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NONUNIVERSAL PROPERTIES OF SELF-INTERACTING POLYMER IN NON-HOMOGENEOUS ENVIRONMENT MODELED BY 3-SIMPLEX FRACTAL LATTICE

Dušanka Marčetić [1], Sunčica Elezović Hadžić[2], Ivan Živić[3]*

[1]University of Banja Luka, Faculty of Natural Sciences and Mathematics, Department of Physics, Mladena Stojanovića 2, Banja Luka, Bosnia and Herzegovina
[2]University of Belgrade, Faculty of Physics, Studentski trg 12, Belgrade, Serbia
[3]University of Kragujevac, Faculty of Science, Radoja Domanovića 12, Kragujevac, Serbia

Abstract: We have studied lattice self-avoiding polygons with attractive interaction between contacts which are nonconsecutively visited nearest neighboring sites. The lattice of choice is 3-simplex fractal lattice and the model represents a ring polymer in non-homogeneous solution whose quality depends on the interaction parameter. It has already been shown, by the renormalization group approach, that polymer on this lattice at any nonzero temperature can exist only in the extended phase. Universal critical exponents, which do not depend on the interaction strength, have also been determined. In this paper we are concerned with two nonuniversal quantities: the connectivity constant related with the free energy of the model and the mean number of contacts related with the internal energy. We have shown that the connectivity constant is an unboundedly increasing function of the interaction strength, while the mean number of contacts is an increasing function asymptotically approaching a limiting value equal to one half, which is the mean number of contacts in the case of Hamiltonian walks on the same lattice. This limiting value is expected, since in the limit of infinite interaction (or zero temperature) each self-avoiding walk on 3-simplex lattice becomes maximally compact and occupies all lattice points, i.e. becomes Hamiltonian walk.

Key words: polymer, self-avoiding polygon, fractal, nonuniversal quantities.

1. INTRODUCTION

Behavior of a linear polymer in dilute solution is well studied topic in polymer science. At high temperatures, i.e. good solvent regime, excluded-volume effects prevail, and polymer is in an extended phase with swollen conformations. At low temperatures, i.e. bad solvent regime, attractive interaction between monomers prevails, and polymer is in a collapsed phase with compact conformations. Transition between high and low temperature phases (collapse transition) happens at some intermediate, the so called θ-temperature, and exactly at this temperature polymer behaves as an ideal polymer chain [1,2].

Self-avoiding walks (SAWs) on a lattice are random walks that never visit the same lattice point more than once [3]. Closed self-avoiding walks, i.e. self-avoiding walks whose starting and ending points coincide are called self-avoiding polygons (SAPs) [4]. In its simplest form, SAWs and SAPs are used to model linear and circular (i.e. ring) polymers, respectively, in good solvents. The property of non self-intersection mimics the excluded volume effects in a real polymer. Introduction of an attractive interaction between contacts, i.e. nearest neighboring lattice sites visited non-consecutively by the self-avoiding walk, converts the ordinary SAW model into the interacting SAW (ISAW) model, and similarly the SAP into the interacting SAP (ISAP). These interacting models are able to capture collapse transition, and have been extensively studied on lattices with translational invariance in two and three-dimensional space [5–18].

Studies of ISAW model on translationally invariant lattices assume that the polymer is

* Corresponding autor: dusanka.marcetic-lekic@pmf.unibl.org

immersed in a homogeneous solution. Usually, various types of inhomogeneities dispersed in solution spoil its translational invariance, so that fractal lattices, with no such symmetry, become more convenient. Moreover, fractal lattices are scale invariant (a property that enables exact application of the renormalization group technique) which has led to many exact results regarding universal properties (properties that do not depend on the interaction parameter and some particular lattice details) of the model on various fractal lattices [19–24]. Specifically, it has been shown that 3-simplex fractal lattice and two-dimensional Sierpinski Gasket lattice do not allow for the collapse transition, implying that the polymer on these two lattices can exist only in the extended phase for all finite values of the interaction parameter [19,20]. It has also been shown that the studied model on these two lattices belongs to the same universality class, and universal critical exponents in the extended phase - metric exponent ν that determines the gyration radius of a polymer and entropic exponents γ and α that govern the scaling laws of the partition function of the walk and polygon models, respectively, have been determined [19,22,25,26].

