

# Homogeneous elastic model for short DNA

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Keywords:

## I.

The homogeneous, isotropic elastic rod model of DNA may be good for random-sequence DNAs that are much longer than a helical repeat. For shorter DNAs, however,

- . Each basepair step type ( $b_i \rightarrow b_{i+1}$  where  $b_i = \text{A,C,G, or T}$ ) may have its own preferred orientation of  $b_i$  relative to  $b_{i+1}$ , and its own elastic constants for deviations from preferred.
- . More generically, each cross-sectional plane of the DNA helix is quite anisotropic. This anisotropy may average away on length scales much larger than 10bp, but for short DNA cannot be ignored.
- . Another kind of anisotropy, also modulated by the helix repeat, is twist–bend (or “twist–roll”) coupling.

How are we going to get values for all these parameters? W. Olson has been working on this for a long time. Her strategy is to examine crystal structures of lots of DNA oligomers, and of DNA–protein complexes. She assumes that on average, each basepair is subjected to random external forces (e.g. crystal forces), the same for every type of basepair junction, analogous to the thermal forces in thermal equilibrium but of an unknown overall magnitude. Then the observed deformations of basepairs in this imagined random external force tell us about the elastic constants for deformation of each basepair type, and the covariances of deformations give the off-diagonal terms.

That’s a strong set of assumptions. However, even if we don’t accept them, it’s clear on more general grounds that a helical elastic body must have an elastic matrix with the general form given below (Marko and Siggia, 1994). And we will set the overall magnitude of the elastic matrix using the very well measured persistence length of DNA. So hopefully the precise details won’t be too critical.

## II. “CAMBRIDGE” CONVENTION

See Fig. 1. These conventions are equivalent to but slightly different from those of (Marko and Siggia, 1994).

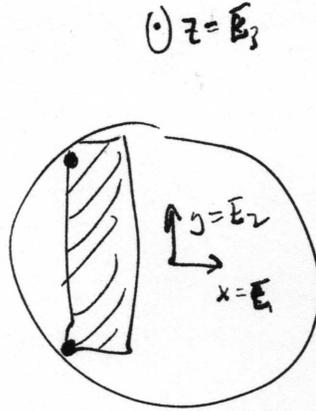


FIG. 1 Similar to a figure in (Marko and Siggia, 1994). The hatched rectangle is a basepair. The black dots are the phosphate backbones. The circle is the outer envelope of the helix, 2nm in diameter. We set up an orthonormal frame where  $\mathbf{E}_3$  is out of the page,  $\mathbf{E}_1$  points to the major groove as shown, and  $\mathbf{E}_2$  completes the triad. “Positive roll” is then defined as a positive rotation about  $\mathbf{E}_2$  as we pass from this basepair to the one on top of it (=“bend into the major groove”). Similarly “positive tilt” is positive rotation about  $\mathbf{E}_1$ , and “twist” is excess rotation about  $\mathbf{E}_3$  (in addition to the natural  $\omega_0 = 2\pi/10.5\text{bp}$ ). See also [http://rutchem.rutgers.edu/~olson/step\\_par.gif](http://rutchem.rutgers.edu/~olson/step_par.gif)

### III. ELASTIC MODEL OF CZAPLA ET AL.

Let  $\ell_0 = 0.34\text{ nm}$ . (Czapla *et al.*, 2006) define a vector  $\Delta\theta$  consisting of the tilt, roll, and twist per basepair. For the continuum limit, let  $\Omega_i = \Delta\theta_i/\ell_0$  be the corresponding rates (per unit length). Czapla *et al* define the elastic deformation free energy per basepair as  $\frac{1}{2}k_B T \Delta\theta^t F \Delta\theta$ . Thus  $F$  is dimensionless.

I define the elastic deformation free energy per length as  $\frac{1}{2}k_B T \Omega^t Q \Omega$ , so  $Q$  has units of length; in the simplest model it’s diagonal, with the bend and twist persistence lengths on the diagonal. Thus  $Q = \ell_0 F$ .

Czapla *et al* discuss the effect of roll–twist coupling on their page 692. This section proposes a simplified model for DNA elasticity. Instead of the full sequence dependence, the model posits interspersed “X-” and “Z-”tracts. The elastic matrix for “Z-”tracts is taken to be

$$F = \begin{bmatrix} (4.84^\circ)^{-2} & 0 & 0 \\ 0 & (4.84^\circ)^{-2} & (5.41^\circ)^{-2} \\ 0 & (5.41^\circ)^{-2} & (4.09^\circ)^{-2} \end{bmatrix} \quad (1)$$

(Here the units are degrees<sup>-2</sup>.) The elastic matrix for “X-”tracts is the same without the offdiagonal terms.

### IV. PERSISTENCE

Let’s work out the persistence length of a polymer with elasticity in the form given above.

