Exact approach to the elasticity of phantom polymer networks via application of homology

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Abstract

Phantom network theory is fundamental in the study of the elastic behavior of polymer networks such as rubbers and gels in statistical mechanics. In this talk we present a theoretical method for calculating the shear modulus rigorously for phantom networks associated with periodic lattices such as the diamond, simple cubic and body-centered cubic lattices, etc. The connectivity structure of a given network is expressed by a simple graph, where its vertices and edges are called cross-links and chains (or network chains), respectively, in polymer physics. In phantom networks each chain corresponds to a constrained Gaussian random walk connecting a pair of cross-links, while there is no interaction among different chains. The connectivity of network chains may lead to nontrivial constraints on them. However, by taking advantage of homology, we generate all sets of chains satisfying the constraints, and derive network configurations with proper loops (i.e., three-dimensional embeddings of the graph) by making no cross-links fixed. We thus obtain the rigorous method for calculating the network elasticity since there are no fixed cross-links. In all the previous studies of phantom networks the positions of some cross-links are fixed in order to make the partition function finite, while it could make the theoretical approach to the elasticity quite nontrivial. This work is in collaboration with Jason Cantarella, Clayton Shonkwiler and Erica Uehara.