DNA Modelling Course
Exercise Session 1
Summer 2006

SOLUTIONS

Calculus of Variations

We are looking for minimizers $\boldsymbol{y}$ of the functional I where

$$I = \int_0^1 F(s, \boldsymbol{y}, \boldsymbol{y}')\ ds. \tag{1.1}$$

and where $\boldsymbol{y}$ fulfills some boundary conditions.
From the Fundamental Lemma of Calculus of Variation we get the necessary Euler-Lagrange equation

$$F_{\boldsymbol{y}}(s, \boldsymbol{y}, \boldsymbol{y}')\ - \frac{d}{ds}\ F_{\boldsymbol{y}'}(s, \boldsymbol{y}, \boldsymbol{y}') = 0. \tag{1.2}$$

Here $\boldsymbol{y} = \phi$ is a function in $\mathbb{R}$. Set

$$F(s, \phi, \phi') = K_2(\phi' - \hat{u}_2)^2/2 + \lambda \cos\phi + \nu \sin\phi. \tag{1.3}$$

Using (1.2) the Euler-Lagrange equation is

$$-(K_2(\phi' - \hat{u}_2))' - \lambda \sin\phi + \nu \cos\phi = 0. \tag{1.4}$$

1. Both boundary conditions are imposed. No Natural boundary condition.
2. We get one Natural boundary condition $K_2(1)(\phi'(1) - \hat{u}_2(1)) = 0$, i.e. $m_2(1) = 0$.
3. Two Natural boundary conditions $K_2(0)(\phi'(0) - \hat{u}_2(0)) = 0$ and $K_2(1)(\phi'(1) - \hat{u}_2(1)) = 0$, i.e. $m_2(0) = m_2(1) = 0$.

Introduction to Link interal

Problem 1

Look at the chapter 9. DNA Supercoiling on the web. Follow the proof of the second part of Theorem 1 (on page 104/5).

Problem 2

1. Suppose $y(\sigma)$ and $x(s)$ can be moved by homotopy to opposite sides of a plane. Denote by $x_L(s)$ the image of the translation

$$T_L : \mathbb{R}^3 \to \mathbb{R}^3,\ x \mapsto x + L,$$

where $L \in \mathbb{R}^3$ perpendicular to the plane. Then $x_L(s)$ is a homotopic image of $x(s)$, $y \cap x_L = \emptyset$ and

$$\frac{1}{2}|L| < |x_L(s) - y(\sigma)| < 2|L|$$

for $|L|$ sufficiently large (e.g. for $|L| > 2\sup_{(s,\sigma)} |x(s) - y(\sigma)|$).

$$\begin{aligned}
|Lk(T_L C_1, C_2)| &= \left| \frac{1}{4\pi} \int_{T_L C_1} \int_{C_2} \frac{(y(\sigma) - x_L(s)) \cdot (y'(\sigma) \times x_L'(s))}{|y(\sigma) - x_L(s)|^3} d\sigma\, ds \right| \\
&\le \frac{1}{4\pi} \int_{T_L C_1} \int_{C_2} \frac{|y(\sigma) - x_L(s)|\, |y'(\sigma) \times x_L'(s)|}{|y(\sigma) - x_L(s)|^3} d\sigma\, ds \\
&\le \frac{1}{4\pi} \int_{T_L C_1} \int_{C_2} \frac{|y(\sigma) - x_L(s)|\, |y'(\sigma)|\ |x_L'(s)|}{|y(\sigma) - x_L(s)|^3} d\sigma\, ds \\
&\le \frac{1}{4\pi} \int_{T_L C_1} \int_{C_2} \frac{2|L|}{(\frac{1}{2}|L|)^3} d\sigma\, ds = \frac{1}{4\pi} \frac{16}{|L|^2} \int_{T_L C_1} \int_{C_2} d\sigma\, ds < \text{const} \frac{1}{|L|^2}.
\end{aligned}$$

And therefore (for $|L|$ sufficiently large)

$$|Lk(C_1, C_2)| = |Lk(T_L C_1, C_2)| = 0.$$

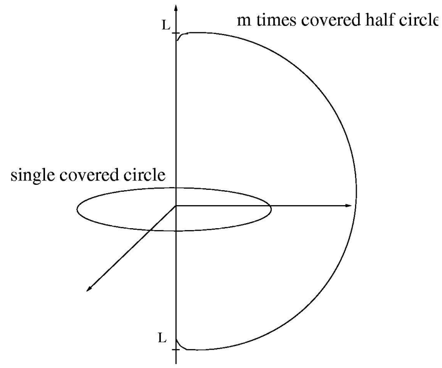
2. The two mini-circles of a double-helix can be deformed by a homotopy to a single covered circle (let it be centered at origin and lie in the horizontal plane) and a multiply (say m times) covered semi-circle plus its chord in the vertical plane. The chord is the vertical straight part that passes through the origin, and the semi-circle is a smooth loop that is outside the unit ball with centre at the origin; the semi-circle and the chord are smoothly closed.

