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SEMI-FLEXIBLE INTERACTING SELF-AVOIDING POLYGONS ON 3- SIMPLEX LATTICE

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ABSTRACT

A model of interacting self-avoiding polygons with bending stiffness is studied on a fractal, 3-simplex, lattice. The model captures the main features of a semi-flexible ring polymer with attractive interactions between non-bonded nearest neighboring monomers adsorbed on a non-homogeneous substrate. Analysis of the recurrence equations on the 3-simplex lattice shows that the model, on this lattice, describes a polymer which is in an extended, random-coil phase in the whole temperature regime. In order to get a better insight into the structure of the conformations, we have extended our study [1] of the number of contacts in the interacting self-avoiding walk model, and focused, here, on the influence of the stiffness on the number of contacts. We found that for fixed interaction strength, the number of contacts is a non-monotonic function of stiffness. Specifically, it decreases with stiffness at first, but eventually, it starts to increase for very stiff polygons.

INTRODUCTION

Self-avoiding walks (SAWs) on a lattice are random walks that may visit some lattice site at most once. They are customary used as a model of linear polymer conformations in solution at high temperatures [2]. By implementing ordinary SAW model with attractive interactions between contacts, i.e., visited sites that are nearest neighbors but not adjacent along the walk (which mimics different solvent qualities) and with an energy penalty for each bend in the walk (which mimics some degree of rigidity of natural polymers), one gets a Semi-flexible interacting self-avoiding walk model (SFISAW). If, instead of open walks, polygons (closed walks) are used, the model represents a ring polymer and is abbreviated as SFISAP.

The simplest lattice where this full model can be studied is the 3-simplex lattice, a finitely ramified fractal lattice on which the weights of the walks can be determined recursively. On this lattice, reduced models: self-avoiding walks (ordinary), interacting self-avoiding walks and semi-flexible self-avoiding walks have already been studied in [3], [4,1] and [5], respectively. In the current paper, we extend our previous study [1], and analyze the full SFISAP model.

METHOD

We use a recurrence scheme for the determination of the generating function, which represents the weighted sum over all different polygons of all possible perimeters, on an, in the limit, infinite lattice. The 3-simplex lattice is constructed iteratively, in steps, and the structure obtained in the *r*-th step is called the *r*-th order generator. One polygon on the third order generator is shown in Figure 1, where the Boltzmann weight factors *u* and *s*, associated with the attractive interaction and bending energy, respectively, are also depicted. In Figure 2, we show six types of the walks that are necessary for the enumeration of all polygons and the determination of their overall weights as well as the generating function. The weights of these six walks (restricted generating functions) are determined recursively. In the context of the renormalization group (RG) approach, these recurrence relations become exact RG equations. Analysis of the fixed points of the equations enables determination of the phases and the critical exponents, whereas numerical iteration gives the values of the non-universal quantities.

We find, by inspection, that the generating function of the SFISAP model on the 3-simplex lattice can be expressed as:

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

where A_{3r} (x,u,s) represents the weight of all walks that traverse 3-simplex generator of order *r* and which may or may not visit its third vertex. This type of the walk, denoted as A_3, is depicted in the first row of Figure 2, where all six types of the walks are shown schematically and where one can notice that the walks are also classified according to the direction of the steps before they enter and leave the generator.

