Supplement for

# Allosteric interactions in a birod model of DNA

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Several calculations have been omitted from the main text for the sake of brevity. They are given in this supplement in detail.

## 1 Pictorial representation of the step-wise procedure to calculate interaction energy (sec. 2 of the main text)

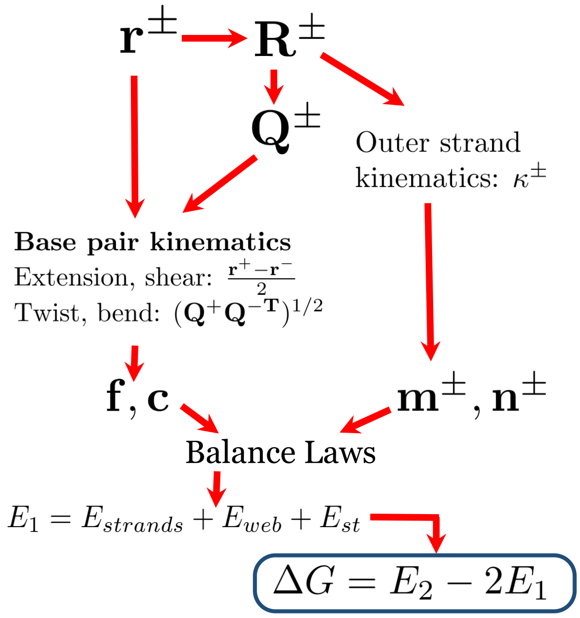


Figure 1: Pictorial representation for the procedure outlined in the sec. 2 of the main text.

## 2 Exponential decay of interaction energy in a 'ladder'

The calculation of interaction energies in a helical birod is considerably involved, so we first illustrate the main concepts in a simpler birod model which we call a 'ladder' because it is not helical. We mimic the binding of a protein by force pairs that tend to widen the ladder as shown in fig. 2. Our goal in this section is to demonstrate the utility of the apparatus in section 2 and 3 of the main text by computing the interaction energy for two force pairs separated by a distance $a$ as shown in fig. 2. We work with a planar 2D birod in this section and assume small elastic deformations in the outer strands and web to keep the calculations tractable. We, ultimately, find that the interaction energy between the force pairs decays exponentially with distance $a$.

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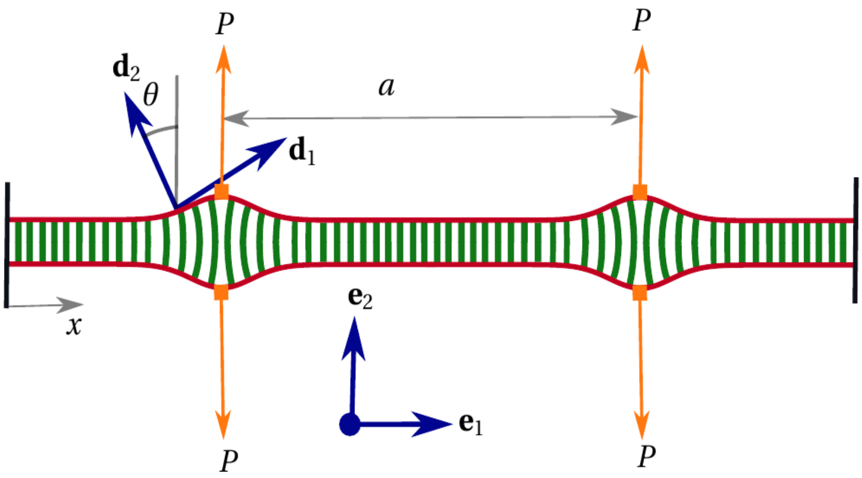


Figure 2: A straight birod, referred to as a ladder, being pulled by two force pairs separated by a distance $a$. We show that the interaction energy between the two force pairs given by $\Delta G = E_a^2 - E_0^1 - E_a^1$ decreases exponentially with $a$.

### 2.1 Step 1: Kinematic description of the two strands

We use the arclength parameter $x$ to describe the mechanics of the birod. In the reference configuration, both the strands $\pm$ are straight, $\mathbf{r}_0^{\pm} = x\ \mathbf{e}_1 \pm \frac{d}{2}\ \mathbf{e}_2$, separated by distance $d$. Here $\mathbf{e}_1$ is a unit vector along the length of the birod, $\mathbf{e}_2$ is a unit vector perpendicular to each birod bridging the gap between them and $\mathbf{e}_3$ is normal to the plane of the birod as shown in fig. 2. We begin by assuming a general displacement in $\mathbf{e}_1 - \mathbf{e}_2$ plane. For the geometry shown in fig. 2 we expect a mirror symmetry for deformation profiles along $\mathbf{e}_1$ such that

$$
\begin{aligned}
\mathbf{r}^{+} &= x\ \mathbf{e}_1 + \frac{d}{2}\ \mathbf{e}_2 + u\ \mathbf{e}_1 + w\ \mathbf{e}_2, \\
\mathbf{r}^{-} &= x\ \mathbf{e}_1 - \frac{d}{2}\ \mathbf{e}_2 + u\ \mathbf{e}_1 - w\ \mathbf{e}_2,
\end{aligned}
\tag{1}
$$

where $u = u(x)$ and $w = w(x)$ are displacements along the $\mathbf{e}_1$ and $\mathbf{e}_2$ directions, respectively.

