Statistical and Hydrodynamic Properties of Graph-shaped Polymers and Quaternions

Tetsuo Deguchi
Ochanomizu University

We study statistical and hydrodynamic properties of graph-shaped polymers, which we call topological polymers, by applying the quaternion method for generating random polygons. We first review topological polymers such as double-ring polymers, tadpole polymers (lassos), and complete bipartite graph polymers, which are synthesized in chemistry. For simplicity, we regard ring polymers as topological polymers. We introduce the algorithm for generating random walks connecting given two points in the three-dimensional space, based on the Hopf map of quaternions [1, 2]. Surprisingly, the computational time of the algorithm is proportional to the number of steps in the random walks, that is, it gives a linear-time algorithm [1]. We compare the results of ideal topological polymers with those of real topological polymer obtained by the molecular dynamical simulation of the Kremer-Grest model. We suggest that for such graphs consisting of only up to trivalent vertices the statistical and hydrodynamic properties of ideal topological polymers are similar to those of the corresponding real topological polymers [2]. Finally, we also suggest enhancement of intra-chain two-point short-distance correlation for real topological polymers [2]. The talk is based on the collaboration with J. Cantarella, C. Shonkwiler and E. Uehara.

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