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Optimizing Lattice Polygon Models to DNA Experimental Knotting Probabilities

We present here the results of optimizing two different lattice models of DNA, where model parameters are tuned by fitting to DNA experimental knotting probabilities obtained by Shaw and Wang (Science, 1993). The resulting knotting probability fits are of similar quality for both models; however, we observe that the model containing a short-range bending potential has a persistence length that is much more agreeable to that of DNA. We next study how knotting probabilities in this optimized bending model change with varying DNA length, where we find remarkable agreement with knotting probability results obtained from an optimized off-lattice freely-jointed chain model.