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SCALING EXPONENT OF COMPACT POLYMER CONFORMATIONS IN NON HOMOGENEOUS MEDIA

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Abstract: We studied compact conformations of a ring polymer adsorbed on the non homogeneous (e. g. porous) substrates. Substrates are represented by the generalization of modified rectangular (MR) lattice – a hierarchically constructed family of fractal lattices embedded in 2d space and parameterized with an integer p >1. Analyzing the exact set of recursive relations for arbitrary value of p, we established an asymptotic form of a number of conformations. As a correction to the leading exponential factor we obtained the stretched exponential factor with the exponent σ = 1/2 on each member of the fractal family. Although it is believed that the critical exponent σ on fractal lattices is determined not only by the fractal dimension of the underlying lattice but also by other lattice parameters, here we found that σ had the same value on different fractals with the same fractal dimension ($d_f = 2$).

Keywords: non-homogeneous media, fractal, polymer, scaling functions, critical exponents.

1. INTRODUCTION

Polymer is a large molecule made up of covalently bonded units called monomers. As solid material, a synthetic polymer can exists in various forms: from ordinary thermoplastics used in everyday life to some highly advanced polymer matrix composites used in marine and aerospace applications. Nature also prefers polymers since all living beings are comprised of polymers such as structural or functional proteins whose performance is directed and controlled by other well known polymers: DNA and RNA.

The conformational properties of a single polymer are best learned when the polymer is immersed in a solvent. Then, due to the thermal agitation, polymer continuously changes its shape and acquires different conformations. Depending on the quality of the solvent and /or temperature, there are three qualitatively different regimes. In good solvent (or high temperature), the regime polymer is in an extended state. Lowering the solvent quality or temperature, at the so called Θ - condition, a polymer undergoes collapse transition from expanded to compact state. In the bad solvent regime (or low temperature) when polymer is in compact state, it occupies compact, globular conformations in order to minimize contacts with the solvent. Statistics of linear polymer conformations in all three regimes are well described by a suitable kind of random walks defined on a lattice [1]. In good solvent regime, when conformations are of the random coil type, self-avoiding random walks are applicable, a concept originally introduced in polymer physics by Montroll [2]. Self avoiding random walks (SAWs) are random walks that never visit some lattice site more than once, i.e. they do not intersect themselves, a property that mimics the self-excluded volume in real polymers. Compact conformations are best represented by Hamiltonian walks (HWs) which are SAWs that visit each lattice site and therefore maximally occupy the lattice. The compact state of a polymer is a principal state in the biological world due to the fact that the functional proteins under normal conditions fold into the unique compact conformation, or to the fact that chromatin in eukaryotic cells is compactly packed into the nucleus.

In this article we study conformations of a ring polymer that are compact and fractal in charac-

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ter, which is directly applicable to chromatin organization in the nucleus as stated in [3−6].These kinds of conformations are generated by the Hamiltonian closed walks (cycles) on fractal lattices, where each walk can be viewed as space-filling fractal curve. Utilizing self-similarity of fractal lattices, through the exact set of recurrence equations, we determine how the number of HWs (Z) grows with the number of lattice sites (N) when $N \to \infty$ (asymptotic law).

2. MODIFIED RECTANGULAR LATTICE AND ITS GENERALIZATION

Modified rectangular (MR) lattice and its generalization (GMR) are fractal lattices embedded in 2d space [7,8]. Each fractal of GMR family is parameterized with an integer p , $2 \le p \le \infty$. The case $p = 2$ corresponds to MR lattice. Construction of fractals is iterative, step by step, as illustrated in Figure 1 and Figure 2. For an arbitrary p , the first four steps of construction are: 1^{st} step − graph of four points in the form of the unit square is constructed; 2^{nd} step − p unit squares are connected in the form of rectangle; 3^{rd} step − p rectangles, as the one obtained in the previous step, are connected in the form of a $p \times p$ square; 4^{th} step − p squares from the previous step are connected in the form of a rectangle. Fractal is obtained after infinitely many steps in which we alternatively generate rectangular and square shapes. The structure obtained in the l^{th} step of the construction is called the l^{th} order generator, and is denoted by G_l . For a given p generator G_l (p) comprises $N_l = 4 \cdot p^{l-1}$ lattice cites, and each fractal lattice obtained when $l \to \infty$ has fractal dimension $d_f = 2$, independently of p .