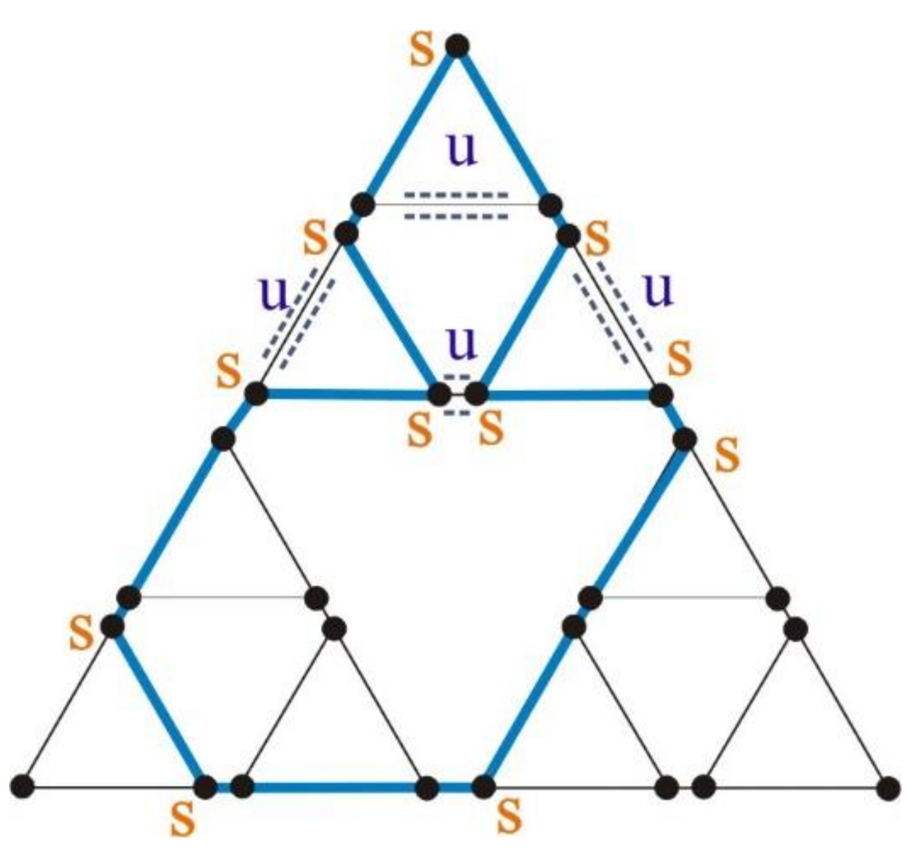


Figure 1. *Self-avoiding polygon on the third order generator of the 3-simplex lattice. Attractive interactions between contacts are marked with double blue dashed lines and weighted with the Boltzmann factor u. Each turn of the walk is weighted with the factor s and assigned to the vertex at which the turn is made. Finally, to each step of the walk the weight x is assigned, so that this polygon contributes term $x^{19}u^4s^{11}$ to the sum given by (1).*

