CONTEMPORARY MATERIALS 2020, BANJA LUKA , 10-11 SEPT. 2020.

NONUNIVERSAL PROPERTIES OF SELF-INTERACTING POLYMER IN NON-HOMOGENEOUS ENVIRONMENT

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ABSTRACT

Non-universal properties of Interacting self-avoiding polygon model have been studied on 3-simplex fractal lattice. Generating function of self-avoiding polygons with self-attraction has been established recursively. Analysis of the generating function has enabled determination of the connectivity constant and the mean number of contacts as functions of the interaction parameter. It is found that both quantities are monotonically increasing functions of the interaction parameter: connectivity constant increases without bounds, while the mean number of contacts asymptotically tends to its limiting value of one-half.

INTRODUCTION

Self-avoiding walks (SAWs) are random walks that never visit the same lattice site more than once. Self-avoiding polygons (SAPs) are SAWs with starting and ending point that coincide. They are used as models of linear (SAWs) and ring (SAPs) polymers in good solvent conditions [1]. Collapse transition of ring polymers can be captured by the Interacting self-avoiding polygon (ISAP) model, obtained from the ordinary SAP model by introducing an attractive interaction between non-consecutively visited nearest neighboring sites, which are called contacts [2]. The central quantity of the ISAP model is the generating function of interacting SAPs of a variable length N:

$$G(x,u) = \sum_{N=0}^{\infty}\sum_{M=0}^{M_{max}} C_N(M)u^M x^N, \qquad (1)$$

where x is the weight of each step, u is the interaction weight (parameter) and M is the number of contacts in each particular polygon. An example of square lattice self-avoiding polygon with attractive interaction between contacts is shown in Figure 1.

Here we study non-universal properties of ISAP model on hierarchically constructed 3-simplex fractal lattice. One self-avoiding polygon with attractive interaction between contacts, on the structure obtained in third stage of construction, is shown in Figure 2.

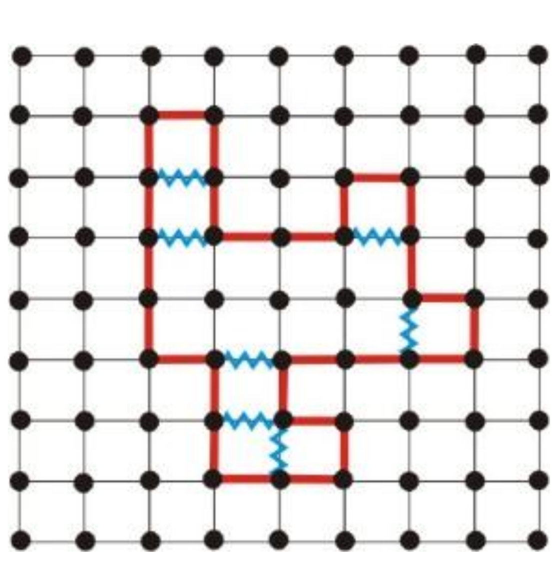


Figure 1. Self-avoiding polygon with N=26 steps and M=7 contacts, on the square lattice. This polygon contributes to the term $x^{26}u^7$ in the generating function (1). Blue, wiggly lines represent attractive interaction between contacts.

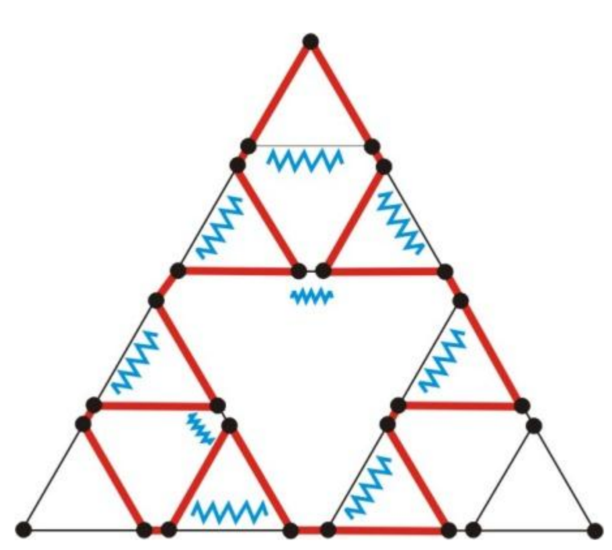


Figure 2. An example of self-avoiding polygon with self-attraction on the third order generator of 3-simplex fractal lattice. This polygon consists of N=23 steps and has M=9 contacts.