In this paper we give our contribution to the understanding of the ISAP model behavior on 3-simplex fractal lattice by studying two non-universal quantities. Precisely, analyzing the generating function of the model, we have obtained the connectivity constant and the mean number of contacts per monomer, related with the model's free energy and the mean number of contacts, respectively, per monomer, in the thermodynamic limit. We determine how each of these quantities depend on the interaction parameter. Numerical study of the comprehensive ISAP model, in the whole temperature range, as presented here, should shed light on relationship between ISAP model and other theoretical models applicable only in some specific temperature domains.

The paper is organized as follows. ISAP model is defined in section 2. Relevant fractal lattice, method for the calculation of the quantities of interest and obtained results are presented in section 3. Finally, summary and conclusions are given in section 4.

2. ISAP MODEL

A self-avoiding polygon representing one possible conformation of circular polymer on the square lattice is shown in Figure 1. Visited lattice sites represent monomers (or collection of monomers) along the polymer backbone, while the steps of the polygon represent chemical bonding between them. Attractive interaction between monomers that are nearest neighbors but not chemically bonded is incorporated through an interaction energy ε ($\varepsilon < 0$) between contacts.

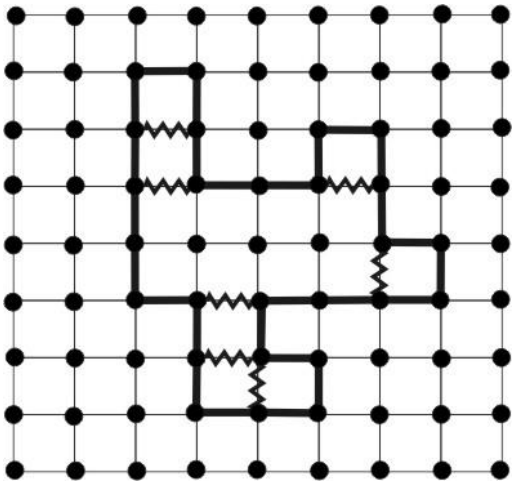

Figure 1. Self-avoiding polygon with N=26 steps and M=7 contacts. This polygon contributes to the term $x^{26}u^7$ in the generating function (4)

This interaction is marked with wiggly line in Figure 1. Assuming that each polygon consists of exactly N steps (has perimeter N), partition function in canonical ensemble is given as

$$Z_N = \sum_{P_N} e^{-\beta E(P_N)}, \quad (1)$$

where P_N stands for polygon of length N, $E(P_N)$ is the energy of each such polygon, and $\beta = 1/kT$. Denoting the number of contacts in each configuration as $M(P_N)$, the energy of this polygon is $E(P_N) = M(P_N)\varepsilon$. Associated Boltzmann weight is $e^{\beta M(P_N)|\varepsilon|} = u^{M(P_N)}$, where it has been taken into account the fact that $\varepsilon < 0$, and interaction parameter $u = e^{\beta|\varepsilon|}$ has been introduced. Then, sum (1) can be written as

$$Z_N(u) = \sum_{P_N} u^{M(P_N)} = \sum_{M=0}^{M_{max}} \mathsf{C}_N(M) u^M, \quad (2)$$

where $\mathsf{C}_N(M)$ is the number of self-avoiding polygons of length N and M contacts, normalized per lattice site. It is convenient to work with variable polymer length controlled by the fugacity $x > 0$ assigned to each step of the polygon (or visited lattice site). Associated grand canonical partition function is

$$G(x,u) = \sum_{N=0}^{\infty} Z_N(u) x^N. \quad (3)$$

In mathematics, this power series represents a generating function for a sequence of numbers $\{Z_N\}$. With (2), expression (3) can also be written as

$$G(x,u) = \sum_{N=0}^{\infty} \sum_{M=0}^{M_{max}} \mathsf{C}_N(M) u^M x^N. \quad (4)$$

Each polygon with M contacts and N steps has a weight $u^M x^N$, so that the generating function is the total weight of all possible polygons from minimal length to maximal infinite length.

