DNA Modelling Course
Exercise Session 5
Summer 2006 Part 2

SOLUTIONS

Problem 1: Fenchel transform

For simplicity we assume that $\nabla\psi : \mathbb{R}^n \to \mathbb{R}^n$ is an invertible function. We thus obtain the existence of a function $\phi : \mathbb{R}^n \to \mathbb{R}^n$ such that $\nabla\psi(\phi(\boldsymbol{x})) = \boldsymbol{x}$. Then we get

$$\begin{aligned}\psi^{**}(\boldsymbol{y}) &= \max_{\boldsymbol{x}}\{\boldsymbol{y}\cdot\boldsymbol{x} - \psi^*(x)\} \\ &= \max_{\boldsymbol{x}}\{\boldsymbol{y}\cdot\boldsymbol{x} - (\boldsymbol{x}\cdot\phi(\boldsymbol{x}) - \psi(\phi(\boldsymbol{x}))\},\end{aligned} \tag{0.1}$$

where the second equality is obtained by using the first order necessary condition for the Fenchel transform $\psi^*(x)$. The first order condition for the maximum (0.1) to exist is

$$\begin{aligned}\boldsymbol{y} &= D(\boldsymbol{x}\cdot\phi(\boldsymbol{x}) - \psi(\phi(\boldsymbol{x}))) \\ &= D(\nabla\psi(\phi(\boldsymbol{x}))\cdot\phi(\boldsymbol{x}) - \psi(\phi(\boldsymbol{x}))),\end{aligned}$$

which after a short calculation reveals

$$\boldsymbol{y} = \phi(\boldsymbol{x}).$$

Inserting the result in (0.1) yields

$$\psi^{**}(\boldsymbol{y}) = \max_{\boldsymbol{x}}\{\boldsymbol{y}\cdot\boldsymbol{x} - (\boldsymbol{x}\cdot\boldsymbol{y} - \psi(\boldsymbol{y}))\} = \psi(\boldsymbol{y}).$$

Problem 2: Effective properties of rods with high intrinsic twist

(a.) We consider the ODE

$$\dot{\boldsymbol{y}}^\epsilon = f(\boldsymbol{y}^\epsilon, t, \tau), \qquad \tau = \frac{t}{\epsilon}, \tag{0.2}$$

where τ is assumed to be periodic with period T. The variable τ can be seen to be a fast variable and t is the slow one. For preparation of the discusson we introduce the inner product $\langle\cdot,\cdot\rangle$ on the vectorspace of T-periodic integrable functions:

$$\langle \boldsymbol{y}, \boldsymbol{x}\rangle \;=\; \frac{1}{T}\int_0^T \overline{\boldsymbol{y}(\tau)}\boldsymbol{x}(\tau)\mathrm{d}\tau.$$

Next, we define the projection operator Π according to

$$\Pi\boldsymbol{y} \;=\; \langle \mathbf{1}, \boldsymbol{y}\rangle \;=\; \frac{1}{T}\int_0^T \boldsymbol{y}(\tau)\mathrm{d}\tau.$$

It is obvious that Π projects a function $\boldsymbol{y}(t,\tau)$ on a function that does not depend on τ, that is $\partial_\tau \Pi = 0$. Using T-periodicity in τ it is likewise obvious that

$$\Pi\partial_\tau \quad = \quad 0. \tag{0.3}$$

We now make the following ansatz for the solution of the equation (0.2) where we demand that the initial state $\boldsymbol{y}^\epsilon(t=0,\tau=0) = \boldsymbol{y}_0$ is independent of ϵ:

$$\boldsymbol{y}^\epsilon(t,\tau) \quad = \quad \boldsymbol{y}^0(t,\tau) \,+\, \epsilon\,\boldsymbol{y}^1(t,\tau) \,+\, \epsilon^2\,\boldsymbol{y}^2(t,\tau) \,+\, ..., \qquad \tau = \frac{t}{\epsilon}. \tag{0.4}$$

We treat the two time scales as if they were independent which is consistent with the separation of scales. Thus we set

$$\frac{\partial}{\partial t} \mapsto \frac{\partial}{\partial t} + \frac{1}{\epsilon}\frac{\partial}{\partial \tau}.$$

The ansatz (0.4) is inserted into the ODE (0.2) and then, equating equal powers in ϵ leads to the following sequence of equations (note that the RHS of (0.2) can be written $f(\boldsymbol{y}^\epsilon, t, \tau) = f(\boldsymbol{y}^0, t, \tau) + \mathcal{O}(\epsilon)$):

$$\epsilon^{-1} \quad : \quad \partial_\tau \boldsymbol{y}^0 \,=\, 0 \tag{0.5}$$

$$\epsilon^{0} \quad : \quad \partial_\tau \boldsymbol{y}^1 \,+\, \partial_t \boldsymbol{y}^0 \,=\, f(\boldsymbol{y}^0, t, \tau). \tag{0.6}$$

1.step: (0.5) immediately yields that $\boldsymbol{y}^0$ does not depend on τ, i.e.,

$$\Pi\boldsymbol{y}^0 \;=\; \boldsymbol{y}^0.$$

2.step: Let $\Pi = \langle \mathbf{1}, \cdot\rangle$ act on (0.6) and use (0.3). This time

$$\Pi f(\boldsymbol{y}^0, t, \tau) \;=\; \Pi\partial_\tau\boldsymbol{y}^1 \,+\, \Pi\partial_t\boldsymbol{y}^0 \;=\; \partial_t\boldsymbol{y}^0.$$

Thus, $\boldsymbol{y}^0$ is determined by the ODE

$$\dot{\boldsymbol{y}}^0 \;=\; \overline{f}(\boldsymbol{y}^0, t),$$

with averaged function

$$\overline{f}(\boldsymbol{y}, t) \;:=\; \Pi f(\boldsymbol{y}, t, \tau),$$

and its solution gives us $\boldsymbol{y}^\epsilon$ up to error $\mathcal{O}(\epsilon)$.

