Discontinuities at the DNA supercoiling transition

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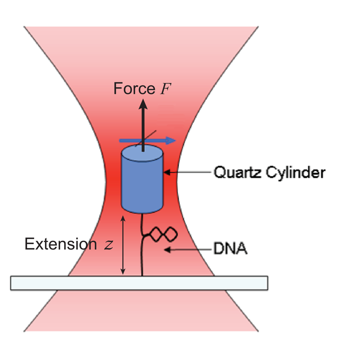
What determines the magnitude of jumps at the supercoiling transition?

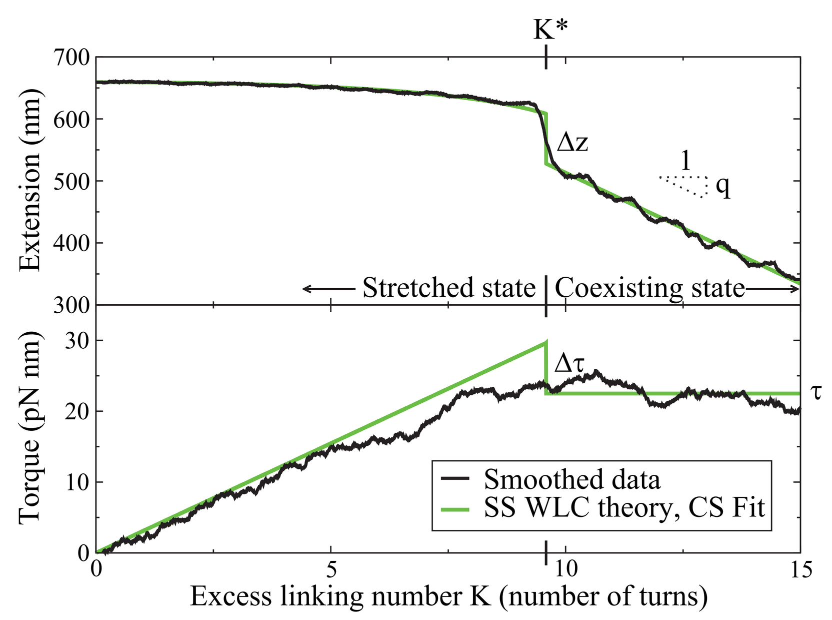
While slowly turning the ends of a single molecule of DNA at constant applied force, a discontinuity was recently observed at the supercoiling transition, when plectonemic DNA is suddenly formed [1].

This can be understood as an abrupt transition into a state in which stretched and plectonemic DNA coexist. We argue that there should be discontinuities in both the extension and the torque at the transition, and provide experimental evidence for both. To predict the sizes of these discontinuities and how they change with the overall length of DNA, we organize a theory for the coexisting plectonemic state in terms of four length-independent parameters. Testing various simple models, we find discrepancies with experiment that can be understood in terms of the four coexisting state parameters.

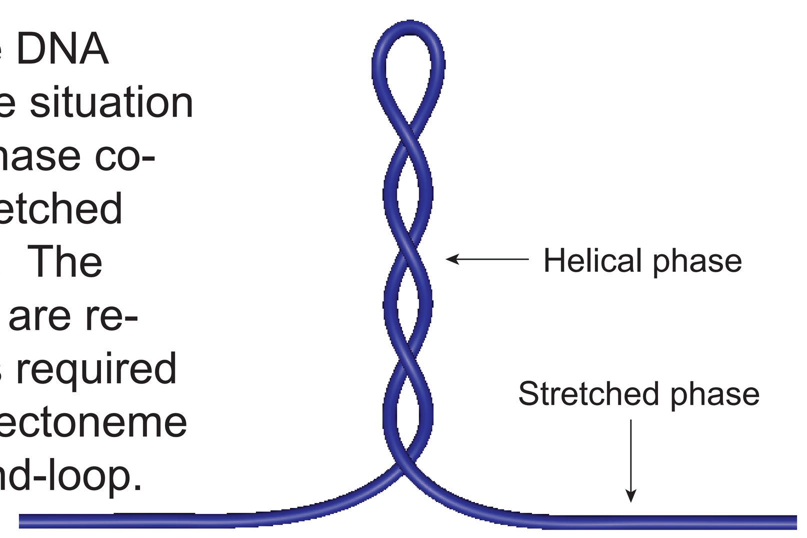
Plectonemes as two-phase coexistence; jumps from interface between phases

We see a jump in the extension at the transition, and predict that there should also be a jump in the torque.





