PHYSICAL REVIEW E **80**, 061131 (2009)

Stiffness dependence of critical exponents of semiflexible polymer chains situated on two-dimensional compact fractals

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(Received 20 July 2009; published 28 December 2009)

We present an exact and Monte Carlo renormalization group (MCRG) study of semiflexible polymer chains on an infinite family of the 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 enumerated by the odd integer b ($3 \leq b < \infty$). For various values of stiffness parameter s of the chain, on the PF fractals (for $3 \leq b \leq 9$), we calculate exactly the critical exponents ν (associated with the mean squared end-to-end distances of polymer chain) and γ (associated with the total number of different polymer chains). In addition, we calculate ν and γ through the MCRG approach for b up to 201. Our results show that for each particular b, critical exponents are stiffness dependent functions, in such a way that the stiffer polymer chains (with smaller values of s) display enlarged values of ν, and diminished values of γ. On the other hand, for any specific s, the critical exponent ν monotonically decreases, whereas the critical exponent γ monotonically increases, with the scaling parameter b. We reflect on a possible relevance of the criticality of semiflexible polymer chains on the PF family of fractals to the same problem on the regular Euclidean lattices.

DOI: 10.1103/PhysRevE.80.061131 PACS number(s): 05.40.Fb, 64.60.De, 64.60.al, 64.60.ae

I. INTRODUCTION

The self-avoiding walk (SAW) is a random walk that must not contain self-intersections. It has been extensively studied as a challenging problem in statistical physics, and, in particular, as a satisfactory model of a linear polymer chain [1]. The pure SAW is a good model for perfectly flexible polymer, where we ignore the apparent rigidity of real polymer, and, consequently, to each step of SAW, we associate the same weight factor (fugacity) x. In most real cases, the polymers are semiflexible with the various degree of stiffness. To take into account this property of polymers, in the continuous space models, the stiffness of the SAW path is modeled by constraining the angle between the consecutive bonds of polymer, while in the lattice models, an energy barrier for each bend of the SAW is introduced. The lattice semiflexible SAW model (also known as persistent or biased SAW model), has been studied some time ago in a series of papers [2], with a focus on the so-called rod-to-coil crossover. Afterwards, it was modified in various ways, in order to describe relevant aspects of different phenomena, such as protein folding [3,4], adsorption of semiflexible homopolymers [5], transition between the disordered globule and the crystalline polymer phase [6,7], behavior of semiflexible polymers in confined spaces [8,9], or influence of an external force on polymer systems [10–13].

In spite of numerous studies, a scanty collection of exact results for semiflexible polymers has been achieved so far, even for the simplest lattice models. A few cases in which some properties of semiflexible SAW can be studied exactly are: directed semiflexible SAWs on regular lattices [5,14], and semiflexible SAWs (with no constraints on the direction) on some fractal lattices [15,16]. In particular, exact values of the end-to-end critical exponent ν and the entropic exponent γ were obtained for these models, and it turned out that in some cases, critical exponents are universal, whereas in other cases, they depend on the stiffness of the polymer chain. Universality arguments, as well as results of approximate and extrapolation methods for similar models, suggest that critical exponents on regular (Euclidean) lattices should not be affected by the value of the polymer stiffness. On the other hand, it is not known what are the effects of rigidity on the critical behavior of SAWs in nonhomogeneous environment. In order to explore further this issue, in this paper we perform the relevant study on the infinite family of the plane-filling (PF) fractal lattices [17,18], which allow for an exact treatment of the problem. These fractals appear to be compact, that is, their fractal dimension d_f is equal to 2. Members of the family can be enumerated by an odd integer b ($3 \leq b < \infty$), and as $b \to \infty$ characteristics of these fractals approach, via the so-called fractal-to-Euclidean crossover [19,20], properties of the regular two-dimensional (2D) lattice. By applying the exact real-space renormalization group (RG) method [21,22], as well as Monte Carlo renormalization group (MCRG) method [23–26], we calculate critical exponents ν and γ. We have performed our calculations for as many as possible members of the fractal family, for various degree of polymer stiffness, in order to study consequent stiffness dependence of the critical exponents, as well as to see the asymptotic behavior of the exponents in the fractal-to-Euclidean crossover region.

This paper is organized as follows. We define the PF family of fractals in Sec. II, where we also present the frame-

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