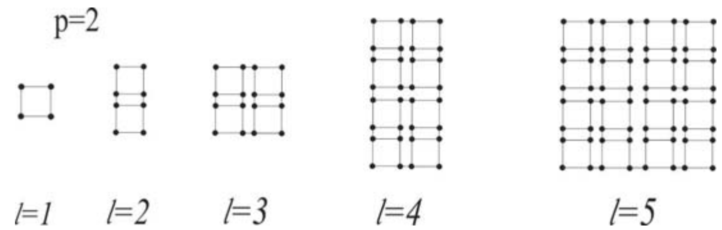

Figure 1. Iterative construction of MR fractal lattice: the first five steps

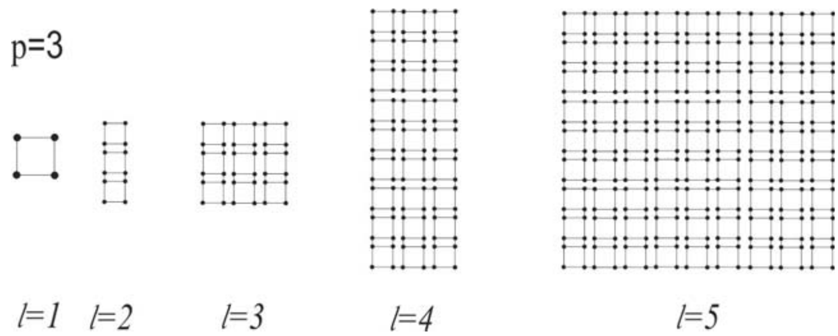

Figure 2. The first five steps of the iterative construction of GMR fractal lattice with $p = 3$

3. RECURSIVE ENUMERATION OF WALKS AND ASYMPTOTICS

In order to enumerate all Hamiltonian cycles on $G_{l+1}(p)$, in Figure 3 we schematically represent all cycles on the coarse grained $G_{l+1}(p)$ − generator of order $l+1$ (square or rectangle) that consists of p generators of order l (rectangles or squares) whose internal structure is not shown. It turns out that for any p there is only one coarse grained cycle. This cycle on $G_{l+1}(p)$ consists of p steps (parts), each one through one of the $G_l(p)$. Steps are denoted by B if they consist of one brunch that enters and leaves $G_l(p)$ through vertices of $G_l(p)$ belonging to different $G_{l-1}(p)$. Actually, step B represents all Hamiltonian walks that enter and leave generator through mentioned vertices, and whose number on $G_l(p)$ is denoted by B_l . Similarly, steps are denoted by D if they consist of two brunches, each of them entering and leaving $G_l(p)$ through vertices of $G_l(p)$ belonging to the same $G_{l-1}(p)$. Step D represents all walks of that type whose number on $G_l(p)$ is denoted by D_l . We can see in Figure 3 that there are two B steps and $p-2$ steps D, so that the overall number of Hamiltonian cycles on $G_{l+1}(p)$ can be expressed as :

$$Z_{l+1} = B_l^2 D_l^{p-2} \quad . \tag{1}$$

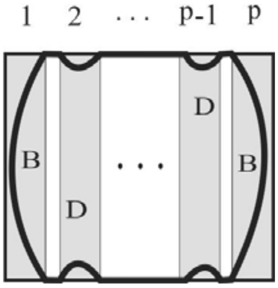

Figure 3. Schematic representation of all Hamiltonian cycles on $G_{l+1}(p)$. Grey rectangles represent $G_l(p)$.

Due to the self-similarity of fractal lattices the numbers of walks of B and D types can be obtained recursively, but in order to achieve this, the other two types of walks, denoted by A and E, are needed. Schematic representation of walks of type A, B and E are given in Figure 4, and that of walk D is given in Figure 5. Recurrence equations are:

$$A_{l+1} = B_l D_l^{p-1}, \tag{2}$$

$$B_{l+1} = A_l^p, \tag{3}$$

$$D_{l+1} = pD_l^{p-1}E_l + (p-1)B_l^2 D_l^{p-2}, \tag{4}$$

$$E_{l+1} = D_l^p \,. \tag{5}$$

This system of non-linear difference equations should be supplemented with the initial conditions − the numbers of walks on the unit square: $A_1 = B_1 = D_1 = E_1 = 1$.

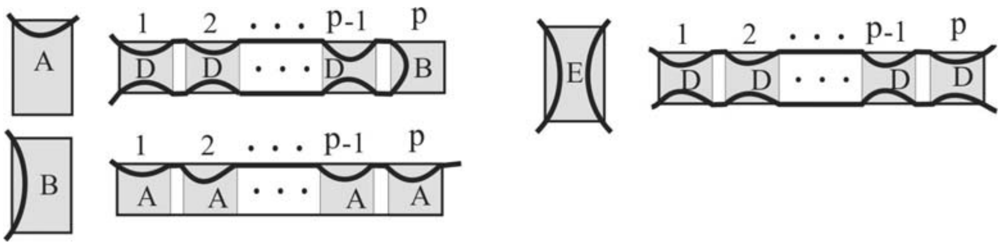

Figure 4. Graphic representation of A, B and E type of walks together with schematic derivation of the corresponding recurrence relations

