DNA Modelling Course
Exercise Session 4
Summer 2006 Part 1

SOLUTIONS

1 Equilibria of an Inextensible and Unshearable Rod without Twist

We are considering an inextensible,unshearable rod with a straight reference configuration $\{\hat{\boldsymbol{r}}, \hat{\boldsymbol{d}}_i\}$ for which

$$(\hat{v}_1, \hat{v}_2, \hat{v}_3) = (0, 0, 1), \qquad (\hat{u}_1, \hat{u}_2, \hat{u}_3) = (0, 0, 0).$$

The equilibrium and inextensibility/unshearability conditions require

$$\left.\begin{aligned} \boldsymbol{n}' &= \boldsymbol{0} \\ \boldsymbol{m}' + \boldsymbol{r}' \times \boldsymbol{n} &= \boldsymbol{0} \\ \boldsymbol{r}' &= \boldsymbol{d}_3 \\ \boldsymbol{d}_i' &= \boldsymbol{u} \times \boldsymbol{d}_i \end{aligned}\right\} \qquad \forall s \in (0, L) \tag{1.1}$$

where

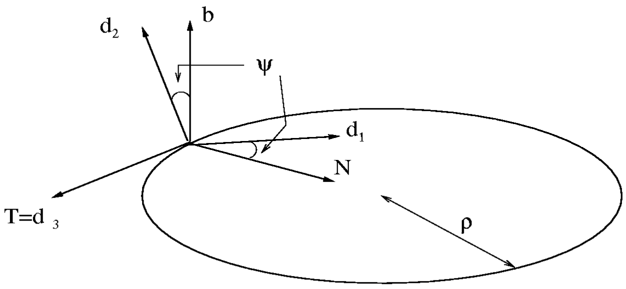
$$\boldsymbol{m} = \mathsf{K}_1(u_1 - \hat{u}_1)\boldsymbol{d}_1 + \mathsf{K}_2(u_2 - \hat{u}_2)\boldsymbol{d}_2 + \mathsf{K}_3(u_3 - \hat{u}_3)\boldsymbol{d}_3$$

and $\boldsymbol{n}$ is an unknown vector function to be determined as part of the solution of (1.1).

We can answer parts (a)-(c) all at once by considering a general untwisted, circular configuration $\{\boldsymbol{r}, \boldsymbol{d}_i\}$. To begin, suppose $\boldsymbol{r}(s)$, $s \in [0, L]$, traces out a circle. Since the rod is inextensible/unshearable, the parameter s is an arclength parameter and the circle radius must be $\rho = L/(2\pi)$. Next, let $\{\boldsymbol{T}(s), \boldsymbol{N}(s), \boldsymbol{B}(s)\}$ be the Frenet frame for the circle and note that we must have $\boldsymbol{d}_3(s) = \boldsymbol{T}(s)$. Also, note that $\boldsymbol{B}(s)$ is actually a constant unit vector, say $\boldsymbol{b}$. A general untwisted, circular configuration may thus be defined (up to a rigid translation and rotation) by

$$\left.\begin{aligned} \boldsymbol{d}_1(s) &= \cos(\psi)\boldsymbol{N}(s) + \sin(\psi)\boldsymbol{b} \\ \boldsymbol{d}_2(s) &= \cos(\psi)\boldsymbol{b} - \sin(\psi)\boldsymbol{N}(s) \\ \boldsymbol{d}_3(s) &= \boldsymbol{T}(s) \end{aligned}\right\} \tag{1.2}$$

where $0 \leq \psi < 2\pi$ is a fixed angle and $\boldsymbol{b}$ is a fixed unit vector. For $\psi = 0$ we have a circle with $\boldsymbol{d}_1(s)$ pointing toward the circle's center and $\boldsymbol{d}_2(s) = \boldsymbol{b}$, and so on.