### 2.2 Step 2: Rotation of the two strands

At each point $x$ on the $\pm$ strands we attach an orthogonal rotation frame which is simply $\mathbf{R}_0^{\pm} = [\ \mathbf{e}_1 \quad \mathbf{e}_2 \quad \mathbf{e}_3] = \mathbf{1}_{3\times 3}$ (the identity matrix) in the reference configuration. The vectors $\mathbf{e}_1$ and $\mathbf{e}_2$ map onto $\mathbf{d}_{1,2}^{+}$ and $\mathbf{d}_{1,2}^{-}$ in the deformed configuration for the positive and negative strand, respectively. The $\mathbf{d}_i$, $i = 1, 2, 3$ are again unit vectors.

$$
\begin{aligned}
\mathbf{d}_1^{\pm} &= \cos\theta\ \mathbf{e}_1 \pm \sin\theta\ \mathbf{e}_2 \approx\ \mathbf{e}_1 \pm \theta\ \mathbf{e}, \\
\mathbf{d}_2^{\pm} &= \mp\sin\theta\ \mathbf{e}_1 + \cos\theta\ \mathbf{e}_2 \approx \pm\theta\ \mathbf{e}_1 +\ \mathbf{e}_2, \\
\mathbf{R}^{\pm} &= \begin{bmatrix} \cos\theta & \mp\sin\theta & 0 \\ \pm\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix} \approx \begin{bmatrix} 1 & \mp\theta & 0 \\ \pm\theta & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.
\end{aligned}
\tag{2}
$$

We assume small $\theta$ to keep the calculations tractable.

### 2.3 Step 3: Extension and rotation of the web

We decompose the kinematics of the web into a macroscopic deformation and a microscopic deformation [1]. The former describes the rigid displacement and rotation, while the latter is related to the force and moment transferred by the web. The macro- displacement vector $\mathbf{r}$ is defined as $\mathbf{r} = \frac{\mathbf{r}^{+} + \mathbf{r}^{-}}{2} = x\ \mathbf{e}_1 + u\ \mathbf{e}_1$ [1]. The macro- rotation tensor is $\mathbf{R}$ defined as $\mathbf{R} = (\mathbf{R}^{+}\mathbf{R}^{-T})^{1/2}\mathbf{R}^{-}$ [1], which in our case is

$$
\mathbf{R} = (\mathbf{R}^{+}\mathbf{R}^{-T})^{1/2}\mathbf{R}^{-} = \mathbf{I}_{3\times 3}. \tag{3}
$$

We define another tensor $\mathbf{P}$ relating $\mathbf{R}^{+}$ and $\mathbf{R}^{-}$ to $\mathbf{R}$. An elastic constitutive relation discussed in further sections connects the micro- rotation tensor $\mathbf{P} = (\mathbf{R}^{+}\mathbf{R}^{-T})^{1/2}$ to the moment transferred by the web.

$$
\mathbf{P} = (\mathbf{R}^{+}\mathbf{R}^{-T})^{1/2} = \begin{bmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix} \approx \begin{bmatrix} 1 & -\theta & 0 \\ \theta & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}. \tag{4}
$$

We need to calculate the Gibbs rotation vector $\boldsymbol{\eta} = \tan\frac{\lambda}{2}\hat{\mathbf{k}}$, where $\lambda$ is obtained from $1 + 2\cos\lambda = \mathrm{tr}(\mathbf{P})$ and $\hat{\mathbf{k}}$ is the eigenvector of $\mathbf{P}$ *i.e.* $\mathbf{P}\hat{\mathbf{k}} = \hat{\mathbf{k}}$. We need $\boldsymbol{\eta}$ in the subsequent section to compute the moment transferred by the web [1].

By direct observations, $\lambda = \theta$ and $\hat{\mathbf{k}} = \mathbf{e}_3$, so that $\boldsymbol{\eta} = \tan\frac{\theta}{2}\,\mathbf{e}_3$. The Gibbs rotation vector in the reference configuration $\boldsymbol{\eta}_0 = 0$.

