

DNA phase transitions in tension and torsion

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The DNA molecule has been modeled for long as an elastic rod capable of resisting stretching, bending and torsion. Indeed, experiments over the last two decades have revealed that DNA undergoes several phase transitions depending on the tension, twist and temperature. In this talk we will focus on two phase transitions -- the B-DNA to L-DNA transition and the B-DNA to S-DNA transition. To model the first transition we will use a fluctuating rod model in which we allow the DNA molecule to have a few possible values of the twisting and bending moduli. This type of situation presents itself when binding of small molecules (for example, intercalators) to DNA can modify the local mechanical properties. Regions of different moduli are also present on the same DNA molecule when it undergoes phase transitions from B-DNA into Z-DNA or L-DNA under high tension and negative twist. One key result of our analysis in this context is that L-DNA could be a mixture of Z-DNA and S-DNA with the fraction of each phase depending on the ion concentration. We will also discuss a non-equilibrium version of this phase transition in which interfaces with discontinuities in both stretch and twist propagate along the DNA. We will use a simple kinetic law to describe the motion of this interface and show that we can easily recover the data in several experiments. Using this model we confirm our argument the L-DNA is indeed a mixture of Z-DNA and S-DNA. The second transition from B-DNA to S-DNA is known as the overstretching transition. To model the second transition we think of dsDNA as a chain composed of n segments of length l , where the transition is studied by means of a Landau quartic potential with statistical fluctuations. The length l is a measure of cooperativity of the transition and is key to characterizing the overstretched phase. By analyzing the different values of l corresponding to a wide spectrum of experiments, we find that for a range of temperatures and ionic conditions, the overstretched form is likely to be a mix of M-DNA and S-DNA. For a transition close to a pure S-DNA state, where the change in extension is close to 1.7 times the original B-DNA length, we find l is approximately 25 base-pairs regardless of temperature and ionic concentration. Our model is fully analytical, yet it accurately reproduces the force-extension curves, as well as the transient kinetic behavior, seen in DNA overstretching experiments.