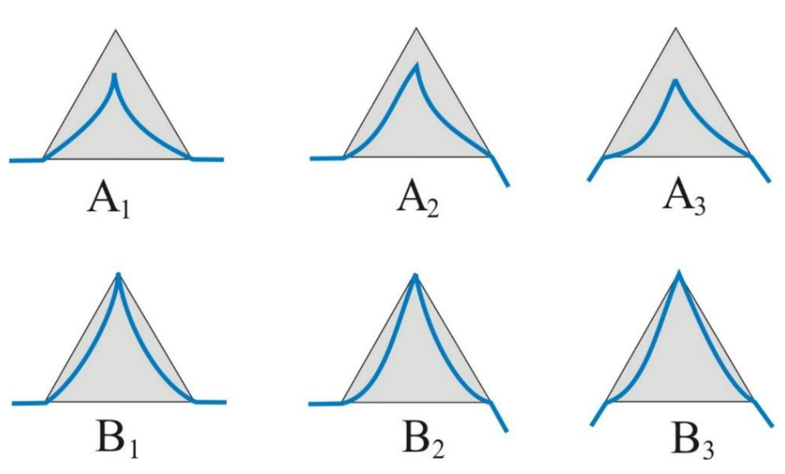
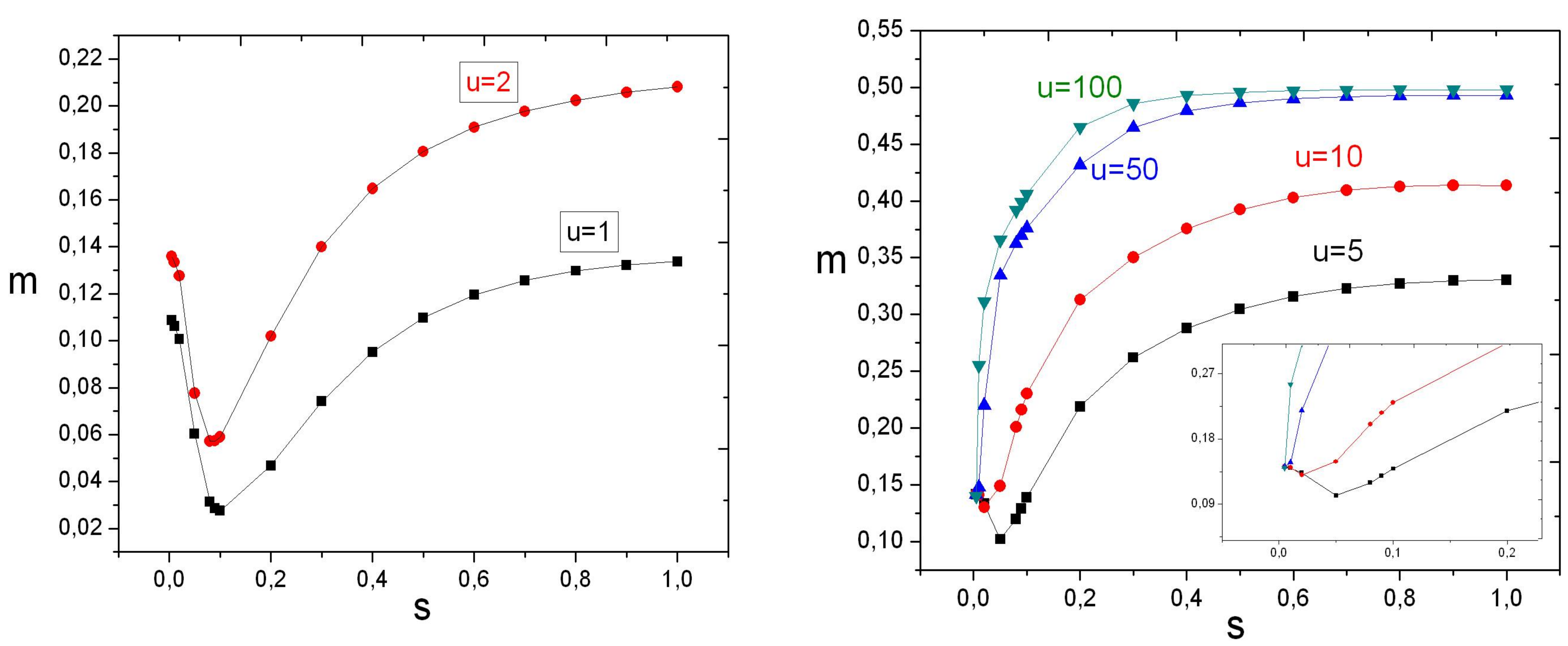


Figure 2. *Schematic representation of the walks necessary for the determination of the generating function given by (1). Walks are classified according to the number of visited corner vertices (A and B) and the direction of the steps with which they enter and leave the triangle (1,2, and 3).*

RESULTS AND DISCUSSION



Graph 1. The mean number of contacts m per step of the polygon, as a function of the stiffness parameter s for fixed, various values of the interaction parameter u. Low values of s correspond to large stiffness and a very stiff polymer ($s \to 0$ is the rigid rod limit).

- The mean number of contacts per step is a non-monotonic function of stiffness and stiffness parameter *s*, as can be seen in Graph 1.
- For fully flexible rings ($s = 1$), values of *m* for various interaction parameters *u*, coincide with those calculated in [1]. By decreasing the stiffness parameter *s* (increasing the stiffness), *m* decreases until it reaches a minimum value for some value of *s* depending on *u*, and then, counterintuitively, starts to increase.
- Non-monotonic behavior of *m* is also found in [6], where the SFISAW model was studied on a simple cubic lattice. However, this non-monotonicity is related to the onset of the different phase regime, while here, there is only an extended (swollen) phase.
- This result might imply that the stiffness promotes collapse transition, and the effect should be studied more thoroughly on fractal lattices which allow for it.

REFERENCES

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