The micro- displacement of the web is defined by $\boldsymbol{w} = \frac{\mathbf{r}^+ - \mathbf{r}^-}{2}$, which is $\boldsymbol{w}_0 = \frac{d}{2}\,\mathbf{e}_2$ in the reference configuration and $\boldsymbol{w} = (\frac{d}{2} + w)\,\mathbf{e}_2$ in the current configuration. We need $\boldsymbol{w}$ and $\boldsymbol{w}_0$ to compute the force transferred by the web.

## 2.4 Step 4: Governing differential equations

We calculate various strains and curvatures associated with the deformation and relate them to the contact force and moment, respectively, which go into the governing equations. For detailed discussion on the relations used in this section we refer the reader to Moakher and Maddocks [1]. The governing equations of the birod consist of three kinetic components: the contact forces in the two strands $\boldsymbol{n}^{\pm}$, the contact moments $\boldsymbol{m}^{\pm}$, and the force $\boldsymbol{f}$ and moment $\boldsymbol{c}$ transferred by the $-$ strand onto the $+$ strand. We compute each of these components as follows:

1. $\boldsymbol{n}^{\pm}$: We need strains in the current configuration $\boldsymbol{v}^{\pm}$ and in the reference configuration $\boldsymbol{v}_0^{\pm}$, in the strands to compute $\boldsymbol{n}^{\pm}$. These strains are:

$$\begin{aligned} \boldsymbol{v}_0^{\pm} &= \frac{\partial \mathbf{r}_0^{\pm}}{\partial x} = \mathbf{e}_1, \\ \boldsymbol{v}^{\pm} &= \frac{\partial \mathbf{r}^{\pm}}{\partial x} = (1 + u_x)\,\mathbf{e}_1 \pm w_x\,\mathbf{e}_2. \end{aligned} \tag{5}$$

   The contact forces $\boldsymbol{n}^{\pm} = \mathbf{R}^{\pm}\mathbf{C}\mathbf{R}^{\pm T}\boldsymbol{v}^{\pm}$ where $\mathbf{C}$ is a second order tensor such that $\mathbf{C}_{11} = EA$, $\mathbf{C}_{22} = GA$ and $\mathbf{C}_{12} = \mathbf{C}_{21} = 0$. Here $E$ is the stretch modulus, $G$ shear modulus and $A$ is the cross-sectional area of the strands. Upon performing the calculation and taking account of the fact that $u, w$ and $\theta$ are small and upon ignoring higher order terms we get,

$$\boldsymbol{n}^{\pm} = EAu_x\,\mathbf{e}_1 \pm GA(w_x - \theta)\,\mathbf{e}_2. \tag{6}$$

2. $\boldsymbol{m}^{\pm}$: For calculating the contact moments $\boldsymbol{m}^{\pm}$ in the respective strands we need the curvature vector $\boldsymbol{\kappa}^{\pm}$ for the two strands, which can, in turn, be obtained by computing the axial vector of the skew-symmetric matrices $\mathbf{U}^{\pm} = \frac{\partial \mathbf{R}^{\pm}}{\partial x}\mathbf{R}^{\pm T}$.

$$\begin{aligned} \mathbf{U}^{\pm} &= \frac{\partial \mathbf{R}^{\pm}}{\partial x}\mathbf{R}^{\pm T} = \begin{bmatrix} 0 & \mp\theta_x & 0 \\ \pm\theta_x & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \\ \boldsymbol{\kappa}^{\pm} &= \pm\theta_x\,\mathbf{e}_3. \end{aligned} \tag{7}$$

   The contact moment $\boldsymbol{m}^{\pm}$ is related to the curvature via a bending rigidity $EI$ such that

$$\boldsymbol{m}^{\pm} = \pm EI\theta_x\,\mathbf{e}_3. \tag{8}$$

   Here, $I$ is the moment of inertia of the cross-section of the outer strands.

3. $\boldsymbol{f}$ and $\boldsymbol{c}$: The force transferred by the web $\boldsymbol{f}$ is proportional to the change in the dimensions of the web quantified by $\boldsymbol{w}$ and $\boldsymbol{w}_0$ in the previous sections such that,

$$2\boldsymbol{f} = \mathbf{R}\mathbf{H}\mathbf{R}^T[\boldsymbol{w} - \mathbf{R}\check{\boldsymbol{w}}_0] \approx Lw\,\mathbf{e}_2, \tag{9}$$

   where $\mathbf{H}$ is a diagonal second order elasticity tensor such that $\mathbf{H}_{22} = L$. Similarly, the moment transferred by the web $\boldsymbol{c}$ is elastically related to $\boldsymbol{\eta}$ and $\boldsymbol{\eta}_0$ calculated in the previous sections:

$$2\boldsymbol{c} = \frac{1}{\alpha}\mathbf{R}\mathbf{G}\mathbf{R}^T(\boldsymbol{\eta} - \mathbf{R}\check{\boldsymbol{\eta}}) - \boldsymbol{\eta} \times (\boldsymbol{w} \times \boldsymbol{f}) \approx K\theta\,\mathbf{e}_3, \tag{10}$$

   where $\alpha = \frac{2}{1 + ||\boldsymbol{\eta}||^2}$, $\mathbf{G}$ is a second order diagonal elasticity tensor and $K = \frac{G_{33}}{2}$.