It is conjectured that the asymptotic, large N behavior, of partition function (1) in high temperature regime is given by

$$Z_N(u) \sim A\mu(u)^N N^{\alpha-3}, \quad (5)$$

where the base μ is called connectivity constant, a non-universal quantity which depends on the interaction parameter u as well as on the lattice details. Assuming that relation (5) holds, it can easily be shown that the radius of convergence of power series (3) is $x_c(u) = \frac{1}{\mu(u)}$, and in this context x_c is called critical fugacity. Also, from the definition of free energy $F = -\frac{1}{\beta}\ln Z$, and relation (5), it follows that the free energy per monomer in the thermodynamic limit is given as

$$f = \lim_{N\to\infty} \frac{F}{N} = -\frac{1}{\beta}\ln \mu, \quad (6)$$

which elucidates the physical meaning of the connectivity constant. Exponent α in the asymptotic relation (5) is universal, and depends only on the lattice dimensionality. It determines the leading singular behavior of the generating function G, and it can be shown that the following relation holds $G(x) \sim const(x_c - x)^{2-\alpha}$ as $x \to x_c$ from below.

The mean number of contacts by definition is

$$\langle M \rangle = \frac{1}{G}\sum_{N=0}^{\infty}\sum_{M=0}^{M_{max}} M C_N(M) u^M x^N, \quad (7)$$

and can be obtained from the generating function as

$$\langle M \rangle = \frac{\partial \ln G}{\partial \ln u}, \quad (8)$$

while the mean number of steps is

$$\langle N \rangle = \frac{1}{G}\sum_{N=0}^{\infty} N Z_N(u) x^N, \quad (9)$$

and is given by

$$\langle N \rangle = \frac{\partial \ln G}{\partial \ln x}. \quad (10)$$

It is assumed that partial derivatives in (8) and (10), for each u, are calculated at the corresponding value of x_c. Combining equations (8) and (10), the mean number of contacts per step is given as

$$m = \frac{\langle M \rangle}{\langle N \rangle} = \frac{u}{x}\frac{\frac{\partial G}{\partial u}}{\frac{\partial G}{\partial x}}, \quad (11)$$

and this quantity determines internal energy per step in the thermodynamic limit, which is equal to $m\varepsilon$.

3. ISAP MODEL ON 3-SIMPLEX LATTICE

Deterministic 3-simplex fractal lattice is constructed iteratively. In the first step of construction three points are joined into the form of the unit triangle. The obtained structure is called the first order generator or initiator. In the second step, three unit triangles are joined into the form of triangle in such a way that the vertices of neighboring triangles are split. Repeating this procedure infinitely many times, full fractal lattice is obtained. The structure obtained in the arbitrary *r*-th step of construction is called *r*-th order generator and it is denoted as G_r. First three generators are shown in Figure 2. The number of lattice sites in G_r is 3^r.

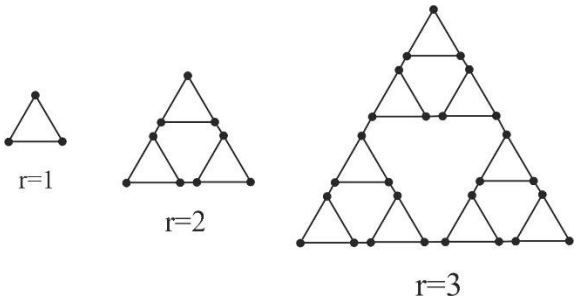

Figure 2. First three steps of the iterative construction of 3-simplex fractal lattice