METHOD

Self-similarity of 3-simplex lattice enables recursive determination of the generating function for interacting SAPs [3,4] :

$$G(x,u) = \frac{1}{3}x^3 + \sum_{r=1}^{\infty}\frac{1}{3^{r+1}}(B_r(x,u))^3, \qquad (2)$$

which is illustrated in Figure 3. Open walks denoted as B and C, necessary for construction of closed walks, are schematically shown in Figure 4 together with the initial walks. Recursive relations for the weights of walks B and C are given by

$$B_r = B_{r-1}^2 + B_{r-1}^3 + (u-1)B_{r-1}C_{r-1}^2; \quad B_1 = x^2 + x^3u, \qquad (3)$$

and

$$C_r = B_{r-1}^2 C_{r-1} + (u-1)C_{r-1}^3; \qquad C_1 = x^3u. \qquad (4)$$

Connectivity constant μ for each u is calculated from the generating function (2) as $\mu(u) = \frac{1}{x_c(u)}$, where $x_c(u)$ is the radius of convergence of series given with (2). Mean number of contacts m is calculated as

$$m = \frac{u}{x}\frac{\frac{\partial G}{\partial u}}{\frac{\partial G}{\partial x}},$$

for each u at the corresponding value of x_c.

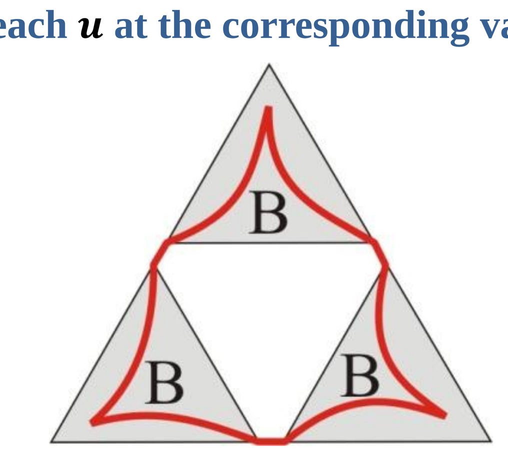


Figure 3. Scheme for recursive determination of weights of all polygons on 3-simplex lattice.

