a large set of studied compact fractals.

1. Introduction

It is well known that polymers show scale invariant properties, so that fractal concepts provide a fruitful mathematical grounds within which different aspects of polymer behavior can be analyzed [1]. Statistics of various lattice walk models which can capture the critical properties of linear polymer chains (i.e., non-trivial power-laws in the behavior of different quantities) has been studied as an ongoing problem in statistical mechanics [2]. The self-avoiding random walk (SAW) model [3], as a canonical model, has been usually applied, in such a way that steps of the walk have been identified with monomers which comprise the polymer chain, while the surrounding solvent has been represented by a lattice. SAW is a random walk that must not contain self-intersections, which means that on a lattice the walker cannot visit a site more than once – such a restriction corre-

sponds to the excluded -volume interactions of monomers within the polymer chain. Less repulsive excluded-volume interactions may be modeled by random walks formed in such a way that they never visit the same bond more than once (bond-avoiding walk) [4]. This model, which we refer to as to the self-avoiding trail (SAT) model has been effectively applied to study the statistic of flexible polymers on regular (Euclidean) [5–8] and semiregular lattices [9,10]. Within the SAT model the lattice sites may be revisited in two ways: by collision (where path touches itself), or by crossing (where path crosses itself), which enables one to generalize this model by assigning the weight w_x to the crossing site, and the weight w_c to the collision site [11,12]. For various values of w_x and w_c assorted types of self-avoiding walk models may be devised. For instance, the case $w_x = w_c = 0$ describes the standard SAW model, while the case $w_x = w_c = 1$ corresponds to the SAT model. The third, intermediate case ($w_x = 0$ and $w_c = 1$), in which the crossings are forbidden and collisions are allowed we refer here to the crossing-avoiding trail (CAT) model. This model coincides with the $O(n)$ model (in the limit $n \to 0$) initially introduced by Blöte and Nienhuis

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on the square lattice [13], which is also known as the vertex-interacting self-avoiding-walk model [14].

In real situations polymers are semiflexible [15,16] with various degrees of flexibility, so that in lattice models, besides the weight (fugacity) x associated with each step of the walk (monomer), an additional weight factor s (the stiffness parameter), corresponding to each bend of a walk on a lattice, should be introduced. The consideration of asymptotic properties (for large number of steps) of various types of self-avoiding walk models, appears to belong to the category of demanding problems in the critical phenomena studies. One of the main issues in semiflexible polymer model studies has been to answer the question if the critical exponents depend on polymer stiffness, and, whether different self-avoiding type models have the same values for critical exponents (belong to the same universality class) for the same polymer flexibility. In the case of flexible noninteracting polymer chains, there is an evidence that SAW and SAT models are in the same universality class for the square lattice [17], as well as in the case of the simple cubic lattice [18]. Moreover, for flexible interacting polymers on square lattice, it has been found that SAT and CAT models are in the same universality class [7], but this fact has been disputed in a recent study of loop models with crossings [19]. Besides, for semiflexible interacting SATs on the square lattice, it was found [20] that the SAT universality class is unaffected by the presence of stiffness, for a very wide range of stiffness weights.

To comprehend the various features of semiflexible polymers within the SAW model numerous studies have been performed. On the other hand, the same facets of the SAT and CAT model have been barely explored, and only a few studies of interacting semiflexible polymers, within the generalized SAT model [11,12] and the pure CAT model [14,21,22] on two dimensional Euclidean lattice have been performed recently. In these studies it was found that, for a wide range of flexibility, the examined critical exponents on regular (Euclidean) lattice are not affected by the value of the polymer stiffness. On the contrary, in recent studies of semiflexible noninteracting SAWs [23] and SATs [24] on fractals it has been found that geometrical critical exponents are stiffness dependant. Studies of random walk models on fractals [25] proved useful because often methods which exploit self-similarity of these lattices, such as real-space renormalization group method, can be applied and give exact results [26,27], thus providing information regarding different aspects of universality. Also, such investigations can provide valuable insight into polymer behavior in real situations occuring in non-homogeneous environment (for instance in living cells, which are crowded with various biomolecules). Since there have been no studies of semiflexible CAT model on fractal lattices so far, we have been motivated to perform a detailed study of the relevant problem on a family of two-dimensional compact fractals. Furthermore, we have explored the impact of excluded volume interaction on the statistics of semiflexible polymers by comparing results for CAT model with the corresponding previously obtained results for SAW and SAT models, on the same family of fractal lattices.

In our attack of the problem we apply the exact and Monte Carlo renormalization group approach to study the CAT model of semiflexible polymer chains on an infinite family of the plane-filling fractals, which appear to be compact, that is, their fractal dimension d_f is equal to 2 for all members of the fractal family, enumerated by an odd integer b ($3 \leq b < \infty$). We calculate the end-to-end distance critical exponents ν (associated with the mean squared end-to-end distance of polymer chain) and the entropic critical exponents γ (associated with the total number of different polymer configurations, averaged over all possible positions of the starting point). We have performed our calculations, for various degrees of polymer rigidity, for a large set of members of the fractal family, in order to attain information about the critical exponents behavior in the limit $b \to \infty$ (i.e. in the fractal–to–Euclidean crossover zone).

The present paper is organized as follows. In Section 2 we define the model of semiflexible CAT on plane-filling family of fractals, where we also present the renormalization group calculation (exact and Monte Carlo) of the critical exponents ν and γ of CATs on the plane-filling fractals, together with their specific results, obtained for various values of the stiffness parameter s. In Section 3 we discuss the evaluated data for CAT model and compare obtained results with the previous findings for SAT and SAW models on the same family of fractals. Summary of the obtained results and the relevant conclusions are given in Section 4.

2. The model and renormalization group method calculation

In this section we describe a renormalization group (RG) approach for studying the critical behaviour of semiflexible polymer chains immersed in a non-homogeneous container with a good solvent. Polymer chains are modeled by crossing-avoiding trails (CATs), whereas the container is modeled by fractals belonging to the plane-filling (PF) family of fractals. The members of PF fractal family are labeled by an odd integer b ($3 \leq b < \infty$), and can be constructed in stages. At the first stage ($n = 1$) of the construction one has a fractal generator which is a part of square lattice (of size b) containing b^2 connected bonds. The subsequent fractal stages are constructed recursively, so that the complete self-similar fractal lattice can be obtained as the result of an infinite iterative process of successive ($n \to n + 1$) enlarging the fractal structure b times, and replacing the smallest parts of enlarged structure with the initial ($n = 1$) structure (see Fig. 1(a)). The way the PF lattices are built implies that each member of the family has the fractal dimension d_f equal to 2, and PF fractals emerge to be compact objects embedded in two-dimensional Euclidean space, that is, they look like square lattices with various degrees of inhomogeneity distributed self-similarly.

To study the statistics of semiflexible polymers within the CAT model, we assign the weight x to each step of the walk performed on a lattice and the stiffness weight factor $s = e^{-E_s/k_B T}$, where $E_s > 0$ is an energy barrier associated with each bend of the polymer, and k_B is the Boltzmann constant. The situation $0 < s < 1$ corresponds to a semiflexible polymer chain, whereas the cases $s = 1$ and $s = 0$ coincide with a flexible and a fully rigid polymer chain, respectively. Then, the weight of a polymer having N monomers (steps in the applied model), with N_b bends, is $x^N s^{N_b}$, and corresponding partition function for the system studied may be written