Past the transition, the DNA coils around itself. The situation is well-described as phase coexistence between stretched and plectonemic DNA. The jumps at the transition are related to the extra parts required to create the helical plectoneme phase: the tails and end-loop.



Simulated coexisting state

Linearity implies the coexisting state is specified by four numbers.

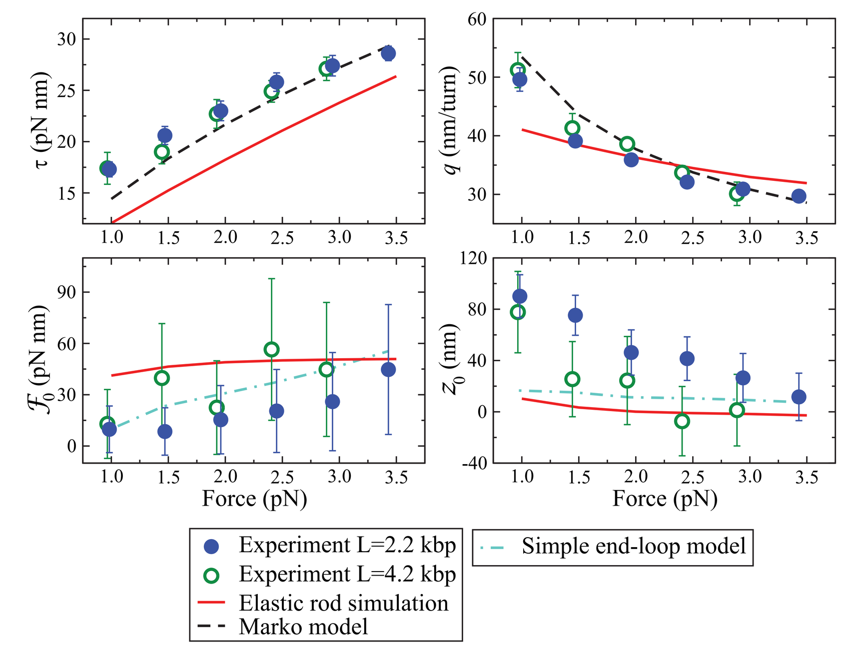
As we twist the coexisting state, a linearly increasing amount of DNA is taken into the plectoneme. (Analogously, increasing the volume of a tube of coexisting liquid and gas will linearly increase the amount of gas.)

This linearity allows us to write the free energy and extension of the coexisting state using two slopes and two intercepts:

$$\mathcal{F}_{\mathrm{CS}}(K,L) = \mathcal{F}_0 + 2\pi\tau K - \frac{\tau^2}{2C}L;$$

$$z_{\mathrm{CS}}(K,L) = -z_0 - qK + \left(\xi(\tau) + \frac{\tau}{2\pi C}q\right)L.$$

(C = DNA torsional modulus; $\xi(\tau)L$ = thermally-shortened DNA extension)

