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Twisted bundle model for DNA toroidal condensates

We consider a model of DNA toroidal condensate that corresponds to a twisted bundle arrangement and compare it to other models of the chain conformation inside the condensate. The latter models correspond to those of a spool-like folding and a constant curvature bending. The ground states of the condensate in different models are obtained by minimizing a total energy given by the sum of the bending energy and a surface energy promoting compaction. It is shown that for the condensates of the same polymer length, the twisted bundle model leads to a lower ground state energy than both the spool model and the constant curvature model. A phase diagram of ground states depending on the chain length and the polymer stiffness is calculated for toroidal and rod-like condensates. We study also the curvature distribution and the thickness to radius ratio in optimal toroid condensates. Our study highlights the role of the twist geometry in DNA packing. The analytical results are supported by Monte Carlo simulations of a bead and spring model.

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