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Force-induced desorption of self-avoiding walks on Sierpinski gasket fractals

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Abstract. In this work we investigate force-induced desorption of linear polymers in good solvents in non-homogeneous environment, by applying the model of self-avoiding walk on two- and three-dimensional fractal lattices, obtained as generalization of the Sierpinski gasket fractal. For each of these lattices one of its boundaries represents an adsorbing wall, whereas along one of the fractal edges, not lying in the adsorbing wall, an external force acts on the self-avoiding walk. The hierarchical nature of the lattices under study enables an exact real-space renormalization group treatment, which yields the phase diagram of polymer critical behavior. We show that for this model there is no low-temperature reentrance in the cases of two-dimensional lattices, whereas in all studied three-dimensional cases the force-temperature dependance is reentrant. We also find that in all cases the force-induced desorption transition is of first order.

1 Introduction

Adsorption of polymer chains on surfaces is a phenomenon of wide occurrence in many industrial and daily processes and it also plays an important role in functioning of biological systems. Recent progress in atomic force microscopy and development of optical and magnetic tweezer techniques made it possible to micromanipulate a single polymer chain [1]. Using these experimental methods one can measure the force needed to detach a chain from an adsorbing surface and monitor the mechanism of some force-driven phase transitions at the level of a single molecule. Such experiments initiated a number of theoretical studies with the aim to obtain a deeper insight into the thermodynamics of force-induced desorption of a polymer. These studies pursue an extensive theoretical work on the polymer adsorption problem performed in the last decades [2–4], and include approaches based on mean-field type approximations, scaling arguments, Monte Carlo simulations and exactly solvable models [5–19].

A common physical situation treated theoretically in the context of force-induced polymer desorption is the following: a linear polymer molecule is tethered at one end to an impenetrable surface, at which the polymer can adsorb, and to the other end of the polymer a force is applied. When the polymer is pulled away from the surface, one expects a critical value of the force $f_c(T)$ (which depends on the temperature T), such that for $f < f_c(T)$ the polymer is adsorbed, while for $f > f_c(T)$ it is desorbed. Thus, the curve $f_c(T)$ can be regarded as a boundary that separates the desorbed phase from the adsorbed phase in the (T, f) plane. This phase transition was usually studied within the models in which the polymer is in a homogeneous environment, whereas in real situations one can expect different kinds of obstacles, which make some parts of the environment not accessible to the polymer. For instance, in biological systems the adsorption of polymer molecules on membranes occurs in cells which are crowded with various biomolecules, that may occupy a large fraction of the cell volume. However, exact treatment of such heterogeneities is difficult, therefore in this paper we use a simplified approach in which the polymer is modeled by a self-avoiding walk (SAW) on deterministic fractal lattices. Such models were often used and proved to be very useful in analytical investigation of various aspects of polymer behavior in non-homogeneous media (see [20] for a recent review). Here, by applying an exact real-space renormalization group (RG) method, in Section 2 we consider SAW on the Sierpinski gasket (SG) fractal, one of its boundary edges representing an adsorbing wall, whereas an external force, directed along the other fractal edge, is pulling the SAW from the wall. We show that unbinding occurs at some critical value of the force and obtain the corresponding phase diagram in the force-temperature plane. In Section 3 we generalize this approach to the Given-Mandelbrot (GM) fractal family, explicitly obtain phase diagrams for several GM fractals, show that for all of them

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