Scaling of Hamiltonian walks on fractal lattices

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We investigate asymptotical behavior of numbers of long Hamiltonian walks (HWs), i.e., self-avoiding random walks that visit every site of a lattice, on various fractal lattices. By applying an exact recursive technique we obtain scaling forms for open HWs on three-simplex lattice, Sierpinski gasket, and their generalizations: Given-Mandelbrot (GM), modified Sierpinski gasket (MSG), and n-simplex fractal families. For GM, MSG and n-simplex lattices with odd values of n, the number of open HWs Z_N, for the lattice with $N \gg 1$ sites, varies as $\omega^N N^\gamma$. We explicitly calculate the exponent γ for several members of GM and MSG families, as well as for n-simplices with $n=3$, 5, and 7. For n-simplex fractals with even n we find different scaling form: $Z_N \sim \omega^N \mu^{N^{1/d_f}}$, where d_f is the fractal dimension of the lattice, which also differs from the formula expected for homogeneous lattices. We discuss possible implications of our results on studies of real compact polymers.

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I. INTRODUCTION

Self-avoiding walks (SAWs) have long been used in the studies of configurational statistics of polymer chains in solution [1]. Due to excluded volume effect, at high temperatures T (good solvent) long polymer chains are in swollen configurations. At low temperatures (poor solvent) polymers are in a collapsed state, caused by the attractive interactions of different sections of a polymer, mediated by a solvent. The transition between these two states occurs at the so-called θ temperature, at which excluded volume and attractive forces balance. Whereas the swollen and θ phases have been well investigated by now, the entropic scaling of the collapsed phase is still an open issue. A closely related problem is the scaling of Hamiltonian walks (HWs), which are SAWs that visit all the sites of the underlying lattice. HWs are believed to represent the $T=0$ limit of collapsed polymers, and they are also used in the studies of polymer melting [2], as well as in the context of protein folding [3].

The number Z_N of HWs on homogeneous lattices with $N \gg 1$ sites is expected to behave as

$$Z_N \sim \omega^N \mu_S^{N^\sigma} N^a. \tag{1.1}$$

Here $\sigma=(d-1)/d$, where d is the dimensionality of the lattice, μ_S is some constant less than 1, and ω is the connectivity constant, defined as

$$\ln \omega = \lim_{N\to\infty} \frac{\ln Z_N}{N}. \tag{1.2}$$

Proposed scaling form for HWs differs from the ordinary SAW case (swollen polymer), where the average number of N-step SAWs, for large N, behaves as $\omega^N N^a$, and where the critical exponent a depends only on d (which is not the case for HWs). The term $\mu_S^{N^\sigma}$ in the HW case is expected on the basis of the exact study of HWs on the Manhattan lattice [4], as well as on the conjecture that the collapsed polymer (globule) has a sharp boundary, so that a surface tension term should arise [5]. The scaling form (1.1) was confirmed by Owczarek [6] for collapsed partially directed SAWs on the square lattice. Baiesi *et al.* [7] recently performed extensive Monte Carlo simulations, which gave strong evidence that Eq. (1.1) is also satisfied for undirected collapsed SAWs on the square lattice. There are hardly any results for higher dimensional lattices. To the best of our knowledge, the only clear indication that for collapsed SAWs on three-dimensional lattices there exists a surface term, as predicted by Eq. (1.1), was obtained by Grassberger and Hegger [8] via Monte Carlo simulations. There are also no results concerning the scaling form for the collapsed SAWs on disordered lattices. Having all that in mind it might be useful to study HWs on fractals.

Fractal lattices are somehow intermediate between homogeneous and disordered ones, and their hierarchical and scale invariant structure often allows an exact recursive treatment of various physical phenomena. The ordinary SAW model (corresponding to the polymer chain at high temperatures) has been studied extensively in the past on different fractals [9–20]. These studies contribute to a better understanding of how dimension and topological structure of underlying space

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