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Supporting Material

Energetics at the DNA supercoiling transition

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Relative DNA extension as function of force and torque

The extension of DNA stretched at a constant force appears shorter than its contour length due to thermal fluctuations. Additionally, before buckling the extension of DNA gets reduced upon twisting. This is due to writhe fluctuations (1). We account for the incomplete stretching as function of force F and torque Γ using the expression for the relative extension derived by Moroz and Nelson, which is given by (2):

$$z(F,\Gamma) = 1 - \frac{1}{2}\left[\frac{p \times F}{k_\mathrm{B}T} - \left(\frac{\Gamma}{2k_\mathrm{B}T}\right)^2 - \frac{1}{32}\right]^{-1/2}, \tag{1}$$

where p denotes the bending persistence length.

Energy E_1 and length reduction ΔL_1 of the initial loop

In order to estimate the free energy E_1 to form the initial loop as well as the corresponding loop length ΔL_1, we calculate the mechanical energy required to extrude a perfect circular loop of radius R out of a stretched DNA molecule. We assume the writhe of such a circular loop to be 1 turn. In this case we can write (3):

$$E_1 = 2\pi RF \times z(F,0) + 2\pi R \frac{1}{2}\frac{k_\mathrm{B}T \times p}{R^2}. \tag{2}$$

The first part of the sum represents the change in potential energy due to shortening of the DNA against the applied force. The second part of the sum represents the bending energy of the DNA within such a loop. We account for incomplete DNA stretching, which essentially lowers the change in potential energy for a given loop length, by introducing $z(F,0)$ as a correction term. For simplicity, the torque dependence of the DNA extension is neglected, since it represents only a minor correction.

Minimizing the initial-loop energy with respect to R provides the energetically favored radius of the initial loop and correspondingly the length reduction ΔL_1:

$$\Delta L_1 = 2\pi R_\mathrm{min} \times z(F,0) = \left[\frac{k_\mathrm{B}T \times p \times z(F,0)}{2F}\right]^{1/2}. \tag{3}$$

Combining Eqs. 2 and 3 one obtains for the initial loop energy:

$$E_1 = 2\pi\left[2k_\mathrm{B}T \times p \times F \times z(F,0)\right]^{1/2}. \tag{4}$$

Postbuckling slope according to the composite model by Marko

The composite model by Marko also allows calculating the postbuckling slope (4), for which an expression has been derived (5). Using only non-reduced parameters it results in:

$$\frac{\mathrm{d}L}{\mathrm{d}N}=\frac{2\pi\left[1-\frac{1}{2}\left(\frac{k_\mathrm{B}T}{p\times F}\right)^{1/2}-\frac{C^2\times P\times g\times\left(\frac{k_\mathrm{B}T}{p\times F}\right)^{3/2}}{8\left(C_\mathrm{s}\times k_\mathrm{B}T\right)^2\times\left(1-\frac{P}{C_\mathrm{s}}\right)}\right]}{\left[\frac{2P\times g}{1-\frac{P}{C_\mathrm{s}}}\right]^{1/2}\times\left(\frac{1}{P}-\frac{1}{C_\mathrm{s}}\right)}, \tag{5}$$

with C being the torsional modulus of DNA, C_s the effective torsional modulus (see Eq. 2, main text), and P the plectonemic twist stiffness. g the negative free energy of stretched, nicked (freely swiveling) DNA given by:

$$g=F-\left(\frac{k_\mathrm{B}T\times F}{p}\right)^{1/2}. \tag{6}$$

Jump size at the buckling transition

The jump size at the buckling transition can be written as:

$$\begin{aligned}L_\mathrm{jump}&=\Delta L_1+\left(\Delta N_\mathrm{b}^\mathrm{p}-1\right)\times\frac{\mathrm{d}L}{\mathrm{d}N}\\&+L_0\times\left[z\left(F,2\pi\frac{C_\mathrm{s}}{L_0}N\right)-z\left(F,2\pi\frac{C_\mathrm{s}}{L_0}\left(N-\Delta N_\mathrm{b}^\mathrm{p}\right)\right)\right],\end{aligned} \tag{7}$$

where the first term of the sum accounts for the length reduction by the initial loop, the second term for the other turns of the plectoneme, and the third one for the extension change due to the abrupt reduction of the torque during the transition.

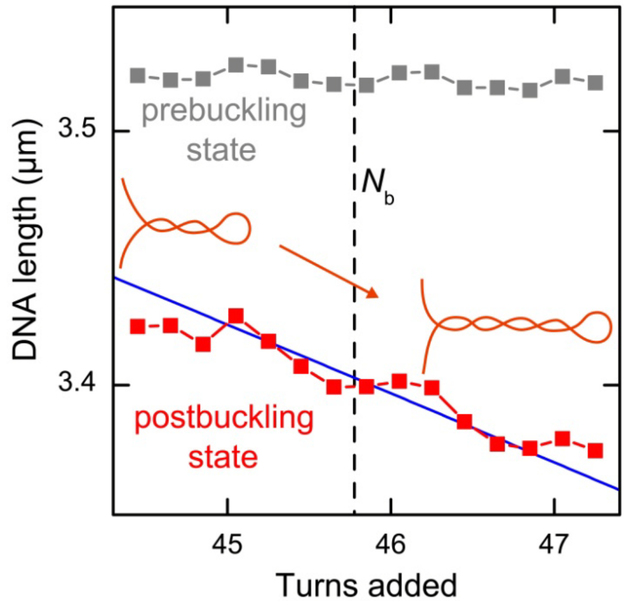

FIGURE S1 Mean position of the pre- and postbuckling state of a 10.9 kbp molecule at 4.0 pN and 320 mM Na^{+} recorded at different amounts of applied supercoils N in the vicinity of the buckling transition. The writhe of the forming plectoneme is not constant over the buckling transition, but increases linearly with the applied supercoils according to Eq. 9 in the main text. This can indeed be seen in the experimental traces as a gradual shift of the postbuckling level, which corresponds to the postbuckling slope (solid blue line). The buckling point defined where pre- and postbuckling state are equally populated is represented by the dashed black line.

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