   Let D_L be the dilatation by L, where $L > 0$. We denote by x_L the image of x of this dilatation. Then we have for some constants $c_1 < c_2$

$$c_1 L < |x_L(s) - y(\sigma)| < c_2 L$$

for L sufficiently large, for the non-straight part of x_L. We denote

$$I_{Lk}(\sigma, s) = \frac{(y(\sigma) - x_L(s)) \cdot (y'(\sigma) \times x_L'(s))}{|y(\sigma) - x_L(s)|^3}.$$



Then

$$\begin{aligned} Lk(D_L C_1, C_2) &= \frac{1}{4\pi} \int_{D_L C_1} \int_{C_2} I_{Lk}(\sigma, s) d\sigma\, ds \\ &= \frac{m}{4\pi} \int_{-L}^{L} \int_{C_2} I_{Lk}(\sigma, s) d\sigma\, ds + \frac{m}{4\pi} \int_{semi-arc} \int_{C_2} I_{Lk}(\sigma, s) d\sigma\, ds. \end{aligned}$$

On the straight part of x_L we have

$$\begin{aligned} x_L(s) &= (0,0,s), & x_L'(s) &= (0,0,1), \\ y(\sigma) &= (\cos\sigma, \sin\sigma, 0), & y'(\sigma) &= (-\sin\sigma, \cos\sigma, 0) \end{aligned}$$

and therefore

$$\begin{aligned} &\int_{-L}^{L} \int_{C_2} I_{Lk}(\sigma, s) d\sigma\, ds \\ &= \int_{-L}^{L} \int_{C_2} \frac{(\cos\sigma, \sin\sigma, -s) \cdot (\cos\sigma, \sin\sigma, 0)}{\sqrt{1+s^2}^3} d\sigma\, ds \\ &= \int_{-L}^{L} \int_{C_2} \frac{1}{\sqrt{1+s^2}^3} d\sigma\, ds = \int_{C_2} d\sigma \int_{-L}^{L} \frac{1}{\sqrt{1+s^2}^3} ds \\ &= 2\pi \int_{-L}^{L} \frac{1}{\sqrt{1+s^2}^3} ds \end{aligned}$$

Now we substitute $s = \sinh z$ and use the facts that $1 + \sinh^2 z = \cosh^2 z$, $\tanh' z = \frac{1}{\cosh^2 z}$, $\sinh' z = \cosh z$, $\tanh(-z) = -\tanh z$ and $\tanh z \rightarrow 1$ for $z \rightarrow \infty$.

$$\begin{aligned} &\int_{-L}^{L} \frac{1}{(\sqrt{1+s^2})^3} ds = \int_{\sinh^{-1} -L}^{\sinh^{-1} L} \frac{\cosh z}{(\sqrt{\cosh^2 z})^3} dz \\ = &\int_{\sinh^{-1} -L}^{\sinh^{-1} L} \frac{1}{\cosh^2 z} dz = \tanh z \Big|_{\sinh^{-1} -L}^{\sinh^{-1} L} \rightarrow 2, \qquad \text{for } L \rightarrow \infty. \end{aligned}$$

Now we calculate the second integral.

$$
\begin{aligned}
& \left| \int_{semi-arc} \int_{C_2} I_{Lk}(\sigma, s) d\sigma\, ds \right| \\
\leq \quad & \int_{semi-arc} \int_{C_2} \frac{|y(\sigma) - x_L(s)|\, |y'(\sigma)|\, |x'_L(s)|}{|y(\sigma) - x_L(s)|^3} d\sigma\, ds \Bigg| \\
\leq \quad & \frac{16}{L^2} \int_{semi-arc} \int_{C_2} d\sigma\, ds \ \leq \ \frac{const}{L} \to \ 0, \qquad \text{for } L \to \infty.
\end{aligned}
$$

This yields

$$Lk(D_L C_1, C_2) = m,$$

that is, a DNA mini-circle with one strand wrapped m times around the other has Link m.