The governing equations from box 4 in [1] are given by,

$$\begin{aligned} \boldsymbol{n}_x &= 0, \\ \boldsymbol{m}_x + \mathbf{r}_x \times \boldsymbol{n} &= 0. \end{aligned} \tag{11a}$$

$$\begin{aligned} \boldsymbol{n}_x^c - 2\boldsymbol{f} &= 0, \\ \boldsymbol{m}_x^c + \mathbf{r}_x \times \boldsymbol{n}^c - \boldsymbol{c} &= 0. \end{aligned} \tag{11b}$$

In the above equations, $\boldsymbol{n} = \boldsymbol{n}^+ + \boldsymbol{n}^- = 2EAu_x\ \mathbf{e}_1$, $\boldsymbol{n}^c = \boldsymbol{n}^+ - \boldsymbol{n}^- = 2GA(w_x - \theta)\ \mathbf{e}_2$, $\boldsymbol{m} = \boldsymbol{m}^+ + \boldsymbol{m}^- + \boldsymbol{w} \times \boldsymbol{n}^c = 0$ and $\boldsymbol{m}^c = \boldsymbol{m}^+ - \boldsymbol{m}^- + \boldsymbol{w} \times \boldsymbol{n} = 2EI\theta_x\ \mathbf{e}_3 + (d/2 + w)\ \mathbf{e}_2 \times 2EAu_x\ \mathbf{e}_1 \approx 2[EI\theta_x - \frac{d}{2}EAu_x]\ \mathbf{e}_3$. Upon substituting these values into the governing equations we get,

$$\begin{aligned}
&EAu_{xx} = 0,\\
&2GA(w_{xx} - \theta_x) - Lw = 0,\\
&2(EI\theta_{xx} - d/2EAu_{xx}) + (1 + u_x)\ \mathbf{e}_1 \times 2GA(w_x - \theta)\ \mathbf{e}_2 - K\theta\ \mathbf{e}_3 = 0.
\end{aligned} \tag{12}$$

We use $\theta_x = w_{xx} - \frac{L}{2GA}w$ and $u_{xx} = 0$ and get,

$$EIw_{xxxx} - (\frac{EIL}{2GA} + \frac{K}{2})w_{xx} + (\frac{L}{2} + \frac{KL}{4GA})w = 0. \tag{13}$$

If we further assume that the outer strands are unshearable ($GA \to \infty$ and $\theta = w_x$), the above equation reduces to a simpler equation.

$$EIw_{xxxx} - \frac{K}{2}w_{xx} + \frac{L}{2}w = 0. \tag{14}$$

### 2.5 Step 5,6 and 7: Interaction Energy

We substitute $w = e^{ms}$, and get eigenvalues $m = \pm\lambda, \pm\mu$. For illustration purposes, we assume $\lambda$ and $\mu$ are real numbers (i.e., $K^2 - 32L > 0$) and the ladder extends from $-\infty$ in the negative $\mathbf{e}_1$ direction to $+\infty$ in the positive $\mathbf{e}_1$ direction with $w = w_x = 0$ at $x = \pm\infty$. Hence, for a force pair at $x = 0$

$$\begin{aligned}
w(x) &= Ae^{\lambda x} + Be^{\mu x} \quad \text{when} \quad x < 0,\\
w(x) &= Ae^{-\lambda x} + Be^{-\mu x} \quad \text{when} \quad x > 0,
\end{aligned} \tag{15}$$

for some constants $A$ and $B$ which could be determined using boundary conditions in step 5. For two force pairs separated by a distance $a$, the displacement profile $w_2(x) = w(x) + w(x - a)$. The elastic energy in the deformed configuration is computed in step 6 and is given by,

$$E[w] = EIw_{xx}^2 + \frac{1}{2}Kw_x^2 + \frac{1}{2}Lw^2. \tag{16}$$

Finally, we compute the interaction energy defined by $\Delta G = E[w_2] - 2E[w]$ in step 7 and find that it decreases exponentially with the distance $a$.