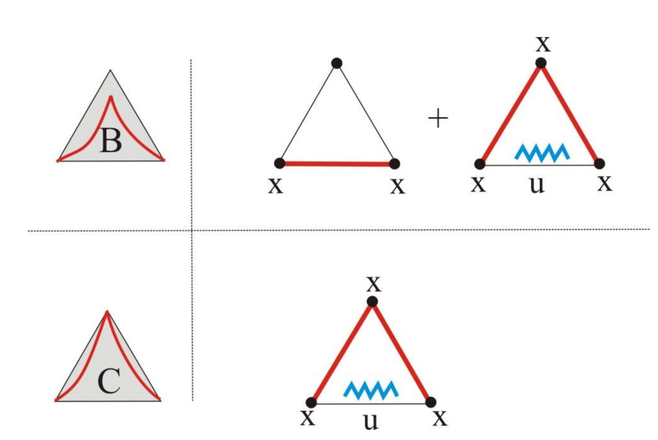
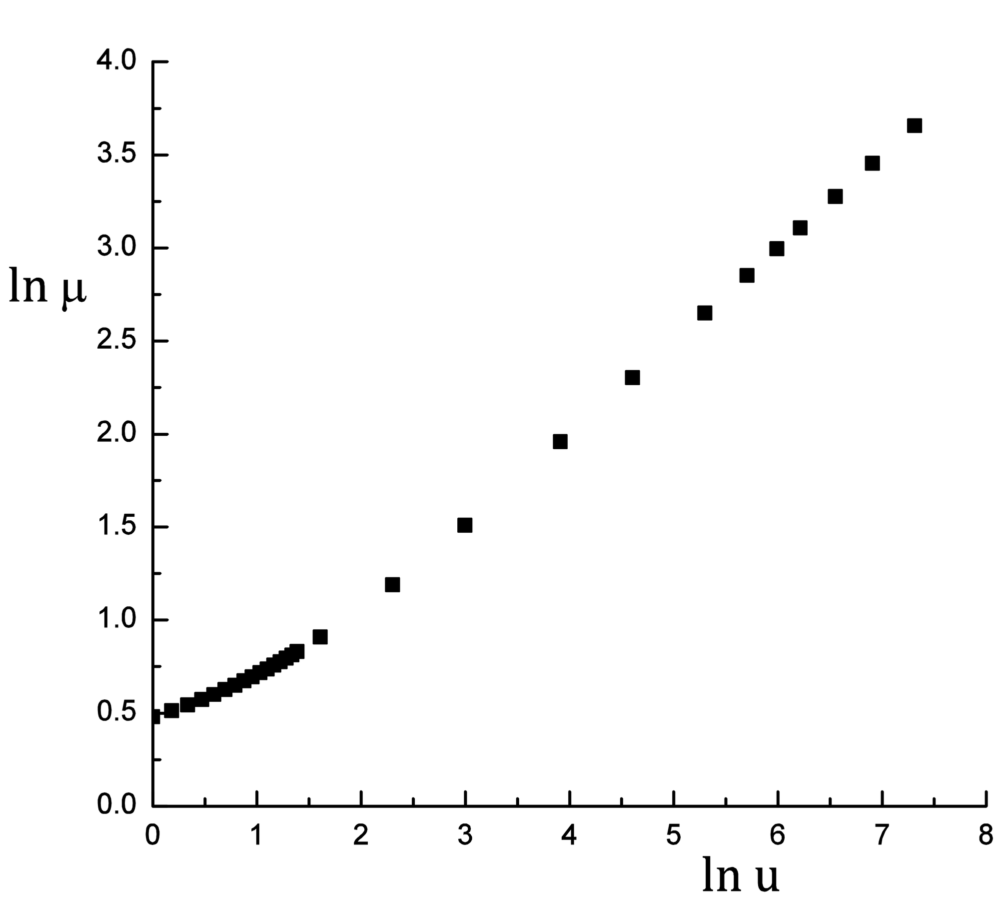
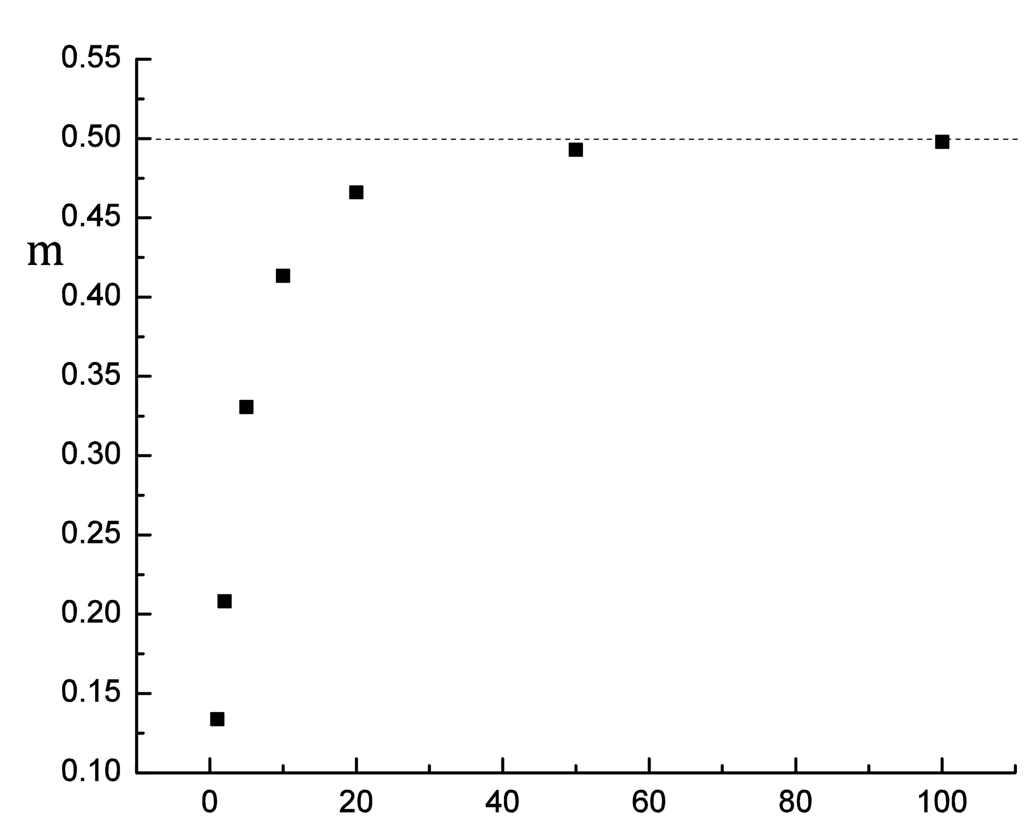


Figure 4. Schematic representation of B and C type of walks on the generator of any order, and B and C walks on the unit triangle from which initial weights in equations (3) and (4) follow.

RESULTS



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



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.

CONCLUSIONS

Connectivity constant increases without bounds as $u \to \infty$, and, in this limit, relation $\mu \sim u^{\frac{1}{2}}$ holds. Mean number of contacts tends to $^1/_2$ as $u \to \infty$, which is Hamiltonian walk limit. This is a conformation of the correspondence between $u \to \infty$ (zero temperature) limit of the ISAP model and Hamiltonian walk model. Our next goal is to investigate whether this correspondence holds in the whole compact regime, on fractal lattices where compact phase exists at nonzero temperatures.

REFERENCES

[1] N. Madras and G. Slade, *The Self-Avoiding walk*, Birkhaüser, Boston, 1993. **[2]** C. Vanderzande, *Lattice models of polymers*, Cambridge University press, Cambridge, 1998. **[3]** D. Dhar and J. Vannimenus, *The collapse transition of linear polymers on fractal lattices*, J. Phys. A: Math. Gen 20 (1987) 199-213. **[4]** D. Dhar and Y. Singh, *Linear and branched polymers on fractals*, in Statistics of linear polymers in disordered media, edited by B. K. Chakrabarti, Elsevier B. V., Amsterdam, The Netherlands, 2005, 149-195.