Using the Frenet formulas we have

$$\boldsymbol{T}' = \kappa \boldsymbol{N} \qquad \text{and} \qquad \boldsymbol{N}' = -\kappa \boldsymbol{T}$$

where $\kappa = 1/\rho$ is the constant curvature of the circle. A straightforward computation gives

$$(u_1, u_2, u_3) = (\kappa \sin(\psi), \kappa \cos(\psi), 0)$$

and so

$$\boldsymbol{m}(s) = \kappa \mathsf{K}_1 \sin(\psi) \boldsymbol{d}_1(s) + \kappa \mathsf{K}_2 \cos(\psi) \boldsymbol{d}_2(s).$$

The equilibrium equation $(1.1)_1$ requires $\boldsymbol{n}(s) \equiv \boldsymbol{c}$ for some constant vector $\boldsymbol{c}$, and equation $(1.1)_2$ then requires

$$\boldsymbol{m}'(s) = \boldsymbol{c} \times \boldsymbol{T}(s), \qquad \forall s \in (0, L),$$

or

$$\kappa^2 \sin(\psi) \cos(\psi) [\mathsf{K}_2 - \mathsf{K}_1] \boldsymbol{T}(s) = \boldsymbol{c} \times \boldsymbol{T}(s), \qquad \forall s \in (0, L). \tag{1.3}$$

Taking the dot product of the above equation with each of the basis vectors $\{\boldsymbol{T}(s), \boldsymbol{N}(s), \boldsymbol{b}\}$ leads to the conclusion

$$\left.\begin{array}{l} \kappa^2 \sin(\psi) \cos(\psi) [\mathsf{K}_2 - \mathsf{K}_1] = 0 \\ \boldsymbol{c} \times \boldsymbol{T}(s) = \boldsymbol{0}. \end{array}\right\} \tag{1.4}$$

The second equation implies that $\boldsymbol{c}$ must be parallel to $\boldsymbol{T}(s)$ for all $s \in (0, L)$. Since $\boldsymbol{c}$ is constant we must have $\boldsymbol{c} = \boldsymbol{0}$. The first equation is satisfied if

$$\left.\begin{array}{ll} \psi = 0, \frac{\pi}{2}, \pi, \frac{3\pi}{2}, & \forall\, \mathsf{K}_1, \mathsf{K}_2 > 0 \\ \mathsf{K}_1 = \mathsf{K}_2 > 0, & \forall\, \psi \in [0, 2\pi). \end{array}\right\} \tag{1.5}$$

(a) Choosing $\psi = 0$ and $\boldsymbol{b} = \boldsymbol{e}_2$ we have an untwisted, circular equilibrium with $\boldsymbol{d}_2 = \boldsymbol{e}_2$ and

$$\boldsymbol{n}(s) = \boldsymbol{0} \quad \text{and} \quad \boldsymbol{m}(s) = \kappa \mathsf{K}_2 \boldsymbol{b}.$$

The end loads $\boldsymbol{g}$ and $\boldsymbol{h}$ at $s = 0, L$ required for this equilibrium are

$$\left.\begin{array}{ll} \boldsymbol{g}(0) = \boldsymbol{0}, & \boldsymbol{g}(L) = \boldsymbol{0}, \\ \boldsymbol{h}(0) = -\kappa \mathsf{K}_2 \boldsymbol{b}, & \boldsymbol{h}(L) = \kappa \mathsf{K}_2 \boldsymbol{b}. \end{array}\right\}$$

(b) Choosing $\psi = \frac{\pi}{2}$ and $\boldsymbol{b} = \boldsymbol{e}_1$ we have an untwisted, circular equilibrium with $\boldsymbol{d}_1 = \boldsymbol{e}_1$ and

$$\boldsymbol{n}(s) = \boldsymbol{0} \quad \text{and} \quad \boldsymbol{m}(s) = \kappa \mathsf{K}_1 \boldsymbol{b}.$$

The end loads $\boldsymbol{g}$ and $\boldsymbol{h}$ at $s = 0, L$ required for this equilibrium are

$$\left.\begin{array}{ll} \boldsymbol{g}(0) = \boldsymbol{0}, & \boldsymbol{g}(L) = \boldsymbol{0}, \\ \boldsymbol{h}(0) = -\kappa \mathsf{K}_1 \boldsymbol{b}, & \boldsymbol{h}(L) = \kappa \mathsf{K}_1 \boldsymbol{b}. \end{array}\right\}$$

Note that this equilibrium is genuinely different from the one in part (a). That is, these equilibria are not related by a rigid translation and rotation. Moreover, if $\mathsf{K}_1 \neq \mathsf{K}_2$, different end moments are required to maintain these equilibria.