$$\begin{aligned}
\Delta G =& \frac{L}{2}\Big(\frac{e^{-\lambda a}\left(A^2\lambda^2\mu - A^2\mu^3 + A^2\lambda^3\mu a - A^2\lambda\mu^3 a - 4AB\lambda\mu^2\right)}{\lambda\mu(\lambda^2 - \mu^2)} + \\
&\frac{e^{-\mu a}\left(4AB\lambda^2\mu + B^2\lambda^3 - B^2\lambda\mu^2 + B^2\lambda^3\mu a - B^2\lambda\mu^3 a\right)}{\lambda\mu(\lambda^2 - \mu^2)}\Big) + \\
&\frac{K}{2}\Big(\frac{e^{-\lambda a}\left(A^2\lambda^3 - A^2\lambda\mu^2 - A^2\lambda^4 a + A^2\lambda^2\mu^2 a + 4AB\lambda^2\mu\right)}{(\lambda^2 - \mu^2)} + \\
&\frac{e^{-\mu a}\left(-4AB\lambda\mu^2 + B^2\lambda^2\mu - B^2\mu^3 - B^2\lambda^2\mu^2 a + B^2\mu^4 a\right)}{(\lambda^2 - \mu^2)}\Big) + \\
&EI\Big(\frac{e^{-\lambda a}\left(A^2\lambda^5 - A^2\lambda^3\mu^2 + A^2\lambda^6 a - A^2\lambda^4\mu^2 a - 4AB\lambda^2\mu^3\right)}{(\lambda^2 - \mu^2)} + \\
&\frac{e^{-\mu a}\left(4AB\lambda^3\mu^2 + B^2\lambda^2\mu^3 - B^2\mu^5 + B^2\lambda^2\mu^4 a - B^2\mu^6 a\right)}{(\lambda^2 - \mu^2)}\Big).
\end{aligned} \tag{17}$$

We follow these steps for a helical birod model of DNA in the main text.

## 3 Kinematics of the − strand

In the main text we gave detailed derivations for the strains, curvatures, etc., for the + strand in our birod. We now shift our attention to the complimentary − strand. The reference configuration of this strand is denoted by position vector $\mathbf{r}_0^-$.

$$\mathbf{r}_0^- = b(\cos(\omega x + \alpha)\ \mathbf{e}_1 + \sin(\omega x + \alpha)\ \mathbf{e}_2) + x\ \mathbf{e}_3. \tag{18}$$

Along the same lines as the + strand, we conceive the deformed configuration to be a helix wrapped around a curved axis defined by curvatures $k_1, k_2$ and $k_3$ along the directors $\mathbf{d}_1$, $\mathbf{d}_2$ and $\mathbf{d}_3$, respectively.

$$\mathbf{r}^-(x) = (b + r^-)(\cos(\omega x + \alpha + \beta^-)\ \mathbf{d}_1 + \sin(\omega x + \alpha + \beta^-)\ \mathbf{d}_2) + \int_0^x (1 + b\xi)\ \mathbf{d}_3 dx. \tag{19}$$

We use the same apparatus *mutatis mutandis* described for the + strand to calculate various quantities of interest. The results are:

$$\mathbf{R}^- = [\boldsymbol{n}^- \quad \boldsymbol{b}^- \quad \boldsymbol{t}^-] = \mathbf{Z}\mathbf{R}_0^-(\mathbf{1} + \mathbf{\Theta}^-). \tag{20}$$

where $\mathbf{\Theta}^-$ is a skew symmetric tensor.

$$\begin{aligned} \mathbf{\Theta}^- &= \begin{bmatrix} 0 & -\theta_3^- & \theta_2 \\ \theta_3^- & 0 & -\theta_1^- \\ -\theta_2^- & \theta_1^- & 0 \end{bmatrix}, \\ \text{where} \quad \theta_1^- &= (r^-\omega + b(\beta_x^- + k_3)), \quad \theta_2^- = -r_x^- \cos k + \beta^- \sin k, \\ \theta_3^- &= \frac{g^-}{\omega \sin k} - \frac{(r_x^- \cos k - \beta^- \sin k)\cos k}{\omega \sin k}. \end{aligned} \tag{21}$$

We compute curvature $\kappa^-$ as follows,

$$\begin{aligned} \Omega^- =& (\boldsymbol{t}_x^-.\boldsymbol{t}_x^-)^{1/2} = \omega \sin k - (r_{xx}^- + \xi)\cos k + (\beta_x^- + k_3)\sin k, \\ \kappa^- =& \Omega^- - \omega \sin k = -(r_{xx}^- + \xi)\cos k + (\beta_x^- + k_3)\sin k. \end{aligned} \tag{22}$$

