外国語要旨

Knot probabilities and scaling exponents of ring polymer chains: effects of topology and excluded volume

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Polymers with various topologies have been successfully synthesized and a dilute solution of ring polystyrenes has been purified with high level in the last decade. A ring polymer has topological isomers: there are a number of topologically different knotted ring polymers. It is an interesting question how much a dilute solution of ring polymers contains non-trivial knotted polymers and how the topological effects change the physical properties of knotted ring polymers.

The purpose of this thesis is to characterize the nature of knotted ring polymers through simulation. We generated the random polygons (RP) and the self-avoiding polygons (SAP) consisting of cylindrical segments by Monte-Carlo method. RP and SAP are the simplest models of a ring polymer in a dilute solution, where the excluded volume effect approximates the screening effect due to counter ions in the solvent. We detected their knot types and estimated the knot probability and the radius of gyrations of knotted RP and knotted SAP. The knot probability is defined by the probability of a given RP or SAP having a specified knot type.

Knot probability

We introduced a new formula for knot probability of RP or SAP:

$$\mathrm{P}(N;r,K) = C_K x^{m(K)-1/2-x}\Gamma(x+1),$$
$$x = \frac{N}{N_K}.$$

where N is the number of segments of RP or SAP. Here one of the segment corresponds to such a part of a ring polymer that has length equal to the persistence length. Here r is the radius of cylinders of SAP and K expresses the type of a given knot. The formula has 3 parameters: the characteristic length N_K, the coefficient C_K, the index $m(K)$.

Our formula well explains the knot probability as a function of N for N is not much smaller than N_K. Here N_K is almost the same for any knot K and grows exponentially as r increases. The best estimates of $m(K)$ is close to an integer. If K is given by a prime knot, the best estimates of $m(K)$ is close to 1. If it is a composite knot, $m(K)$ is close to the number of the constituent prime knots.

For the knot probability of a prime knot, only C_K depends on K. And C_K and N_K depend on radius r. Thus if we normalized N with N_K, there is only one parameter for the formula: C_K.

Radius of gyration

The mean square radius of gyration of a polymer $\langle R_g^2 \rangle$ in a solution obeys the scaling law with the number of monomers N: $\langle R_g^2 \rangle \propto N^{2\nu}$, where ν is the scaling exponent.

ν is 0.5 for a ring polymer without topological constraint in Θ solvent, 0.59 for a ring polymer in good solvent. Here the phrase "without topological constraint" means that we estimate the statistical value of ring polymers whose topology contains all of possible knot types.

If we take ring polymers which have a given knot type, their mean square radius of gyration is different from that of ring polymers without topological constraint. The mean square radius of gyration of ring polymers with 0_1 knot is the largest in the all knot types. That of ring polymers with 3_1 knot is the second largest. We know little of the scaling exponent for ring polymers with topological constraint. We calculated the mean square radius of gyration of RP and SAP with various knot types and evaluated the best estimates of the effective scaling exponent of knotted RP and SAP.

References

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