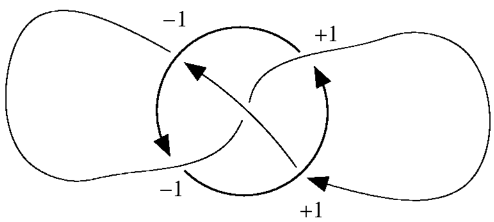
DNA Modelling Course
Exercise Session 2
Summer 2006 Part 2

SOLUTIONS

Problem 1: The linking number of the Whitehead link

We have given a projection of two curves. First orient the two curves. Assign to each crossing between the two curves $+1$ or -1 depending on the sign of the crossing. (For instance, move the curves such that they lie perpendicular to each other in the crossings. Then, if you have to turn the curve above $+\frac{\pi}{2}$ to line up with the correct orientation of the curve below assign $+1$ to the crossing. If you have to turn the curve above $-\frac{\pi}{2}$ to line up with the right orientation of the curve below assign -1 to the crossing.) Then sum over each crossing the corresponding $+1$ or -1 and divide the sum by 2.
For the Whitehead link we get $Lk = \frac{1}{2}(-1+1-1+1) = 0$. We have seen in the



previous Problem, that a link which can be 'physically unlinked' has $Lk = 0$. But the contrary is not true! The Whitehead link is an example of a link with $Lk = 0$, where the two curves cannot be 'physically unlinked'.

Problem 2: Properties and Computation of Writhe integral

Problem 2a.)

This follows of the fact $a \times b = -b \times a$ for all $a, b \in \mathbb{R}^3$ and the bilinearity of the scalar product.

Problem 2b.)

Look at the chapter 9. Supercoiling on the web. Follow the proof of the lemma on page 6-7.

Problem 2c.)

- Translation $x \mapsto x + a,\ a \in \mathbb{R}^3$

$$\begin{aligned}(x+a)(\sigma) - (x+a)(s) &= x(\sigma) - x(s),\\ (x+a)'(\sigma) \times (x+a)'(s) &= x'(\sigma) \times x'(s)\end{aligned}$$

- Rotation $x \mapsto Rx,\ RR^t = I,\ |R| = 1$
  It holds for any rotation R

$$\begin{aligned}Ra \cdot Rb &= a \cdot b\\ Ra \times Rb &= R(a \times b)\end{aligned}$$

  In particular, every rotation is isometric and leaves volume invariant. The derivative of the rotated curve it the rotated tangent, i.e. $(Rx)' = Rx'$. This completes the proof.

- Dilation $x \mapsto \lambda x,\ \lambda > 0$
  Both, the scalar product and the cross product are bi-linear, therefore

$$\begin{aligned}&(\lambda x(\sigma) - \lambda x(s)) \cdot (\lambda x'(\sigma) \times \lambda x'(s))\\ =\ &(\lambda x(\sigma) - \lambda x(s)) \cdot (\lambda^2 (x'(\sigma) \times x'(s)))\\ =\ &\lambda^3\ (x(\sigma) - x(s)) \cdot (x'(\sigma) \times x'(s))\end{aligned}$$

  and the Writhe integrand remains invariant.

Problem 2d.)

Using the results from Problem 3, it is sufficient to consider a reflection in the (e_1, e_2)-plane. We denote by Ix the reflection of x in the (e_1, e_2)-plane. Then

$$\begin{aligned}&\frac{(Ix(\sigma) - Ix(s)) \cdot ((Ix)'(\sigma) \times (Ix)'(s))}{|Ix(\sigma) - Ix(s)|^3}\\
=\ &\frac{\begin{pmatrix} x_1(\sigma) - x_1(s)\\ x_2(\sigma) - x_2(s)\\ -x_3(\sigma) + x_3(s)\end{pmatrix} \cdot \begin{pmatrix} x_1'(\sigma)\\ x_2'(\sigma)\\ -x_3'(\sigma)\end{pmatrix} \times \begin{pmatrix} x_1'(s)\\ x_2'(s)\\ -x_3'(s)\end{pmatrix}}{\left|\begin{matrix} x_1(\sigma) - x_1(s)\\ x_2(\sigma) - x_2(s)\\ -x_3(\sigma) + x_3(s)\end{matrix}\right|^3}\\
=\ &-\frac{\begin{pmatrix} x_1(\sigma) - x_1(s)\\ x_2(\sigma) - x_2(s)\\ x_3(\sigma) - x_3(s)\end{pmatrix} \cdot \begin{pmatrix} x_1'(\sigma)\\ x_2'(\sigma)\\ x_3'(\sigma)\end{pmatrix} \times \begin{pmatrix} x_1'(s)\\ x_2'(s)\\ x_3'(s)\end{pmatrix}}{|x(\sigma) - x(s)|^3}\\
=\ &-\frac{(x(\sigma) - x(s)) \cdot (x'(\sigma) \times x'(s))}{|x(\sigma) - x(s)|^3}.\end{aligned}$$

The Writhe of the reflection of the curve x in the plane is the negative of the Writhe of the curve.