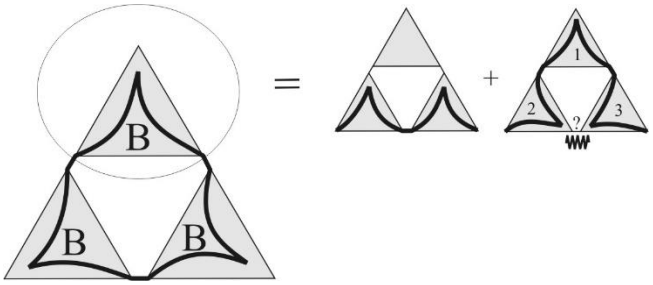

Figure 3. Schematic representation of all self-avoiding polygons on an arbitrary order generator of 3-simplex lattice. Each polygon on generator G_{r+1} consists of three open self-avoiding walks, denoted by B, one through each G_r. For B walk through upper G_r two possible different realizations through its sub-generators G_{r-1} are schematically shown

We will utilize self-similar structure of the 3-simplex lattice, and following [20] determine the generating function (3) of ISAP model recursively. We notice that each polygon on G_{r+1} can be formed from open self-avoiding walks through its sub-generators G_r. One such polygon on G_{r+1}, and its three composing parts, open self-avoiding walks through each G_r, are schematically shown in Figure 3. Self-avoiding walks that start at one apex of any generator of order r and end at any of the other two apexes of the same generator are denoted as B type of the walks. These are walks of different length which include both, walks that visit and walks that do not visit the third apex of the generator. The overall weight of all polygons on G_{r+1} is product of the overall weights of its composing parts through G_r. If the weight of all walks of type B on G_r is denoted by

B_r, then the weight of all polygons on G_{r+1} is equal to $(B_r)^3$. Normalizing this weight per lattice site of G_{r+1} and summing over generators of all order r, we obtain the generating function

$$G(x,u) = \frac{1}{3}x^3 + \sum_{r=1}^{\infty} \frac{1}{3^{r+1}} (B_r(x,u))^3. \quad (12)$$

The first term, $\frac{1}{3}x^3$, is the weight per site of the only one polygon on the unit triangle. For determination of the weights of walks B on G_r we will set recursive equations on the basis of Figure 3. Two possible situations on encircled G_r are schematically represented in the upper right part of the figure. The first scheme represents all walks of type B on G_r that traverse only two of its sub-generators G_{r-1}, and the weight of all such walks is $(B_{r-1})^2$. The second scheme represents all walks of type B on G_r that traverse each of its three sub-generators G_{r-1}, and one can notice that if the walks B through sub-generators denoted as 2 and 3 visit their third apex, then an additional interaction between apexes of these two neighboring triangles occurs. In order to account properly for this interaction, among all walks of type B on sub-generators 2 and 3, we will distinguish those walks that visit the third apex of these generators and denote them as C (see Figure 4), while their weights on G_{r-1} will be denoted as C_{r-1}. If the additional interaction was not present, the weight of all walks in second scheme would be $(B_{r-1})^3$. Since among all walks of type B through generators 2 and 3, only walks of type C contribute to this interaction, we will subtract their contribution from the weight $(B_{r-1})^3$ and add an additional term with the new interaction incorporated. It then follows that recursion relation for the weight B_r can be written as

$$B_r = B_{r-1}^2 + B_{r-1}^3 - B_{r-1}C_{r-1}^2 + uB_{r-1}C_{r-1}^2, \quad (13)$$

that is

$$B_r = B_{r-1}^2 + B_{r-1}^3 + (u-1)B_{r-1}C_{r-1}^2. \quad (14)$$

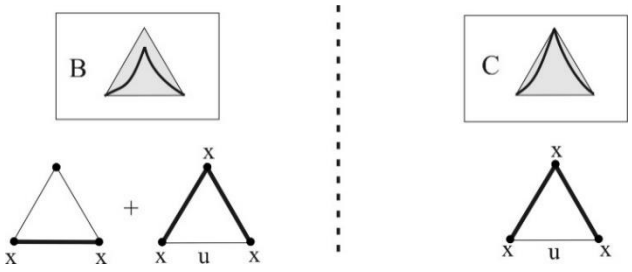

Figure 4. Schematic representation of walks of type B , as well as their subset, the walks C, together with their weighted initial conformations on the unit triangle

