Lattice models of Polymers with applications to DNA topology experiments

Chris SOTEROS（University of Saskatchewan）

Abstract

Due to their conformational freedom, it was conjectured in the 1960s by Frisch and Wasserman and by Delbruck (FWD) that long polymers in solution should be knotted (self-entangled) with high probability. DNA is a large molecule with conformational freedom and knots and links have been observed in experiments on DNA. Knots and links however are obstructions to normal cellular processes such as replication and hence understanding the entanglement statistics of polymers and in particular DNA is an important area of study for polymer modellers. Lattice polygon models of ring polymers were an important starting point for such models and they have proved useful for answering fundamental questions about polymer and DNA topology. Indeed the FWD conjecture was first proved using a lattice polygon model (by Sumners and Whittington and by Pippenger in 1988). Many questions remain open about the details of the knot and link distribution and also the typical "size" of the knotted or linked parts for lattice polygon models. After a general overview of these topics, I will discuss two directions of recent research.

One direction involves developing improved lattice models for modelling the 1993 DNA knot probability experiments due to Shaw and Wang and to Rybenkov et al.

With M Schmirler, we recently developed a lattice model with a short-range bending rigidity term and a long-range screened Coulomb potential that fits well with the Shaw and Wang knot probability results for varying salt concentrations and which yields estimates of knot probabilities for varying DNA lengths that are comparable to those of the off-lattice model of Rieger and Virnau (2016).

Persistence length measurements for our lattice model are consistent with those reported for DNA. This is an improvement over earlier lattice models which were based on a short-range nearest-neighbour contact interaction. Motivated by DNA nano-channel experiments, another direction involves using lattice models to study the knot and link statistics for polygons confined to a tubular sublattice. We have previously provided strong evidence that the scaling form for the number of n-edge embeddings of a knot or link L in a simple cubic lattice tube is consistent with the 1990's conjectured scaling form for unconfined lattice polygons and consistent with knot and link localization. Recently we have focussed in on the region where two polymers under confinement are overlapping. For this, we considering two polygons (2SAPs) in a lattice tube which each span the same length of the tube. Forcing the two polygons to overlap ensures that all but exponentially few are linked, an FWD style result for linking.

This was previously proved for 2SAPs in large enough tubes and we have recently proved that it holds for all tube sizes which admit non-trivial links. We have also explored the link distribution as a function of tube size as well as, for fixed link-types, the characteristics of typical conformations. The work on 2SAPs is jointwork with J Eng, P Pongtanapaisan and R Scharein.