We obtain the moment $\boldsymbol{m}^-$ as follows,

$$\boldsymbol{m}^- = EI\kappa^-(\cos k \cos\frac{\alpha}{2}\ \mathbf{f}_1 + \cos k \sin\frac{\alpha}{2}\ \mathbf{f}_2 + \sin k\ \mathbf{f}_3), \tag{23}$$

where $\mathbf{f}_1,\ \mathbf{f}_2,\ \mathbf{f}_3$ are given as follows.

$$\mathbf{f}_1 = \Big(\sin(\omega x + \frac{\alpha}{2})\ \mathbf{d}_1 - \cos(\omega x + \frac{\alpha}{2})\ \mathbf{d}_2\Big), \quad \mathbf{f}_2 = \Big(\cos(\omega x + \frac{\alpha}{2})\ \mathbf{d}_1 + \sin(\omega x + \frac{\alpha}{2})\ \mathbf{d}_2\Big), \quad \mathbf{f}_3 = \ \mathbf{d}_3. \tag{24}$$

# 4 Evaluation of material properties of the web

In this section, we consider a deformation of the double-helical structure induced by a stretching force $F$ and torque $T$ on one end. We assume that the helix retains its helical configuration, but with changed geometrical parameters. Thus, $r$, $\beta$ and $e$ are independent of $x$. Our goal is to compute the strains and curvatures, then evaluate the energy, and then identify the stretch modulus, twist modulus and twist-stretch coupling modulus of the double-helical structure from this energy expression. The computation of strains, curvatures, etc., of the helix proceeds as in the main text.

$$\begin{aligned} \mathbf{r}^+ &= (a + r)(\cos\omega x(1+\beta)\ \mathbf{e}_1 + \sin\omega x(1+\beta)\ \mathbf{e}_2) + x(1+e), \\ \mathbf{r}^+ &= -(a + r)(\cos\omega x(1+\beta)\ \mathbf{e}_1 + \sin\omega x(1+\beta)\ \mathbf{e}_2) + x(1+e), \end{aligned} \tag{25}$$

We assume $r, \beta, e \sim O(\varepsilon)$, hence

$$\begin{aligned} \mathbf{r}^+ &= (a + r)(\cos\omega x\ \mathbf{e}_1 + \sin\omega x\ \mathbf{e}_2) + a\omega\beta x(-\sin\omega x\ \mathbf{e}_1 + \cos\omega x\ \mathbf{e}_2) + x(1+e)\ \mathbf{e}_3, \\ \mathbf{r}_x^+ &= (a + r)\omega(-\sin\omega x\ \mathbf{e}_1 + \cos\omega x\ \mathbf{e}_2) + a\omega\beta(-\sin\omega x\ \mathbf{e}_1 + \cos\omega x\ \mathbf{e}_2) - a\omega^2, \\ &\beta x(\cos\omega x\ \mathbf{e}_1 + \sin\omega x\ \mathbf{e}_2) + (1 + (ex)_x)\ \mathbf{e}_3, \\ &= -a\omega^2\beta x(\cos\omega x\ \mathbf{e}_1 + \sin\omega x\ \mathbf{e}_2) + \omega(a + r + a\beta)(-\sin\omega x\ \mathbf{e}_1 + \cos\omega x\ \mathbf{e}_2) + (1 + (ex)_x)\ \mathbf{e}_3. \end{aligned} \tag{26}$$

The inextensibility condition gives,

$$\begin{aligned} &|\mathbf{r}_x^+| = |\mathbf{r}_{0x}^+|, \\ &(ex)_x + \omega^2 a(r + \beta) = 0, \end{aligned} \tag{27}$$

$\boldsymbol{t}_0^+$, $\boldsymbol{n}_0^+$ and $\boldsymbol{b}_0^+$ are the tangent, normal and binormal to the + strand in the reference configuration. We calculate tangent $\boldsymbol{t}^+$ to the deformed configuration.

$$\begin{aligned} \boldsymbol{t}^+ =& -\sin k\beta x(\cos\omega x\ \mathbf{e}_1 + \sin\omega x\ \mathbf{e}_2) + (\sin k + \omega r\cos k + \beta\sin k) \\ & (-\sin\omega x\ \mathbf{e}_1 + \cos\omega x\ \mathbf{e}_2) + (\cos k - \omega\sin k(r + a\beta))\ \mathbf{e}_3, \\ =& \boldsymbol{t}_0^+ + \omega\beta x\sin k\ \boldsymbol{n}_0^+ + (\omega r + \beta\tan k)\boldsymbol{b}_0^+, \end{aligned} \tag{28}$$

Next, we calculate the curvature $\kappa^+$.