(c) If $\mathsf{K}_1 \neq \mathsf{K}_2$, there are four genuinely different equilibria, one for each of the values $\psi = 0$, $\frac{\pi}{2}$, π and $\frac{3\pi}{2}$. If $\mathsf{K}_1 = \mathsf{K}_2$, there is a one-parameter family of genuinely different equilibria, one for each $\psi \in [0, 2\pi)$.

2 Equilibria of an Inextensible and Unshearable Rod with Twist

(a) We are given a straight, uniformly twisted configuration $\{\boldsymbol{r}, \boldsymbol{d}_i\}$ for which

$$(v_1, v_2, v_3) = (0, 0, 1), \qquad (u_1, u_2, u_3) = (0, 0, \eta)$$

where $\eta = \frac{2\pi\vartheta}{L}$. The configuration $\{\boldsymbol{r}, \boldsymbol{d}_i\}$ is an equilibrium (with $\{\hat{\boldsymbol{r}}, \hat{\boldsymbol{d}}_i\}$ serving as the reference) if the equations (1.1) are satisfied with

$$\boldsymbol{m}(s) = \eta \mathsf{K}_3 \boldsymbol{d}_3(s) = \eta \mathsf{K}_3 \boldsymbol{e}_3.$$

Equation $(1.1)_3$ is clearly satisfied and equation $(1.1)_1$ requires $\boldsymbol{n}(s) \equiv \boldsymbol{c}$ for some constant vector $\boldsymbol{c}$. Equation $(1.1)_2$ then requires

$$\boldsymbol{m}'(s) = \boldsymbol{c} \times \boldsymbol{e}_3, \qquad \forall s \in (0, L),$$

or

$$\boldsymbol{c} \times \boldsymbol{e}_3 = \boldsymbol{0}. \tag{2.6}$$

We see that equilibrium holds with $\boldsymbol{m}(s) = \eta \mathsf{K}_3 \boldsymbol{e}_3$ and $\boldsymbol{n}(s) = \gamma \boldsymbol{e}_3$ for any constant $\gamma \in \mathbb{R}$. The end loads $\boldsymbol{g}$ and $\boldsymbol{h}$ at $s = 0, L$ required for this equilibrium are

$$\left.\begin{array}{ll} \boldsymbol{g}(0) = -\gamma \boldsymbol{e}_3, & \boldsymbol{g}(L) = \gamma \boldsymbol{e}_3, \\ \boldsymbol{h}(0) = -\eta \mathsf{K}_3 \boldsymbol{e}_3, & \boldsymbol{h}(L) = \eta \mathsf{K}_3 \boldsymbol{e}_3. \end{array}\right\}$$

(b) A uniformly twisted, circular configuration can be defined using the apparatus described in parts (a)-(c). In particular, we now assume $\psi = \eta s$ for some constant twist rate $\eta \in \mathbb{R}$. A straightforward computation gives

$$(u_1, u_2, u_3) = (\kappa \sin(\psi), \kappa \cos(\psi), \eta)$$

and so

$$\boldsymbol{m}(s) = \kappa \mathsf{K}_1 \sin(\psi)\boldsymbol{d}_1(s) + \kappa \mathsf{K}_2 \cos(\psi)\boldsymbol{d}_2(s) + \eta \mathsf{K}_3 \boldsymbol{d}_3(s).$$

The equilibrium equation $(1.1)_1$ requires $\boldsymbol{n}(s) \equiv \boldsymbol{c}$ for some constant vector $\boldsymbol{c}$, and equation $(1.1)_2$ then requires

$$\boldsymbol{m}'(s) = \boldsymbol{c} \times \boldsymbol{T}(s), \qquad \forall s \in (0, L),$$

or

$$\begin{aligned}
&\kappa^2 \sin(\eta s)\cos(\eta s)[\mathsf{K}_2 - \mathsf{K}_1]\boldsymbol{T}(s) \\
&\quad + \kappa\eta[\mathsf{K}_3 + \cos(2\eta s)(\mathsf{K}_1 - \mathsf{K}_2)]\boldsymbol{N}(s) \\
&\qquad + 2\kappa\eta \sin(\eta s)\cos(\eta s)[\mathsf{K}_1 - \mathsf{K}_2]\boldsymbol{b} = \boldsymbol{c} \times \boldsymbol{T}(s), \qquad \forall s \in (0, L).
\end{aligned} \tag{2.7}$$