This equation involves weights C_{r-1}, for which, by the similar reasoning, recursion relation is established

$$C_r = B_{r-1}^2 C_{r-1} + (u-1)C_{r-1}^3. \quad (15)$$

Initial values for relations (14) and (15) are defined on the unit triangle. In order that each polygon of perimeter N has weight x^N, to each vertex visited by the walks B on the unit triangle, a weight x is assigned. Also, weight u is assigned to contacts. Initial weighted walks are shown in Figure 4, from which their starting weights are given as

$$B_1 = x^2 + x^3u, \quad (16)$$

and

$$C_1 = x^3u. \quad (17)$$

Interaction parameter u enters not only initial values, but also recursion equations (14) and (15). But, defining new variable A_r as $\sqrt{(u-1)}\,C_r = A_r$, these equations become

$$B_r = B_{r-1}(B_{r-1} + B_{r-1}^2 + A_{r-1}^2), \quad (18)$$

and

$$A_r = A_{r-1}(B_{r-1}^2 + A_{r-1}^2), \quad (19)$$

so that interaction parameter is removed. It now enters initial conditions only, which are given with expression (16) for variable B, and with

$$A_1 = x^3u\sqrt{u-1}, \quad (20)$$

for variable A.

3.1. Calculation and results

In order to determine connectivity constant, we first notice that the generating function (12) can be obtained as $G = \lim_{r\to\infty} P_r$, where P_r is defined recursively as

$$P_{r+1} = P_r + \frac{1}{3^{r+1}}(B_r)^3, \quad (21)$$

with the initial value $P_1 = \frac{1}{3}x^3$. Iterating equation (21), together with recurrence equations (18) and (19), starting from their initial values, for each $u \geq 1$ we determine radius of convergence $x_c(u)$ of the generating function and find connectivity constant μ as $\mu(u) = \frac{1}{x_c(u)}$. Numerical results for some chosen values of u are given in Table 1, and overall results are shown graphically in Figure 5.

Table 1. Numerically calculated values of the connectivity constant μ for some values of the interaction parameter u. The last digit is rounded off.

u	1.0	1.5	2	5	10	50	100	200	500
μ	1.618034	1.749171	1.869979	2.483085	3.288930	7.086544	10.00648	14.14508	22.36178

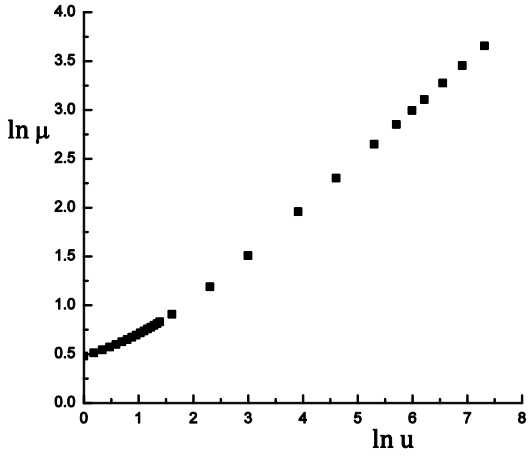

Figure 5. Logarithm of the connectivity constant μ versus logarithm of the interaction parameter u