This property and the fact that Writhe of a curve is independent of the orientation of the curve implies that the Writhe of any curve which has a plane of symmetry (i.e. is a mirror image of itself) is zero.

Problem 2e.)

If the curve lies in a plane, then

$$(x(\sigma) - x(s)) \perp (x'(\sigma) \times x'(s)) \qquad \forall \sigma, s.$$

Therefore the Writhe integrand vanishes pointwise.

Problem 2f.)

The curve $x(s)$ is symmetric with respect to the plane $X = \frac{l}{2}$ (if the length of the links is assumed to be l). We denote by Ix the reflection of x in this plane and by $\tilde{x}$ the curve x with the opposite orientatin, i.e. $\tilde{x}(s) = x(L - s)$ for all $s \in [0, L]$.

The symmetry implies $Ix = \tilde{x}$. Then by Problem 4 we get $Wr(x) = -Wr(Ix) = -Wr(\tilde{x}) = -Wr(x)$. The last equality is true because Writhe is independent of the orientation of the curve. Thus $Wr(x) = 0$.

Problem 2g.)

First we paremeterize the curve, e.g. for $s \in [1, 4]$ we define

$$\boldsymbol{x}(s) = \begin{cases} \begin{pmatrix} 1-s \\ s \\ 0 \end{pmatrix} & \text{for } s \in [0,1) \\ \begin{pmatrix} 0 \\ 1-s \\ 0 \end{pmatrix} & \text{for } s \in [1,2) \\ \begin{pmatrix} s \\ 0 \\ s \end{pmatrix} & \text{for } s \in [2,3) \\ \begin{pmatrix} 1 \\ 0 \\ 1-s \end{pmatrix} & \text{for } s \in [3,4) \end{cases} \tag{0.1}$$

We split the double integral into a sum of 16 double integrals, of which most vanish.

$$\begin{aligned} Wr(C) &= \frac{1}{4\pi}\sum_{i,j}\int_{I_i}\int_{I_j} I_{Wr}(\sigma,s)d\sigma\, ds \\ &= \frac{1}{2\pi}\left(\int_{I_1}\int_{I_3}+\int_{I_2}\int_{I_4}\right) I_{Wr}(\sigma,s)d\sigma\, ds \\ &= \frac{1}{2\pi}\,(a+b), \end{aligned}$$

where we denote

$$a=\int_{I_1}\int_{I_3} I_{Wr}(\sigma,s)d\sigma\, ds=\int_0^1\int_0^1 \frac{1}{(1-s-\sigma)^2+\sigma^2+s^2)^{\frac{3}{2}}}d\sigma\, ds,$$

and

$$b=\int_{I_2}\int_{I_4} I_{Wr}(\sigma,s)d\sigma\, ds=\int_0^1\int_0^1 \frac{-1}{(1+(1-\sigma)^2+(1-s)^2)^{\frac{3}{2}}}d\sigma\, ds.$$

We calculate the double integral a (with Maple, for instance)

$$\begin{aligned} a &= \int_0^1\int_0^1 \frac{1}{(1-s-\sigma)^2+\sigma^2+s^2)^{\frac{3}{2}}}d\sigma\, ds, \\ &= \int_0^1\int_{-1}^0 \frac{1}{(s+\sigma)^2+(\sigma+1)^2+s^2)^{\frac{3}{2}}}d\sigma\, ds=\frac{2\pi}{3}. \end{aligned}$$

Then we calculate the double integral b

$$\begin{aligned} b &= \int_0^1\int_0^1 \frac{-1}{(1+(1-\sigma)^2+(1-s)^2)^{\frac{3}{2}}}d\sigma\, ds, \\ &= -\int_{-1}^0\int_{-1}^0 \frac{1}{(1+\sigma^2+s^2)^{\frac{3}{2}}}d\sigma\, ds, \\ &= -\int_0^1\int_0^1 \frac{1}{(1+\sigma^2+s^2)^{\frac{3}{2}}}d\sigma\, ds \;=-\int_0^1 \left.\frac{\sigma}{(1+s^2)\sqrt{1+\sigma^2+s^2}}\right|_0^1 ds \\ &= -\int_0^1 \frac{1}{(1+s^2)\sqrt{2+s^2}}\, ds \;=-\arctan\left(\frac{s}{\sqrt{2+s^2}}\right)\Bigg|_0^1 = -(\frac{\pi}{6}-0)=-\frac{\pi}{6}. \end{aligned}$$

Hereby we used the facts

$$\int \frac{1}{(\sigma^2+z^2)^{\frac{3}{2}}}d\sigma = \left.\frac{\sigma}{z^2\sqrt{\sigma^2+z^2}}\right|$$

and

$$\arctan'(x)=\frac{1}{1+x^2}.$$

Now we get

$$Wr(C)=\frac{1}{2\pi}\,(a+b)=\frac{1}{2\pi}\,(\frac{2\pi}{3}-\frac{\pi}{6})=\frac{1}{4}.$$

We note, that, in general, the Writhe of a curve is not an integer.