$$\begin{aligned} \boldsymbol{t}_x^+ =& -(\omega\sin k 2\omega\beta\sin k + \omega^2 r\cos k)(\cos\omega x\ \mathbf{e}_1 + \sin\omega x\ \mathbf{e}_2) \\ & - \omega^2\sin k\beta x(-\sin\omega x\ \mathbf{e}_1 + \cos\omega x\ \mathbf{e}_2). \\ K^2 =& \omega\sin k + 2\omega\beta\sin k + \omega^2 r\cos k. \\ \kappa^+ =& K - \omega\sin k = 2\omega\beta\sin k + \omega^2 r\cos k. \end{aligned} \tag{29}$$

We go on to calculate the normal in the deformed configuration $\boldsymbol{n}^+$.

$$\begin{aligned}\boldsymbol{n}^+ =& -(\cos\omega x\ \mathbf{e}_1 + \sin\omega x\ \mathbf{e}_2) - \omega\beta x(-\sin\omega x\ \mathbf{e}_1 + \cos\omega x\ \mathbf{e}_2),\\ =&\boldsymbol{n}_0^+ - \omega\beta x\sin k\boldsymbol{t}_0^+ + \omega\beta x\cos k\boldsymbol{b}_0^+.\end{aligned} \tag{30}$$

We are now in a position to calculate the deformed Frenet-Serret frame $\mathbf{R}^+$.

$$\mathbf{R}^+ = [\boldsymbol{n}^+ \quad \boldsymbol{b}^+ \quad \boldsymbol{t}^+] = \mathbf{R}_0^+(\mathbf{1} + \boldsymbol{\Theta}^+). \tag{31}$$

where $\boldsymbol{\Theta}^+$ is a skew symmetric tensor.

$$\begin{aligned}\boldsymbol{\Theta}^+ = \begin{bmatrix} 0 & -\theta_3^+ & \theta_2^+ \\ \theta_3^+ & 0 & -\theta_1^+ \\ -\theta_2^+ & \theta_1^+ & 0\end{bmatrix},\\ \text{where} \qquad \theta_1^+ = \omega r + \beta\tan k, \quad \theta_2^+ = \omega\beta x\sin k, \quad \theta_3^+ = \omega\beta x\cos k.\end{aligned} \tag{32}$$

For the negative strand we follow the same procedure.

$$\begin{aligned}\mathbf{R}^- &= [\boldsymbol{n}^- \quad \boldsymbol{b}^- \quad \boldsymbol{t}^-] = \mathbf{R}_0^-(\mathbf{1} + \boldsymbol{\Theta}^-),\\ \boldsymbol{\Theta}^- &= \boldsymbol{\Theta}^+,\\ \kappa^- &= \kappa^+.\end{aligned} \tag{33}$$

After performing all the calculations

$$\begin{aligned}E = \int_0^L (EI(2\omega\beta\sin k + \omega^2 r\cos k)^2 + \frac{1}{2}H_1\omega^2(r + a\beta)^2 + \frac{1}{2}L_1 r^2) - M\theta - F\Delta x,\\ \Delta x = eL, \qquad \theta = \beta L.\end{aligned} \tag{34}$$

We substitute $r = -\frac{e}{\omega^2 a} - a\beta$ from eqn. (27) and compute the elastic constants as follows.

$$\begin{aligned}&\frac{\partial E}{\partial\beta} = 0, \qquad \frac{\partial E}{\partial e} = 0.\\ &S = \frac{\partial^2 E}{\partial e^2}, \quad g = \frac{\partial^2 E}{\partial e\partial\beta}, \quad C = \frac{\partial^2 E}{\partial\beta^2}.\end{aligned} \tag{35}$$

Then, by trial and error we pick values of $L_1, L_2, L_3, H_1, H_2, H_3, K_c, K_e, EI$ to match the $S, g, C$ known from experiments. Our choice of the material parameters $L_1, H_2, K_c$, etc., is not unique.

# 5 Choice of eigenvalues obtained in section 5

In section 5, we solve the governing differential equation eqn. 3.33 by substituting $y(x) = y_0 e^{-\lambda x}$ where $y = (r, f, \xi, k_3, \beta^\pm, n_i^c, n_i)$ $i = 1, 2, 3$. We look for the values of $\lambda$ corresponding to a non-trivial solution of the governing equations. For this we need to solve the eigenvalue problem $\mathcal{A}(\lambda)\mathbf{v}_0 = 0$, where $\mathcal{A}$ is a function of $\lambda$ and elastic constants (eqn. 4.1) and $\mathbf{v}_0 = [r_0, f_0, \xi_0, k_{30}, \beta_0^+, \beta_0^-, n_{i0}^c, n_{i0}]^T \quad i = 1, 2, 3$. We set $\det\mathcal{A}(\lambda) = 0$ and get following solutions for $\lambda$.