We decouple strain modes by finding an orthogonal matrix  $T$  with  $TFT^t = D = \text{diagonal}$  and defining  $\Psi = T\Delta\theta$ . Then the elastic free energy per basepair is  $\frac{1}{2}\Psi^t D \Psi$ , and so  $\langle(\Psi_1)^2\rangle = 1/D_{11}$

etc. And

$$\langle (\Delta\theta_1)^2 \rangle = \sum_j (T_{j1})^2 / D_{jj}$$

Now connect these expressions to persistence length  $\xi$ . By definition,

$$\langle \hat{\mathbf{t}}_i \cdot \hat{\mathbf{t}}_{i+1} \rangle = e^{-\ell/\xi}$$

If we choose coordinates for which  $\hat{\mathbf{t}}_i = \hat{\mathbf{z}}$ , and  $\theta_i$  are the angles relating basepair  $i + 1$  to  $i$ , then

$$\hat{\mathbf{t}}_{i+1} = \begin{bmatrix} \theta_1 \\ \theta_2 \\ 1 - ((\theta_1)^2 + (\theta_2)^2)/2 + \dots \end{bmatrix}; \quad \langle \hat{\mathbf{t}}_i \cdot \hat{\mathbf{t}}_{i+1} \rangle = 1 - \frac{1}{2} \langle (\theta_1)^2 + (\theta_2)^2 \rangle$$

Since in the small  $\ell$  limit this must equal  $1 - (\ell/\xi) + \dots$ , we get a formula for  $\xi$  in terms of the matrices  $T$  and  $D$ .

We can check that result by generating a lot of random matrices from the Gaussian distribution specified by  $D$ , working out the corresponding chains, and evaluating numerically the desired correlator. Let  $\hat{\mathbf{e}}_i$ ,  $i = 1, 2, 3$  be the three unit vectors fixed in space. Then each elastic rod segment has an orientation specified by the orthogonal matrix  $h_{ia} = \mathbf{E}_a \cdot \hat{\mathbf{e}}_i$ . If we take such an orientation and rotate  $\{\mathbf{E}_a\}$  by a small angle  $\epsilon$  about  $\mathbf{E}_3$  (a twist rotation), we find a new orientation specified by

$$h'_{ia} = [h(\mathbf{1} + \epsilon J^{(3)})]_{ia}, \quad \text{where } J^{(3)} = \begin{bmatrix} 0 & -1 & \\ 1 & 0 & \\ & & 0 \end{bmatrix}$$

Similarly for the other two rotations; the  $J^{(i)}$  are mathematically the spin-one rotation generators from quantum mechanics. Define  $\mathcal{R}_0 = \exp[\omega_0 J^{(3)}]$ .

To generate random rotation matrices, we now draw  $\Psi$  vectors from three Gaussians defined by the entries of  $D$ . For each such vector we form  $\Delta\theta = T^t \Psi$ , combine with the  $J$ 's, exponentiate to get a rotation matrix, and left multiply by  $\mathcal{R}_0$ .<sup>1</sup> Build up successive segment orientations from products of these small rotations, then evaluate  $\langle \hat{\mathbf{t}}_i \cdot \hat{\mathbf{t}}_{i+k} \rangle$ . I carried out these steps and confirmed that the correlator had exponential falloff.

To test the procedure I started with the usual, simple choice of elasticity matrix (diagonal and isotropic), and found the expected value of the persistence length by the above procedure. Then I repeated with more realistic forms.

## V. PROPOSED ELASTIC MATRIX

Czapla et al. offered the matrix Eq. 1 merely as an example. To get something a bit more based on crystallographic data, but still neglecting sequence (as well as shift, slide, and  $\Delta$ rise),

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<sup>1</sup> This trick amounts to defining a Gaussian on a curved manifold (the rotation group) by the exponential of a Gaussian on a linear space (its Lie algebra). Alternatively we could add  $\omega_0 T^{(3)}$  prior to exponentiating. In the continuum limit this procedure is equivalent to the one indicated in the text; for finite steps the latter method works slightly better (gives persistence close to the continuum value).

I took Olson's published covariance matrices for the  $\theta_i$  of various basepair steps and just averaged them. See [http://rutchem.rutgers.edu/~olson/cov\\_matrix.html](http://rutchem.rutgers.edu/~olson/cov_matrix.html). The elastic matrix should be an unknown overall constant times the inverse of the averaged covariance matrix.

It's encouraging that the entries of the elastic matrix that are forbidden by the (approximate) symmetry of DNA (Marko and Siggia, 1994) are indeed much smaller than the (11), (22), (23), and (33) entries. I set these exactly to zero, proceeded as above, and finally set the overall constant to get  $\xi = 45$  nm, appropriate for DNA in the salt conditions of experiments we study. This gave

$$F = \begin{bmatrix} 0.0601 & 0 & 0 \\ 0 & 0.0334 & 0.0116 \\ 0 & 0.0116 & 0.0335 \end{bmatrix} \quad (2)$$

(Again the units are degrees<sup>-2</sup>.)

## References

- Czapla, L., D. Swigon, and W. K. Olson, 2006, *Journal of Chemical Theory and Computation* **2**(3), 685.  
 Marko, J., and E. Siggia, 1994, *Macromolecules* **27**, 981, Erratum *Ibid.* **29** (1996) 4820.