



Statistical mechanics of polymer chains grafted to adsorbing boundaries of fractal lattices embedded in three-dimensional space



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HIGHLIGHTS

- Self-avoiding walk model of polymers near an adsorbing fractal surface is studied.
- Polymers are situated on three-dimensional lattices of Sierpinski gasket family of fractals.
- Exact and very precise Monte Carlo results are obtained for various polymer configurations.

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ABSTRACT

We study the adsorption problem of linear polymers, immersed in a good solvent, when the container of the polymer–solvent system is taken to be a member of the Sierpinski gasket (SG) family of fractals, embedded in the three-dimensional Euclidean space. Members of the SG family are enumerated by an integer b ($2 \leq b < \infty$), and it is assumed that one side of each SG fractal is impenetrable adsorbing boundary. We calculate the surface critical exponents γ_{11} , γ_1 , and γ_s which, within the self-avoiding walk model (SAW) of polymer chain, are associated with the numbers of all possible SAWs with both, one, and no ends grafted to the adsorbing surface (adsorbing boundary), respectively. By applying the exact renormalization group method, for $2 \leq b \leq 4$, we have obtained specific values for these exponents, for various types of polymer conformations. To extend the obtained sequences of exact values for surface critical exponents, we have applied the Monte Carlo renormalization group method for fractals with $2 \leq b \leq 40$. The obtained results show that all studied exponents are monotonically increasing functions of the parameter b , for all possible polymer states. We discuss mutual relations between the studied critical exponents, and compare their values with those found for other types of lattices, in order to attain a unified picture of the attacked problem.

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1. Introduction

The conformational characteristics of flexible polymer chains, immersed in various types of solvent, near an adsorbing substrate have been extensively studied because of their practical importance in technology and biological physics, and, as a surface critical phenomenon of modern statistical physics [1–3]. In almost all theoretical studies of the linear polymer

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adsorption, the model of the so-called self-avoiding random walk (SAW) has been used. SAW is simply defined as a random walk that must not contain self-intersections, so that steps of the walk have been identified with monomers comprising the polymer chain of length N , while the solvent surrounding has been represented by a lattice that has one adsorbing impenetrable boundary. Within that model, different thermodynamic ensemble approaches may be applied for studying finite length polymer chains [4,5]. In this paper we utilize the grand canonical ensemble formalism to study the behavior of very long chains in the thermodynamic limit $N \rightarrow \infty$. We assume that polymer, being immersed in a good solvent (i.e. interactions between the contiguous monomers of the chain are not taken into account), interacts with the adsorbing surface and thereby for a large enough strength of monomer–surface interaction it undergoes phase transition from the bulk (desorbed) phase to the adsorbed chain phase. The number of adsorbed monomers M is a function of temperature T , so that the ratio M/N can be figured as an order parameter for an adsorption transition appearing at the critical temperature T_a . At high temperatures ($T > T_a$), the number of adsorbed monomers M is vanishingly small and the polymer is situated in the bulk, while at low temperatures ($T < T_a$) the number M is proportional to N and polymer is adsorbed on the attractive surface. At the transition temperature $T = T_a$, the number of adsorbed monomers behaves according to the scaling law $M \sim N^\phi$, where ϕ is the so-called crossover critical exponent, which has been studied for an adsorption problem of polymers on planar (homogeneous) [6–9] and porous (fractal) [10–15] boundaries of polymer containers.