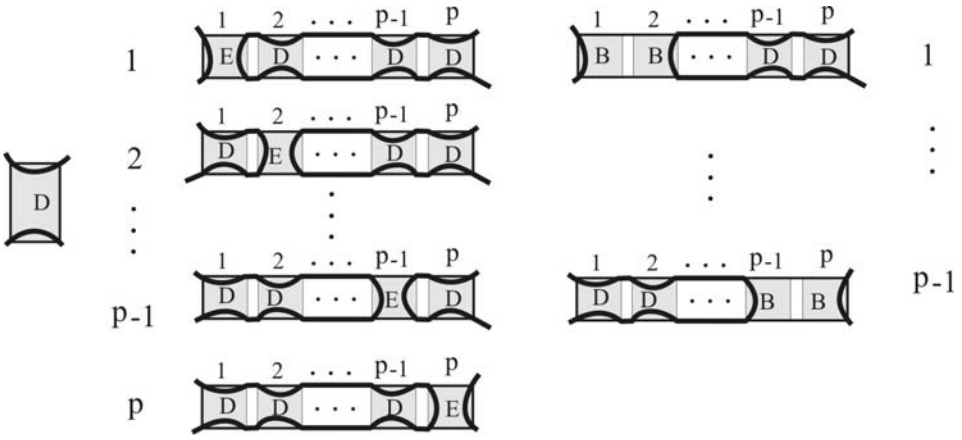

Figure 5. Schematic representation of D type of walks and illustration of obtaining recurrence relation

The numerical iteration shows that variables A_l, B_l, D_l and E_l grow very fast with each iteration l, so that we rescale them dividing A_l, B_l and E_l by D_l, and obtain new, rescaled variables defined as: $x_l = A_l / D_l$, $y_l = B_l / D_l$ and $z_l = E_l / D_l$. Recurrence equations for rescaled variables, that follow from equations (2), (3) and (5) are:

$$x_{l+1} = \frac{y_l}{(p-1)y_l^2 + pz_l}, \tag{6}$$

$$y_{l+1} = \frac{x_l^p}{(p-1)y_l^2 + pz_l}, \tag{7}$$

$$z_{l+1} = \frac{1}{(p-1)y_l^2 + pz_l}, \tag{8}$$

while equation (4) turns to

$$D_{l+1} = D_l^p[(p-1)y_l^2 + pz_l]. \tag{9}$$

By numerical iteration we obtain that $x_l, y_l \to 0$ for large l, while $z_l \to const$ whose value depends on the parity of l. With these facts, combining equations (6) and (7) for $l >> 1$ it follows that $y_l \approx const\ y_{l-2}^p$, meaning that

$$y_l \approx \begin{cases} C_1 \lambda_e^{p^{\frac{l}{2}}}, & \text{for even } l \\ C_2 \lambda_o^{p^{\frac{l-1}{2}}}, & \text{for odd } l. \end{cases} \quad (10)$$

From equation (9) for $l >> 1$ we have $D_{l+1} \sim const\, D_l^{\ p}$ so that variable D asymptotically grows as $D_l \sim const\ \omega_1^{\ p^l}$, where ω_1 can be obtained numerically as $\ln \omega_1 = \lim_{l\to\infty} \frac{\ln D_l}{p^l}$ for each value of p . In rescaled variables relation (1) becomes $Z_{l+1} = y_l^{\ 2} D_l^{\ p}$, from which, together with the asymptotic given by (10), asymptotic for D_l and relation for the number of lattice cites $N_l = 4 \cdot p^{l-1}$, it is derived that the number of Hamiltonian cycles on GMR lattices for arbitrary p asymptotically behaves as

$$Z_l \sim \begin{cases} const\ \omega^{N_l} \mu_e^{\ N_l^\sigma}, & \text{for even } l \\ const\ \omega^{N_l} \mu_o^{\ N_l^\sigma}, & \text{for odd } l, \end{cases} \quad (11)$$

where the connectivity constant $\omega = \omega_1^{\frac{p}{4}}$ and constant μ in the stretched exponential factor depend on p , but μ also depends on the parity of l for given p .

We obtained that $\mu_e = (\lambda_o)^{\frac{1}{\sqrt{p}}}$ while $\mu_o = \lambda_e$. Exponent σ in the stretched exponential factor is equal to $1/2$ for all p . Values of ω, λ_e and λ_o as functions of p are given in Table 1 for $2 \le p \le 10$, and graphical presentations of ω, μ_o and μ_e are given in Figures 6 and 7.

