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Semi-flexible compact polymers on fractal lattices

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ABSTRACT

Semi-flexible compact polymers modeled by Hamiltonian walks with bending rigidity are studied on 3 and 4-simplex fractal lattices. Hamiltonian walks are weighted according to the number of bends in the walk, and total weights are obtained by an exact recursive treatment. Asymptotic form of the partition function, with temperature dependent scaling parameters, as well as the corresponding critical exponents, is determined. Various thermodynamic quantities are calculated numerically and presented graphically, and the possibility of phase transition between a compact molten globule and an ordered 'crystal' state is investigated. No phase transition is found on either of these two lattices, meaning that fractal geometry here prevents any kind of orientational order.

1. Introduction

Flexible linear polymer in solution can exploit quite different parts of conformational space depending on the solvent quality and/or temperature [1]. In a good solvent or at high temperatures, excluded volume interactions prevail and polymer takes extended 'random coil' conformations which are usually well described by self-avoiding random walks (SAW) i.e. random walks without intersections. At some lower, the so called θ temperature, polymer collapses, it undergoes phase transition into the low temperature compact phase. This happens when attractive monomer–monomer interactions mediated by the solvent cause polymer to shrink and take compact, globular conformations, expelling the solvent molecules out from the globule. The low temperature phase is 'liquid' like and still with large entropy.

In order to mimic real polymer behavior, various lattice models are introduced [2], and particularly the collapse transition is captured by the Interacting self-avoiding walk (ISAW) model, where attractive interaction between neighboring, nonconsecutive bonds in the walk is incorporated in the ordinary SAW model. However, bio-polymers such as DNA or proteins are not flexible, their persistence length L_p is comparable with the contour length L, i.e. $L_p \sim L$, in contrast to flexible polymers for which $L_p \ll L$, or rigid-rod polymers for which $L_p \gg L$. Polymer stiffness, or its resistivity to making bends, can be introduced into the ISAW model by adding an energy penalty to each bend in the conformation. The obtained model is a semi-flexible ISAW model whose analysis [3–7] showed the existence of an ordered compact crystal phase besides the extended and compact disordered phase. The full phase diagram of semi-flexible polymer reveals that the polymer can undergo collapse transition followed by 'freezing' transition into the crystal phase by lowering the temperature, or it can 'freeze' directly from the extended phase when bending energy becomes large enough. As for the order of phase transitions, it is shown that transitions from both other phases to the crystal phase are of first order in three dimensional space [3,4], while in two dimensions, coil–crystal transition stays first order and the globule–crystal transition becomes second order, as found in Ref. [7].

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surface sites, so that the exponent σ should take on the value equal to $(d-1)/d$. The stretched exponential factor also appears on fractal lattices, and the reason for its appearance is not in the boundary sites, but is in the sites which are loosely connected via Hamiltonian walks and are designated as 'maximally isolated sites' in Ref. [31].

Free energy of the SHW model on 4-simplex lattice is an analytic function of temperature which excludes the possibility of finite order phase transition. The first derivative of free energy determines persistence length which is a continuous, monotonically decreasing function of stiffness weight, as we see in Fig. 13(b). This is a reasonable result, since for small s bends are rare and there are many steps between them, while for larger s bends become more frequent with fewer steps in between. Specific heat, as a second derivative of free energy, is shown in Fig. 14, where a smooth peak is displayed. This maximum does not change with the length of the walks so it does not signal any divergency in specific heat. It is, as we think, the characteristic peak of systems with a finite number of discrete energy levels, i.e. anomaly of the Schottky type.

Finally, we return to the ground state of our model, which is highly degenerate since there is an exponentially large number of ground state conformations. The SHW model on 4-simplex lattice belongs to the class of geometrically frustrated systems (see for example Ref. [32]). Minimization of energy and compactness of the walks are in conflict with 4-simplex geometry since in order to minimize energy, the polymer should be arranged in long, straight segments with bends on the lattices' edges only, but this cannot be fulfilled on 4-simplex lattice if the constraint of Hamiltonian walks is to be preserved. This is not the case with the SHW model on square lattice, where ground state conformations consists of all parallel segments whose length is equal to the linear dimension of the lattice and degeneracy is only two-fold due to two possible directions of segment orientations. There are no bends on any unit square in the interior of square lattice, while on each unit square of 4-simplex lattice there are at least two bends. Although 4-simplex lattice is similar to square lattice in the sense that they both have coordination number of four and the fractal dimension of 4-simplex lattice is two, 4-simplex lattice is highly anisotropic and any kind of ordered or even 'quasi' ordered state on this lattice is impossible. To conclude, we can say that the compact phase on 4-simplex lattice can exist in a disordered, 'liquid' like phase only, which is in accordance with the results for the semi-flexible ISAW model on 4-simplex lattice, obtained in Ref. [29], where the crystal phase was not found either.

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