DNA Modeling Course
Exercise Session 5
Summer 2006 Part 2

Introduction

This session is concerned with the effect of a high intrinsic twist rate on the effective bending properties of an elastic rod. In Problem 1 we again consider the Fenchel transform. Together with the results of Problem 1 of Session 4 you are now in position to compute the Legendre transform of the strain energy functions in Problem 2. In Problem 2 we will derive the effective strain energy function for the averaged Hamiltonian system governing the equilibrium dynamics in the limit as intrinsic twist tends to infinity. The analysis is used to show that for a rod with locally anisotropic constitutive relation for bending, there is an effective bending law in the infinite intrinsic twist limit, and that the effective constitutive law is isotropic. In the last part of the exercise the effective strain energy density function has to be computed explicitly for a non-diagonal stiffness matrix which constitutes a coupling term between bending and twisting.

Problem 1: Fenchel transform

Let $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^n$ and consider a smooth function $\psi(\boldsymbol{x}) \in \mathbb{R}$ with Fenchel transform $\psi^*(\boldsymbol{y}) \in \mathbb{R}$ defined as

$$\psi^*(\boldsymbol{y}) = \max_{\boldsymbol{x} \in R^n} \left[\boldsymbol{y} \cdot \boldsymbol{x} - \psi(\boldsymbol{x}) \right]. \tag{2.1}$$

Show that the Fenchel transform $\psi^{**}(\boldsymbol{y})$ of $\psi^*(\boldsymbol{x})$ equals the function ψ, that is,

$$\psi^{**}(\boldsymbol{y}) \;=\; \psi(\boldsymbol{y}) \qquad \text{for } \boldsymbol{y} \in \mathbb{R}^n.$$

Hint: Use the first order necessary condition!

Problem 2: Effective properties of rods with high intrinsic twist

(a.) Consider the following ODE

$$\dot{\boldsymbol{y}}^\epsilon \;=\; f(\boldsymbol{y}^\epsilon, t, \tau), \qquad \tau = \frac{t}{\epsilon}, \tag{3.1}$$

where τ is assumed to be periodic with period T. As shown in class one can use multiscale analysis in order to show that the effective dynamics

$\boldsymbol{y}^\epsilon(t,\tau) \to \boldsymbol{y}^0(t)$ in the limit $\epsilon \to 0$ obeys an averaged ODE

$$\begin{aligned}\dot{\boldsymbol{y}}^0 &= \overline{f}(\boldsymbol{y}^0, t),\\ \overline{f}(\boldsymbol{y}, t) &= \frac{1}{T}\int_0^T f(\boldsymbol{y}, t, \tau)\,(d)\tau.\end{aligned}$$

Implement the formal asymptotic procedure in order to obtain the above result. To this end, expand the solution $\boldsymbol{y}^\epsilon$ wrt. the smallness parameter ϵ, insert the expansion into equation (3.1) and compare the coefficients of different powers of ϵ. Note that the two time scales have to be treated as if they were independent which is consistent to the separation of scales between t and τ.

(b.) Next, we apply the asymptotic result to the specific problem of an elastic rod with high intrinsic twist.

As before we denote $\boldsymbol{u}$ the strain vector satisfying $\boldsymbol{d}_i' = \boldsymbol{u} \times \boldsymbol{d}_i$, $i = 1, 2, 3$. The components $u_i = \boldsymbol{u} \cdot \boldsymbol{d}_i$ wrt. the frame $\{\boldsymbol{d}_i\}$ are gathered in a triple u. In the same way we gather the three components $m_i = \boldsymbol{m} \cdot \boldsymbol{d}_i$ of the moment vector $\boldsymbol{m}$ in a triple $m = (m_1, m_2, m_3)$. The strain energy density function W is assumed to be of the standard quadratic form

$$W(w, s) = \frac{1}{2} w \cdot \boldsymbol{K} w, \qquad \boldsymbol{K} \in \mathrm{Mat}(3 \times 3, \mathbb{R}^+),$$

and the constitutive relations are of the form

$$m_i = \frac{\partial}{\partial w_i} W(u - \hat{u}),$$

where $\hat{u} = (\hat{u}_1, \hat{u}_2, \hat{u}_3)$ are the components wrt. $\{\boldsymbol{d}_i\}$ in the minimum energy unstressed configuration.