$$\begin{aligned}&x_1 = -1.5\times 10^4(1+i), \quad x_2 = -1.5\times 10^4(-1+i), \quad x_3 = -4\times 10^3, \quad x_4 = 1.2\times 10^3(-1-3.2i),\\ &x_5 = 1.2\times 10^3(-1+3.2i), \quad x_6 = -0.68, \quad x_7 = -0.42, \quad x_8 = -0.36, \quad x_9 = -5.2\times 10^{-10},\\ &x_{10} = -1.9i, \quad x_{11} = 1.9i, \quad x_{12} = -3.8i, \quad x_{13} = 3.8i, \quad x_{14} = -6.2i, \quad x_{15} = 6.2i,\\ &x_{16} = 5.2\times 10^{-10}, \quad x_{17} = 0.36, \quad x_{18} = 0.42, \quad x_{19} = 0.68, \quad x_{20} = 2.3\times 10^3(1.4-i),\\ &x_{21} = 2.3\times 10^3(1.4+i), \quad x_{22} = 1.5\times 10^4(1-i), \quad x_{23} = 1.5\times 10^4(1+i).\end{aligned} \tag{36}$$

Among these 23 eigenvalues we neglect the eigenvalues $x_{1,2,3,4,5,20,21,22,23}$ whose magnitude is $> 10^3$ because the corresponding decay length is tiny which leads to large numerical errors given that we need to compute third derivatives. Then, there are small eigenvalues $x_{9,16}$ whose magnitude is close to zero ($< 10^{-3}$) and purely imaginary eigenvalues $x_{10,11,12,13,14,15}$ which when substituted in $e^{-\lambda x}$ result in a constant or a sinusoidal function, respectively, that do not decay to 0 as $x \to \pm\infty$. Hence, we must neglect these too. This leaves us with $x_{6,7,8,17,18,19}$, which are used in section 5.

# 6 Results for $\alpha = \pi$ radians

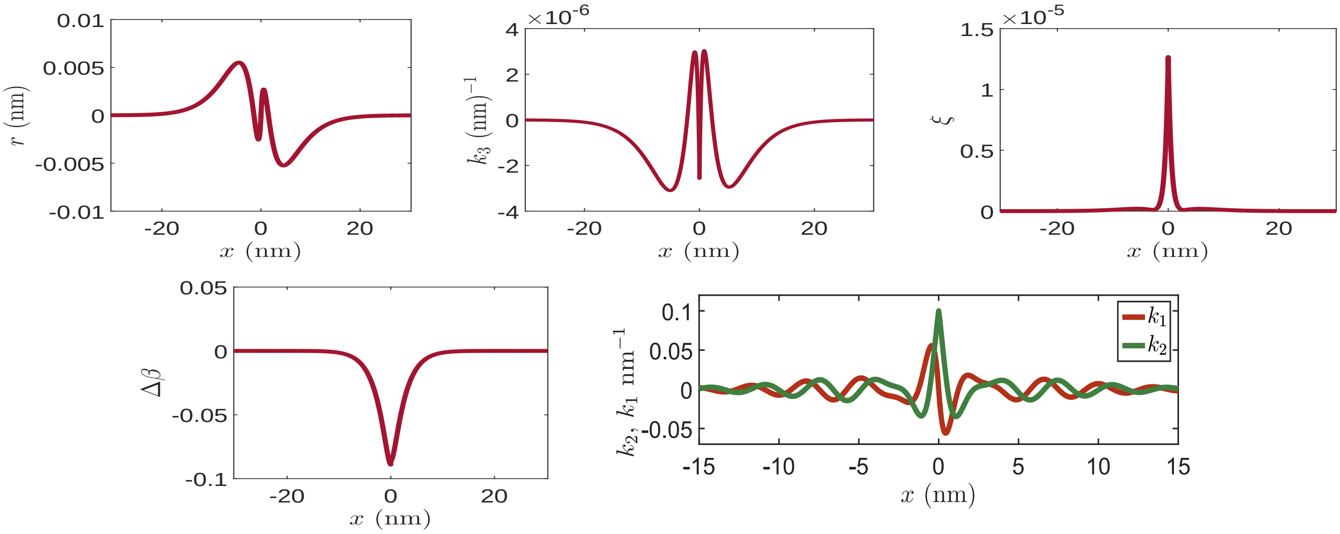


Figure 3: Variation of strain variables for $\alpha = \pi$ radians. Notice that the curves are symmetric about the site of protein binding. As mentioned in section 6, the curves are not symmetric if we choose $\alpha = 2.1$ radians.

# References


[1] Moakher, M. and Maddocks, J.H., 2005. A double-strand elastic rod theory. Archive for rational mechanics and analysis, 177(1), pp.53-91.