Taking the dot product of the above equation with each of the basis vectors $\{\boldsymbol{T}(s), \boldsymbol{N}(s), \boldsymbol{b}\}$ leads to the conclusion

$$\left.\begin{aligned}
&\kappa^2 \sin(\eta s)\cos(\eta s)[\mathsf{K}_2 - \mathsf{K}_1] = 0 \\
&\kappa\eta[\mathsf{K}_3 + \cos(2\eta s)(\mathsf{K}_1 - \mathsf{K}_2)] = \boldsymbol{c} \cdot \boldsymbol{b} \\
&2\kappa\eta \sin(\eta s)\cos(\eta s)[\mathsf{K}_1 - \mathsf{K}_2] = -\boldsymbol{c} \cdot \boldsymbol{N}(s).
\end{aligned}\right\} \tag{2.8}$$

Because $\boldsymbol{c} \cdot \boldsymbol{b}$ is a constant, independent of $s \in (0, L)$, the only way $(2.8)_2$ can hold is if $\mathsf{K}_1 = \mathsf{K}_2$. In this case, we obtain

$$\left.\begin{aligned}
\boldsymbol{c} \cdot \boldsymbol{b} &= \kappa\eta\mathsf{K}_3 \\
\boldsymbol{c} \cdot \boldsymbol{N}(s) &= 0.
\end{aligned}\right\}$$

Since $\boldsymbol{c}$ is constant and $\boldsymbol{c} \cdot \boldsymbol{N}(s) = 0$, it follows that $\boldsymbol{c} \cdot \boldsymbol{T}(s)$ is constant. Moreover, since $\boldsymbol{T}(s)$ spans the plane normal to $\boldsymbol{b}$ as s varies, it follows that $\boldsymbol{c}$ must be parallel to $\boldsymbol{b}$. In particular, we must have $\boldsymbol{c} = \kappa\eta\mathsf{K}_3\boldsymbol{b}$. Thus, equilibrium holds only when $\mathsf{K}_1 = \mathsf{K}_2$, in which case we have

$$\left.\begin{aligned}
\boldsymbol{n}(s) &= \kappa\eta\mathsf{K}_3\boldsymbol{b} \\
\boldsymbol{m}(s) &= \kappa \mathsf{K}_1 \sin(\eta s)\boldsymbol{d}_1(s) + \kappa \mathsf{K}_2 \cos(\eta s)\boldsymbol{d}_2(s) + \eta \mathsf{K}_3 \boldsymbol{d}_3(s).
\end{aligned}\right\}$$

3 Computation of Unit Quaternion

The rotation matrix $\boldsymbol{Q}$ is given by

$$\boldsymbol{Q} = \begin{pmatrix} \cos(s) & -\sin(s) & 0 \\ \sin(s) & \cos(s) & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

The axis of rotation $\boldsymbol{k}$ is in the nullspace of $\boldsymbol{Q} - \boldsymbol{Q}^T$ such that we obtain

$$\boldsymbol{k} = \begin{pmatrix} k_1 \\ k_2 \\ k_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

For the angle of rotation ϕ we have the relation

$$\mathrm{tr}(\boldsymbol{Q}) = 1 + 2\cos\phi \;=\; 1 + 2\cos(s),$$

which immediately provides us with

$$\phi = \pm s.$$

The correct sign is obtained by verifying the result. Thus, we get

$$\phi = -s.$$

The unit quaternion is now obtained as

$$q_i(s) \;=\; k_i \sin(\phi/2), \qquad i = 1, 2, 3, \qquad q_4 = \cos(\phi/2),$$

such that

$$\boldsymbol{q} = \begin{pmatrix} q_1 \\ q_2 \\ q_3 \\ q_4 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \sin(-s/2) \\ \cos(-s/2) \end{pmatrix}.$$

Note that we obtain

$$\boldsymbol{q}(s=0) \;=\; \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \qquad \boldsymbol{q}(s=2\pi) \begin{pmatrix} 0 \\ 0 \\ 0 \\ -1 \end{pmatrix}.$$