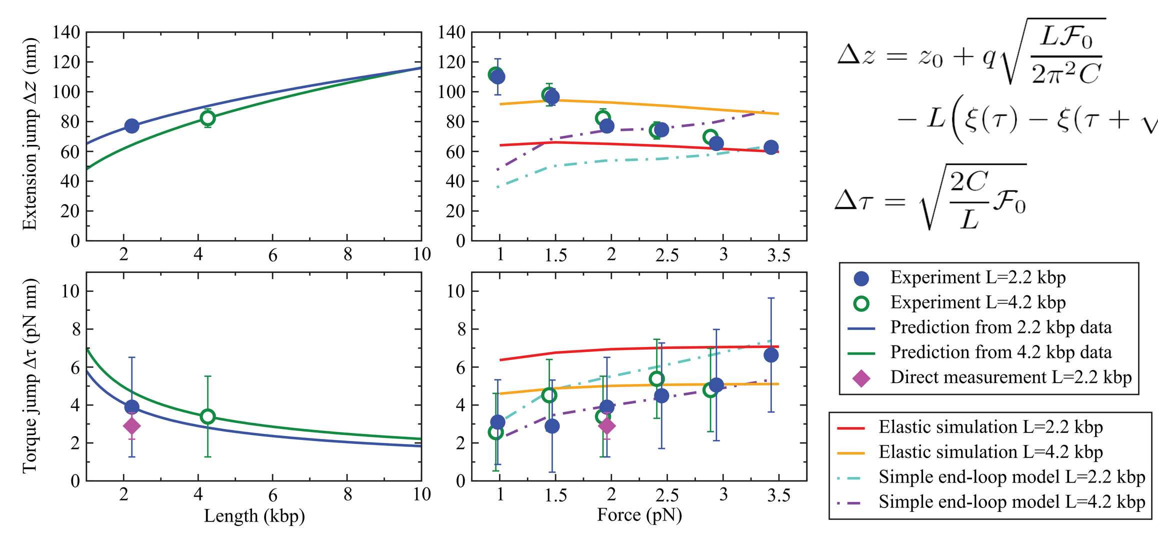


These four values — the torque τ, slope q, free energy offset $\mathcal{F}_0$, and extension offset z_0 — can be obtained from experimental data. We expect them to be independent of contour length L.

Testing plectoneme models

Models can predict the four coexisting state parameters. A model proposed by John Marko [2] matches τ and q well (black dashed line above), but does not attempt to predict $\mathcal{F}_0$ or z_0.

Our "simple end-loop" model for the intercepts $\mathcal{F}_0$ and z_0 includes an extra circular loop to mimic the end of the plectoneme. We also use an elastic rod simulation with measured elastic moduli as well as electrostatic and entropic repulsion. Both models produce z_0 that is too small at low applied forces, leading to extension jumps smaller than experiment (below).

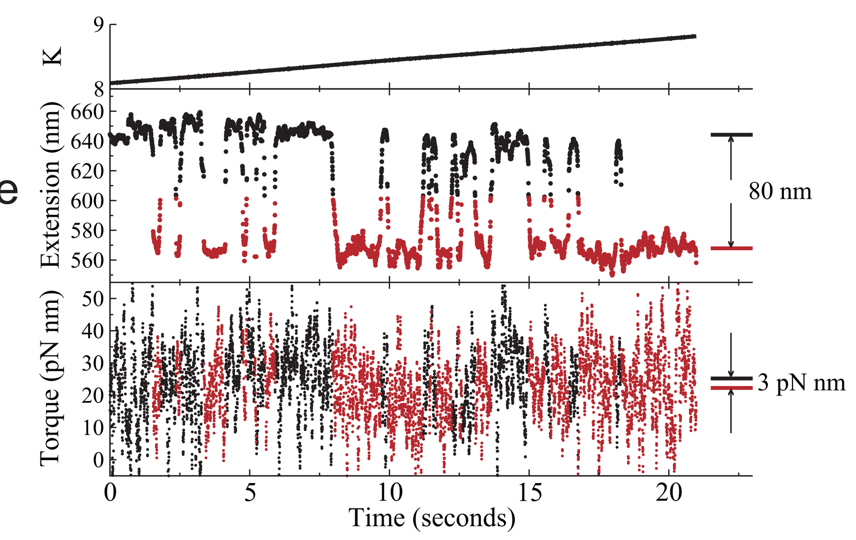


$$\Delta z = z_0 + q\sqrt{\frac{L\mathcal{F}_0}{2\pi^2 C}} - L\left(\xi(\tau) - \xi\left(\tau + \sqrt{2C\mathcal{F}_0/L}\right)\right)$$

$$\Delta\tau = \sqrt{\frac{2C}{L}\mathcal{F}_0}$$

Direct observations of thermal hopping and torque jump

Sufficiently near the transition that the two states have a difference in free energy of order k_BT, we see thermal hopping.



We use the previously published extension data [1] to sort the torque data into pre- and post-transition, providing a new, direct measurement of the torque jump (purple diamond on previous plots).

Corrections to our current framework do not seem to help with low-force agreement.

Bending anisotropy, kinking:
- Attempting to fit z_0 produces poor fit for $\mathcal{F}_0$.

Entropic corrections:
- Circular loop correction [3] is very small.

Multiple plectonemes:
- Entropy due to plectoneme location causes unwanted length-dependence if $\mathcal{F}_0$ is of order k_BT.

Conclusions

- Extension and torque jumps at the transition to the plectonemic state can be understood in terms of two-phase coexistence.
- Simple models predict reasonable free energies, but have an extension jump that is too small at low applied forces.

Preprint and references

- http://arxiv.org/abs/0811.3645
- [1] S. Forth, C. Deufel, M. Y. Sheinin, B. Daniels, J. P. Sethna, and M. D. Wang, Phys. Rev. Lett. 100, 148301 (2008).
- [2] J. F. Marko, Phys. Rev. E 76, 021926 (2007).
- [3] T. Odijk, J. Chem. Phys. 105, 1270 (1996).