

THE KNOT SPECTRUM OF CONFINED RANDOM EQUILATERAL POLYGONS

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Preprint no. 2013-15

Abstract

It is well known that genomic materials (long DNA chains) of living organisms are often packed compactly under extreme confining conditions using macromolecular self-assembly processes but the general DNA packing mechanism remains an unsolved problem. It has been proposed that the topology of the packed DNA may be used to study the DNA packing mechanism. For example, in the case of (mutant) bacteriophage P4, DNA molecules packed inside the bacteriophage head are considered to be circular since the two sticky ends of the DNA are close to each other. The DNAs extracted from the capsid without separating the two ends can thus preserve the topology of the (circular) DNAs. It turns out that the circular DNAs extracted from bacteriophage P4 are non-trivially knotted with very high probability and with a bias toward chiral knots. In order to study this problem using a systematic approach based on mathematical modeling, one needs to introduce a DNA packing model under extreme volume confinement condition and test whether such a model can produce the kind of knot spectrum observed in the experiments. In this paper we introduce and study a model of equilateral random polygons confined in a sphere. This model is not meant to generate polygons that model DNA packed in a virus head directly. Instead, the average topological characteristics of this model may serve as benchmark data for totally randomly packed circular DNAs. The difference between the biologically observed topological characteristics and our benchmark data might reveal the bias of DNA packed in the viral capsids and possibly lead to a better understanding of the DNA packing mechanism, at least for the bacteriophage DNA. The purpose of this paper is to provide information about the knot spectrum of equilateral random polygons under such a spherical confinement with length and confinement ratio in a range comparable to circular DNAs packed inside bacteriophage heads.