As one can see in Table 1 and Figure 5, connectivity constant is a monotonically increasing function of the interaction parameter u. Two limiting values of u should be commented on. Firstly, the case $u = 1$ corresponds to $|\varepsilon| = 0$ or $T = \infty$, that is, to non-interacting SAW model, for which connectivity constant has been calculated exactly to be $\mu(u = 1) = \frac{2}{\sqrt{5}-1}$ [25]. Our numerical value agrees with the exact value, and it is calculated with more than twenty significant figures, although only seven are presented. Secondly, limit $u \to \infty$ corresponds to $T \to 0$ or $|\varepsilon| \to \infty$, that is zero temperature or infinite interaction energy limit. At zero temperature, free energy is equal to internal energy, and in the thermodynamic limit it can be expressed as $f = -m|\varepsilon|$, where m is the mean number of contacts. Combining this expression and equation (6), relation $\ln \mu = m \ln u$ can be established. In the next paragraph it would be shown that $m \to \frac{1}{2}$ when $u \to \infty$. Thus, relation $\mu \sim u^{\frac{1}{2}}$ should hold in this limit, from which it follows that connectivity constant increases with u without a bound.

Mean number of contacts, m, given by equation (11) can be obtained as the limit $m = \lim_{r\to\infty} m_r$, where

$$m_r = \frac{u}{x}\frac{P'_{ru}}{P'_{rx}}. \tag{22}$$

In this expression P'_{ru} is a new variable which stands for the partial derivative of P_r with respect to u, i.e. $P'_{ru} = \frac{\partial P_r}{\partial u}$, and similarly $P'_{rx} = \frac{\partial P_r}{\partial x}$. Recursion relations for the new variables are obtained after taking the partial derivatives of equation (21), and are given as

$$P'_{r+1,u} = P'_{ru} + \frac{1}{3^r}(B_r)^2 B'_{ru}, \tag{23}$$

and

$$P'_{r+1,x} = P'_{rx} + \frac{1}{3^r}(B_r)^2 B'_{rx}, \tag{24}$$

where $B'_{ru} = \frac{\partial B_r}{\partial u}$ and $B'_{rx} = \frac{\partial B_r}{\partial x}$ are another two new variables. Recursion relations for these variables are obtained from relation (18), which in turn need two more variables A'_{ru} and A'_{rx} defined similarly as previous variables. In this way, iterating altogether ten recursive equations, starting from the initial values, we obtain mean number of contacts numerically. Results are presented in Table 2 and Figure 6. It should be mentioned that in order to get five significant figures in the value of m, critical value x_c should be calculated with more than twenty significant figures.

Table 2. Numerically calculated values of the mean number of contacts m for some values of the interaction parameter u. The last digit is rounded off.

u	1	5	10	50	200	500	1000	1500
m	0.13383	0.33064	0.41348	0.49299	0.49937	0.49985	0.49995	0.49997

From the Table 2 and Figure 6, one can perceive that the mean number of contacts is monotonically increasing function of the interaction parameter u, which asymptotically tends to the limiting value equal to 0.5. Increasing the value of u, walks with larger number of contacts, with large weights, become more probable, and in the limit $u \to \infty$ only compact walks with maximal number of contacts contribute to the partition function. These self-avoiding walks with maximal number of contacts visit each site of the lattice, so they are Hamiltonian walks by definition. If the coordination number of lattice is q, and we consider a compact polygon or compact open walk, then starting from some visited lattice site (which is not starting or ending point in the case of the open walk) there are $q-2$ nonconsecutively visited nearest neighboring sites. These are contacts shared by two sites, so that the maximal number of contacts per lattice site is $\frac{q-2}{2}$. Coordination number of each lattice site of 3-simplex lattice is 3 (except the three apexes of the largest generator), so that, theoretically, maximal number of contacts is $\frac{1}{2}$. Our calculation shows that this is exactly the $u \to \infty$ limit of the mean number of contacts of the studied ISAP model on 3-simplex lattice. Moreover, this also confirms correspondence between the ISAW model on 3-simplex lattice in the

limit of zero temperature or infinite attractive interaction and the Hamiltonian walk model on the same lattice.