The analysis in the limit of infinite intrinsic twist requires to refer the equilibrium equations to a director frame $\{\boldsymbol{D}_i\}$ that is independent of the twist $\hat{U}_3$ in the unstressed configuration.

We rotate the frame $\{\boldsymbol{d}_i\}$ about the $\boldsymbol{d}_3$ axis through an angle $\Omega(s)$ to obtain the new set of directors $\{\boldsymbol{D}_i\}$ satisfying

$$[\boldsymbol{D}_1, \boldsymbol{D}_2, \boldsymbol{D}_3] = [\boldsymbol{d}_1, \boldsymbol{d}_2, \boldsymbol{d}_3]\boldsymbol{R}^T(\Omega), \quad \boldsymbol{R}(\Omega) = \begin{pmatrix} \cos\Omega & \sin\Omega & 0 \\ -\sin\Omega & \cos\Omega & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

The $\{\boldsymbol{D}_i\}$ frame has an associated strain vector $\boldsymbol{U}$ satisfying

$$\boldsymbol{D}_i' = \boldsymbol{U} \times \boldsymbol{D}_i,$$

and the triple of components $U_i = \boldsymbol{U} \cdot \boldsymbol{D}_i$ is denoted U, respectively $\hat{U}$ for the triple in the unstressed configuration. We have the relations

$$\begin{aligned} U &= \boldsymbol{R}(\Omega)[u + \Omega' \boldsymbol{e}_3],\\ u &= \boldsymbol{R}^T(\Omega)[U - \Omega' \boldsymbol{e}_3] \end{aligned}$$

In order to refer the equilibrium conditions to the natural frame it is necessary to consider the components $M_i = \boldsymbol{m} \cdot \boldsymbol{D}_i$ of the moment vector $\boldsymbol{m}$. Then the components M in the natural frame are related to the components m in the $\{\boldsymbol{d}_i\}$ frame via

$$M \;=\; \boldsymbol{R}(\Omega)m.$$

The rod equilibrium equations are now derived as a seven degree of freedom, canonical Hamiltonian system

$$\boldsymbol{z}' \;=\; \begin{pmatrix} \boldsymbol{0} & \mathrm{Id} \\ -\mathrm{Id} & \boldsymbol{0} \end{pmatrix} \nabla H(\boldsymbol{z}, s, \Omega)$$

with associated Hamiltonian

$$H(\boldsymbol{z}, s, \Omega) \;=\; [\widehat{W}^{\Omega}]^*(M, s) \;+\; \boldsymbol{n} \cdot \boldsymbol{D}_3,$$

where $[\widehat{W}^{\Omega}]^*(M, s)$ is the Legendre transform of the density function

$$\widehat{W}^{\Omega}(U, s) = W(\boldsymbol{R}^T(\Omega)(U - \hat{U}), s).$$

Compute $[\widehat{W}^{\Omega}]^*(M, s)$ in terms of the Legendre transform W^* of the strain energy function W.

For applying the averaging result in part (a.) we explicitly separate the dependence of the Hamiltonian H on the independent variable s and the angle function Ω and emphasize that the Hamiltonian is always 2π-periodic in Ω and the dependence only enters through the Legendre transform W^*. With it, we are in position to average over Ω, which can be seen to be a fast variable $\Omega = s/\epsilon$. State the averaged Hamiltonian by resorting to part (a.).

(c.) It remains to consider the explicit form of the averaged Hamiltonian $\overline{H}(\boldsymbol{z}, s)$ which can be done whenever the strain energy function W is quadratic. Explicitly compute the averaged Hamiltonian in the case

$$W(u - \hat{u}, s) \;=\; \frac{1}{2}(u - \hat{u}) \cdot \boldsymbol{K}(u - \hat{u}), \qquad \boldsymbol{K} \;=\; \begin{pmatrix} K_1 & 0 & 0 \\ 0 & K_2 & K_{23} \\ 0 & K_{23} & K_3 \end{pmatrix}.$$

What is the effective strain energy density function $\overline{W}$? (Hint: To this end, you have to use the result of Problem 1).