Table1. Values of parameters ω, λ_e and λ_o appearing in scaling form (10) for $2 \le p \le 10$

p	2	3	4	5	6	7	8	9	10
ω	1.1687	1.1474	1.1293	1.1151	1.1039	1.0948	1.0872	1.0809	1.0755
λ_e	0.4621	0.5537	0.6141	0.6574	0.6903	0.7164	0.7377	0.7555	0.7706
λ_o	0.1660	0.1154	0.08999	0.07430	0.06352	0.05561	0.04953	0.04469	0.04075

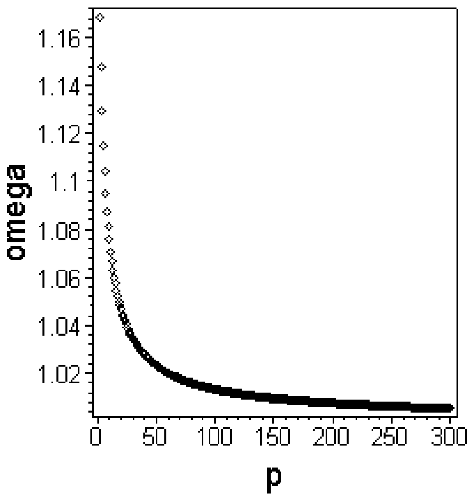

Figure 6. Connectivity constant ω as a function of p.

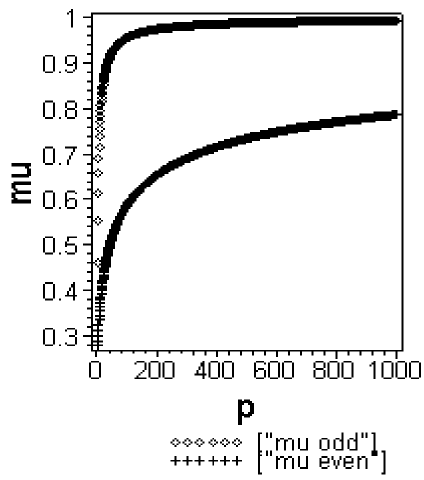

Figure 7. Constant λ for even and odd values of l as a function of p.

4. DISCUSSION OF THE RESULTS

In this paper we established an asymptotic form given by the equation (11) for the number of Hamiltonian cycles on GMR fractal lattices. As a correction to the leading exponential factor we obtained the stretched exponential factor with $\sigma = 1/2$ on the whole fractal family. It is well known that the bases ω and μ in the scaling form (11) depend on lattice details, but it is expected that σ on homogeneous lattices depends only on lattice dimension due to its origin in surface correction [10,11]. Contrary to homogeneous lattices, as pointed out in [12−14], σ on fractal lattices should be of non-universal character, meaning that it should depend not only on the fractal dimension but on other lattice parameters too. Here we found the same value of σ on the whole family of similar, but slightly different lattices, with the same fractal dimension. Although lattice dependent on fractals, we see that σ is less sensitive on lattice details than ω and μ. Furthermore, it follows from Figure 7 that the connectivity constant ω slightly decreases with p, although for all p lattices have the same coordination number (three). Due to the high anisotropy of horizontal and vertical directions for each p, by varying p we obtained two branches for the base μ in the stretched exponential factor (for even and odd values of l) as depicted in Figure 7. In the end, we can say that this is an instructive example of a study of how topological properties of lattices influence scaling parameters of Hamiltonian walks.

5. ACKNOWLEDGMENT

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ЕКСПОНЕНТ СКАЛИРАЊА КОМПАКТНИХ ПОЛИМЕРНИХ КОНФОРМАЦИЈА У НЕХОМОГЕНИМ СРЕДИНАМА

Сажетак: Проучавали смо компактне конформације прстенастих полимера адсорбованих на нехомогене (нпр. порозне) супстрате. Супстрати су представљени генерализацијом модификоване правоугаоне (МП) решетке − хијерархијски конструисаном фамилијом фракталних решетки смјештених у дводимензионални простор и параметрисаних са цијелим бројем p, p > 1. Анализом егзактног система рекурентних релација за произвољну вриједност p, успоставили смо асимптотски облик функције скалирања укупног броја конформација. Као корекцију на водећи експоненцијални фактор добили смо проширени експоненцијални фактор са експонентом σ = 1/2 на сваком фракталу разматране фамилије. Иако се сматра да критични експонент σ на фракталним решеткама не одређује само фрактална димензија решетке већ и њени остали параметри, овдје смо добили да σ има исту вриједност на различитим фракталним решеткама исте фракталне димензије (d_f= 2).

Кључне ријечи: нехомогене средине, фрактал, полимер, функције скалирања, критични експоненти.