DNA Modelling Course
Exercise Session 1
Summer 2006 Part 2

Calculus of Variations

Compute the Euler-Lagrange equations for $\phi(s)$ and Natural boundary conditions (if any) for the functional

$$\int_0^1 K_2(s)(\phi' - \hat{u}_2)^2/2 + \lambda\cos\phi + \nu\sin\phi \, ds \tag{1.1}$$

with imposed boundary conditions, and given constants ν and λ.

1. $\phi(0) = 0$ and $\phi(1) = 0$,
2. $\phi(0) = 0$,
3. no boundary conditions on ϕ.

Notice that the Euler-Lagrange equation is moment balance.

Introduction to Link integral

The rest of the exercise session concerns some properties of the Link integral:

$$Lk(C_1, C_2) = \frac{1}{4\pi}\int_{C_1}\int_{C_2} \frac{(y(\sigma) - x(s)) \cdot (y'(\sigma) \times x'(s))}{|y(\sigma) - x(s)|^3} d\sigma \, ds$$

where C_1 (or $y(\sigma)$) and C_2 (or $x(s)$) are two smooth non-intersecting closed curves in $\mathbb{R}^3$ (for the Link integral non-intersection of $y(\sigma)$ and $x(s)$ is important, but self-intersection of $y(\sigma)$ with itself, or $x(s)$ with itself, is not a significant difficulty). Here σ and s are arc-length parametrizations so that $y'(\sigma)$ and $x'(s)$ are unit vectors.

In the first problem, we will show that Lk is a homotopy invariant. By this we mean, that it is constant under deformations of $y(\sigma)$ and $x(s)$ in which y and x do not intersect each other. In the second part we will show by explicit calculation that in a simple case (which is important for DNA) the Link integral is an integer for any class of curves $y(\sigma)$ and $x(s)$.

Problem 1

Introduce the unit vector field $e(\sigma, s) = \frac{y(\sigma)-x(s)}{|y(\sigma)-x(s)|}$ and notice that because the curves y and x do not intersect, $e(\sigma, s)$ is well-defined and smooth for all σ and s. It is also periodic because $y(\sigma)$ and $x(s)$ are periodic.

1. Show that the Link integral can be rewritten as:

$$\frac{1}{4\pi}\int_{C_1}\int_{C_2}[e, e_s, e_\sigma]\, d\sigma\, ds,$$

where e_σ and e_s are partial derivatives of $e(\sigma, s)$ (at fixed y and x), and the triple bracket $[a, b, c]$ denotes the scalar triple product $[a, b, c] = a \cdot (b \times c)$. Notice that any derivative of $[a, b, c]$ satisfies the 'product rule':

$$[a, b, c]' = [a', b, c] + [a, b', c] + [a, b, c']$$

2. First order variations δx and δy of the curves x and y generate a first order variation $\delta e(s, t)$ in the unit vector field $e(s, t)$ (the detailed expression is not important here).

Show that the first variation of the Link integral is identically zero for all doubly-periodic unit vector fields e. You must integrate by parts (in s on the δe_s and in σ on the δe_σ term) using the appropriate product rule. You must also use skew-symmetry properties of the triple product, and the fact that because $e(\sigma, s)$ is a unit vector field,

$$e \cdot e_s = e \cdot e_\sigma = e \cdot \delta e = 0,$$

or in other words e_s, e_σ and δe are co-planar so that $[e_s, e_\sigma, \delta e] = 0$. This computation is valid at all non-intersecting y and x (so that e is smooth), and suffices to show that Lk is a homotopy invariant.

Problem 2

To prove that Lk is actually an integer in the most general case (where for example y could be a knotted curve, in addition to being entangled with x) is best done with some rather abstract machinery (see for example Dubrovin, Fomenko & Novikov, 1985, Modern geometry-methods and applications, Vol. 2, Series Graduate Texts in Mathematics, Springer-Verlag). However, there are simple and important cases.

1. If $y(\sigma)$ and $x(s)$ can be moved by homotopy to opposite sides of a plane (in particular if y and x are not linked to each other in an intuitive sense), then $Lk(y, x) = 0$. To see this, show that Lk can be bounded above by an arbitrarily

small number by the homotopy in which $x(s)$ (say) is moved to infinity by translation along the normal to the separating plane.

Unfortunately the converse is not true; the Whitehead link is an example of two curves with Lk=0, but which are topologically linked, and which cannot be moved arbitrarily far apart under homotopy.
For the Whitehead link Lk=0, as by crossing one curve with itself, you can 'physically unlink' the two curves. As seen in Problem 1, this deformation doesn't change the link.

2. For mini-circles, where the double-helix is not itself knotted, the two curves representing the two DNA strands can be homotopied (with considerable stretching) to a single covered unit circle (centered at origin) in one plane ($x(s)$ say), intersected by a multiply covered 'loop' (with all coverings in the same orientation) in an orthogonal plane ($y(\sigma)$ say). Recall that self-intersection of y gives no difficulties.

Evaluate the Link integral in the form Link integral by explicit integration after choosing explicit parametrizations where the second loop $y(\sigma)$ is formed by a straight segment $[-L, L]$ of the z-axis plus a smooth closure lying outside the ball of radius L and the unit circle $x(s)$ is in the xy plane. You need to show

- that the contribution to the Lk integral from the part of the curve $y(\sigma)$ outside the ball of radius L is arbitrarily small for L$\rightarrow\infty$ (which is a homotopy under which Lk is invariant).

- that the remaining part of the integral concerning the Link between the straight part of y and the circle x is an integer. What is the interpretation of this integer ?
  (Hint: Use substitution by $sinh\, z$ and the fact that $tanh'\, z = \frac{1}{cosh^2 z}$ and $tanh\, z \rightarrow 1$ for $z \rightarrow \infty$.)