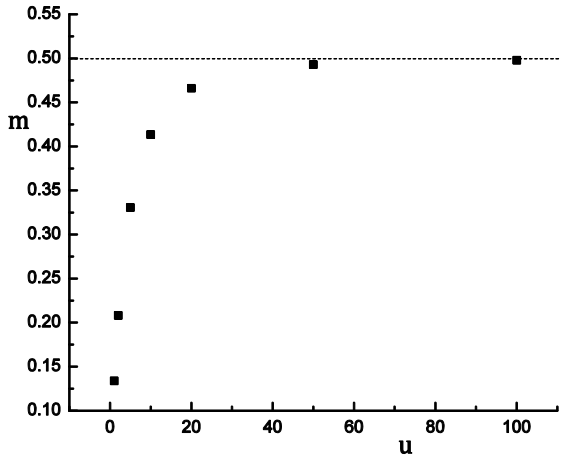

Figure 6. Mean number of contacts m as a function of the interaction parameter u. Horizontal dashed line set at the value $m^* = 0.5$ denotes asymptotic limiting value of m

4. SUMMARY AND CONCLUSIONS

In the present paper we have studied Interacting Self-Avoiding Polygon model on 3-simplex fractal lattice. The model represents a circular polymer in dilute solution which is non-homogeneous and represented by 3-simplex fractal lattice. We have determined dependence of the connectivity constant and the mean number of contacts on the interaction parameter. We have found that the connectivity constant increases boundlessly with the interaction parameter, while the mean number of contacts increases with the interaction parameter, but asymptotically reaches its limiting value of 0.5. This limiting value is the mean number of contacts in the case of Hamiltonian walks on 3-simplex lattice, which confirms that the zero temperature or infinite interaction strength limit of the ISAW model is Hamiltonian walk model. ISAW model on 3-simplex lattice does not undergo a collapse transition at any finite temperature, and compact phase is possible only at absolute zero. It would be very instructive to conduct similar research on some fractal lattices for which it has been proven that the collapse transition exists for non-zero temperature. Such studies could explore the compact phase and resolve the issue of whether the Hamiltonian walk model corresponds to ISAW model in all compact regime, or only at zero temperature. Also, a correspondence between presented theoretical model and a real polymer behavior in non-homogeneous media could be properly examined.

5. ACKNOWLEDGMENT

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НЕУНИВЕРЗАЛНЕ ОСОБИНЕ САМОИНТЕРАГУЈУЋЕГ ПОЛИМЕРА У НЕХОМОГЕНОМ ОКРУЖЕЊУ МОДЕЛОВАНОМ 3-СИМПЛЕКС ФРАКТАЛНОМ РЕШЕТКОМ

Сажетак: Проучавали смо самонепресијецајуће полигоне са привлачном интеракцијом између контаката дефинисаних као неузастопно посјећени сусједни чворови на решетки. Решетка по избору је 3-симплекс фрактална решетка, и модел представља прстенасти полимер у нехомогеном растварачу чији квалитет зависи од интеракционог параметра. Примјеном методе ренормализационе групе, до сада је показано да се полимер на тој решетки и било којој ненултој температури може налазити само у проширеној фази. Универзални критични експоненти, који не зависе од јачине интеракције, такође су одређени. Нас у овом раду занимају двије неуниверзалне величине: константа повезаности која одређује слободну енергију модела и средњи број контаката који одређује унутрашњу енергију. Показали смо да је константа повезаности неограничено растућа функција јачине интеракције, док је средњи број контаката растућа функција која се асимптотски приближава граничној вриједности једнакој једна половина, што је заправо средњи број контаката за случај Хамилтонових шетњи на истој решетки. Та гранична вриједност је и очекивана, јер у лимесу бесконачне интеракције (или нулте температуре) свака самонепресијецајућа шетња на 3-симплекс решетки постаје максимално компактна и посјети све чворове решетке, тј. постаје Хамилтонова шетња.

Кључне ријечи: полимер, самонепресијецајући полигон, фрактал, неуниверзалне особине.

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