Discontinuities at the DNA supercoiling transition

Bryan C. Daniels[1], Scott Forth[1], Maxim Y. Sheinin[1], Michelle D. Wang[1,2], and James P. Sethna[1]

***Short Abstract* — Twisting a single molecule of DNA at constant applied force, a recent experiment resolved a sudden transition to a state with a lower end-to-end distance (extension). This comes from the formation of a supercoiled structure known as a plectoneme, and the extension jump at the transition can be connected to the extra free energy and length required to form the "end loop" of the plectoneme. We use experimental data to determine these parameters, and compare them to various model predictions. We also predict a jump in torque at the transition, which is validated by further analysis of the experimental data.**

***Keywords* — DNA, plectonemes, polymer physics, phase transitions, entropy**

I. Purpose

MUCH like a rope or garden hose, as a single molecule of DNA is twisted, it eventually begins to wrap around itself to form a superhelical twisted structure known as a plectoneme. This effect is seen in single molecule experiments by measuring the end-to-end distance (extension) as a function of added turns, while holding constant the applied force along the DNA. For small added turns, the extension remains relatively constant, whereas once a plectoneme has formed, the extension linearly decreases with increasing turns [1]. It is known that this state can be understood as a coexistence between usual extended DNA and supercoiled plectonemic DNA [2]. Analogously to liquid-gas phase coexistence, where decreasing the volume linearly converts gas to liquid, here adding turns linearly converts straight to plectonemic DNA.

Recently, a jump in the extension was observed at the transition when the plectoneme first forms [3]. In the phase transition analogy, this jump comes from the interface between the two phases, which requires extra free energy and extension; here the interface corresponds to the "end loop" and "tails" of the plectoneme.

II. Results

Using the phase coexistence model, we have calculated the relevant parameters of the interface and explored their subsequent predictions. We have also tested various DNA elasticity models that predict values for the measured parameters.

A. Torque jump

At this abrupt transition, we also expect a jump in the torque, and can predict its size. We find that further analysis of the experimental data reveals a torque jump that agrees with the expected sign and size.

B. Length-dependence

We predict that the size of the extension jump should increase slightly with increasing overall DNA length. Although this is not discernable in the current experiments, we expect that future experiments should be able to resolve this length-dependence.

C. End-loop models

We expect that the interface should behave mostly like an extra circular loop of DNA. However, using this simple model does not account for the large size of the extension jump at low forces. Attempting to more faithfully match the equilibrium shape of the plectoneme, we implemented an elastic rod model that successfully forms superhelical plectonemes, but it does not seem to help the agreement at low forces.

D. Entropic effects

Since thermal fluctuations are important at this scale, we have explored the effects of entropic contributions to the free energy. We also tested the possibility that multiple plectonemes are forming: we find that this is unlikely in our experiment, but may become important for experiments using longer DNA.

III. Conclusion

A natural generalization of Marko's phase coexistence model predicts a torque jump and length dependence of the extension jump, and motivates going beyond simple elastic DNA models in order to better match the data at low applied force.

Acknowledgments: Support is acknowledged from NSF Grants DMR-0705167 and MCB-0820293, NIH Grant GM059849, and the Cornell Nanobiotechnology Center.

[1]Laboratory of Atomic and Solid State Physics, Physics Department, Cornell University, Ithaca, NY. E-mail: bdaniels@physics.cornell.edu

[2]Howard Hughes Medical Institute, Cornell University, Ithaca, NY.

References

[1] Strick TR, et al. (1995) The Elasticity of a Single Supercoiled DNA Molecule. *Science* **271**, 1835.

[2] Marko JF (2007) Torque and dynamics of linking number relaxation in stretched supercoiled DNA. *PRE* **76**, 021926.

[3] Forth S, et al. (2008) Abrupt Buckling Transition Observed during the Plectoneme Formation of Individual DNA Molecules. *PRL* **100**, 148301.