However, a complete picture about the adsorption problem requires knowledge of power-law exponents (dubbed critical exponents, within the parlance of the statistical mechanics of polymers) that describe asymptotic numbers of polymer configurations grouped according to the different ways of anchoring to the adsorbing boundary. In terms of the SAW polymer model, these exponents are defined through the following formulas for numbers of possible different configurations averaged over the number of sites on the impenetrable surface

$$C_{11}(N, T) \sim \mu^N N^{\gamma_{11}-1}, \quad C_1(N, T) \sim \mu^N N^{\gamma_1-1}, \quad C_s(N, T) \sim \mu^N N^{\gamma_s-1}, \quad (1)$$

valid for large number N of SAW steps. Here C_{11} , C_1 , and C_s , are average numbers of all possible SAWs with both, one, and no ends anchored to the boundary respectively, while γ_{11} , γ_1 , and γ_s , are respective surface critical exponents that take different values in various polymer phases. Besides, it is assumed that numbers C_{11} , C_1 , and C_s depend on the temperature T through the connectivity constant μ . So far, the surface critical exponents γ_{11} , γ_1 , and γ_s , have been studied mostly for SAWs in the vicinity of the boundary surfaces of homogeneous (Euclidean) containers [6,8,16,17], while the case of inhomogeneous polymer containers was studied only for SAWs immersed in a good solvent on Sierpinski gasket (SG) fractals embedded in two-dimensional space [18,19] and on n -simplex fractals [20]. In this paper we study the surface critical exponents for polymer chain situated on fractals that belong to the three-dimensional (3d) Sierpinski gasket family. Each member of the SG family is labeled by an integer b ($2 \leq b \leq \infty$), and it is assumed that one side of each SG fractal is impenetrable adsorbing wall. By applying the renormalization group (RG) method for the SAW model that includes monomer–surface interactions we have performed a detailed and extensive study for a large sequence of b values.

This paper is organized as follows. In Section 2 we describe the 3d SG fractals for general scaling parameter b , and introduce the SAW model in the case when a boundary of 3d SG fractal is an adsorbing surface. Then, we present the framework of the general RG method for studying the polymer adsorption problem on these fractals. In Section 3 we perform an exact RG analysis and display results for the studied critical exponents γ_{11} , γ_1 , and γ_s , for $b = 2, 3$ and 4 fractals, in different polymer state regimes. In Section 4 we describe the Monte Carlo renormalization group (MCRG) method for calculating surface critical exponents, and present results found for $2 \leq b \leq 40$. The obtained results are discussed in Section 5, and summarized in Section 6.

2. Framework of the renormalization group approach

In this section we describe the RG approach to calculating the critical exponents γ_{11} , γ_1 , and γ_s for the adsorption problem of SAWs immersed in a container with a good solvent, modeled by fractals belonging to the 3d SG family of fractals. We start with recalling the fact that each member of the 3d SG fractal family is labeled by an integer $b \geq 2$ and can be constructed in stages. At the first stage ($r = 1$) of the construction (the so-called fractal generator) there is a tetrahedron of base b containing $b(b+1)(b+2)/6$ upward oriented unit tetrahedrons. 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 ($r \rightarrow r+1$) enlarging the fractal structure b times, and replacing the smallest parts of enlarged structure with the initial ($r = 1$) structure. In the case under study, we take that one of the four boundaries of the 3d SG fractal is an impenetrable adsorbing surface (wall), which is itself a 2d SG fractal with the fractal dimension $d_s = \ln[b(b+1)/2]/\ln b$, whereas the fractal dimension of the complete 3d SG fractal is $d_f = \ln[b(b+1)(b+2)/6]/\ln b$.

In the terminology that applies to the SAW model of polymer adsorption, we assign the weight x to each step of the walk performed on a lattice in the bulk (away from the adsorbing surface) and the weight xw to each step performed on the adsorbing surface. Here w is the Boltzmann factor $w = e^{-\epsilon_w/k_B T} > 1$, where ϵ_w is the energy of a monomer lying on the attractive wall, and $k_B T$ is the product of the Boltzmann constant and the temperature of the solvent. In order to prevent the tendency of chain towards being always adsorbed (and promote an unbinding transition), it is necessary [10,13] to introduce one additional factor $t = e^{-\epsilon_t/k_B T} < 1$ in such a way that xt is the weight of those steps that are performed in the layer adjacent to the wall, while ϵ_t is the energy of the corresponding repulsive interaction between the surface and monomers

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