(b.) The constitutive relations in the natural frame $\{\boldsymbol{D}_i\}$ variables become

$$M_i \,=\, \frac{\partial}{\partial U_i}\widehat{W}^{\Omega}(U,s),$$

and, by using the results from the last exercise session and exploiting orthogonality of the matrix $\boldsymbol{R}$ we obtain the Legendre transform of $\widehat{W}^{\Omega}$ as

$$[\widehat{W}^{\Omega}]^*(M,s) \,=\, W^*(\boldsymbol{R}^T M,s) \,+\, \hat{U}\cdot M.$$

Again we use former results from Session 4 in order to obtain

$$W^*(m,s) \,=\, \frac{1}{2}m\cdot\boldsymbol{K}^{-1}m,$$

and, conclusively,

$$[\widehat{W}^{\Omega}]^*(M,s) \,=\, \frac{1}{2}m\cdot(\boldsymbol{R}(\Omega)\boldsymbol{K}^{-1}\boldsymbol{R}^T(\Omega))M \,+\, \hat{U}_1M_1 \,+\, \hat{U}_2M_2.$$

The Hamiltonian is now given by

$$H(\boldsymbol{z},s,\Omega) \,=\, [\widehat{W}^{\Omega}]^*(M,s) \,+\, \boldsymbol{n}\cdot\boldsymbol{D}_3. \qquad (0.7)$$

Averaging In order to obtain a system that is suitable to applying the averaging result from part (a.) we incorporate a high twist into the model by setting $\hat{u}_3(s) = -\frac{1}{\epsilon}$ with $\epsilon \ll 1$. The Hamiltonian is dependent on the parameter ϵ through the identity $\Omega(s) = \frac{s}{\epsilon}$ obtained from integrating

$$\Omega' \,=\, -\hat{u}_3.$$

Now, the Hamiltonian system reads

$$\dot{\boldsymbol{z}}^{\epsilon} \quad = \quad \begin{pmatrix} \boldsymbol{0} & \mathrm{Id} \\ -\mathrm{Id} & \boldsymbol{0} \end{pmatrix}\nabla H(\boldsymbol{z}^{\epsilon},s,\Omega), \qquad \Omega = \frac{s}{\epsilon}.$$

Now, we observe that for any initial condition $\boldsymbol{z}^{\epsilon}(0) = \boldsymbol{z}_0$ independent of ϵ the solution $\boldsymbol{z}^{\epsilon}$ is given by $\boldsymbol{z}^0$ up to error ϵ where $\boldsymbol{z}^0$ is the solution of

$$\dot{\boldsymbol{z}}^{0} \quad = \quad \begin{pmatrix} \boldsymbol{0} & \mathrm{Id} \\ -\mathrm{Id} & \boldsymbol{0} \end{pmatrix}\nabla \overline{H}(\boldsymbol{z}^{0},s),$$

where $\overline{H}$ is given by

$$\begin{aligned}
\overline{H}(\boldsymbol{z},s) &= \overline{W}^*(M,s) \,+\, \hat{U}_1M_1 \,+\, \hat{U}_2M_2 \,+\, \boldsymbol{n}\cdot\boldsymbol{D}_3,\\
\overline{W}^*(M,s) &= \frac{1}{2\pi}\int_0^{2\pi} W^*(\boldsymbol{R}^T(\Omega)M,s)\mathrm{d}\Omega.
\end{aligned}$$

(c.)

$$W^*(\boldsymbol{R}^T M, s) \;=\; \frac{1}{2} M \cdot (\boldsymbol{R}(\Omega)\boldsymbol{K}^{-1}\boldsymbol{R}^T(\Omega))M,$$

where the stiffness matrix $\boldsymbol{K}$ is given by

$$\boldsymbol{K} \;=\; \begin{pmatrix} K_1 & 0 & 0 \\ 0 & K_2 & K_{23} \\ 0 & K_{23} & K_3 \end{pmatrix}.$$

The inverse $\boldsymbol{K}^{-1}$ is

$$\boldsymbol{K}^{-1} \;=\; \begin{pmatrix} 1/K_1 & 0 & 0 \\ 0 & K_3/D & -K_{23}/D \\ 0 & -K_{23}/D & K_2/D \end{pmatrix}, \qquad D = K_2K_3 - (K_{23})^2,$$

and a straightforward calculation reveals

$$\widehat{K} \;:=\; \boldsymbol{R}(\Omega)\boldsymbol{K}^{-1}\boldsymbol{R}^T(\Omega) \;=$$
$$\begin{pmatrix} \frac{\cos^2\Omega}{K_1} + \frac{K_3\sin^2\Omega}{D} & \sin\Omega\cos\Omega(-\frac{1}{K_1} + \frac{K_3}{D}) & -\frac{\sin\Omega K_{23}}{D} \\ \sin\Omega\cos\Omega(-\frac{1}{K_1} + \frac{K_3}{D}) & \frac{\sin^2\Omega}{K_1} + \frac{\cos^2\Omega K_3}{D} & -\frac{\cos\Omega K_{23}}{D} \\ -\frac{\sin\Omega K_{23}}{D} & -\frac{\cos\Omega K_{23}}{D} & \frac{K_2}{D} \end{pmatrix}.$$

Using $\int_0^{2\pi}\cos^2(x)dx = \int_0^{2\pi}\sin^2(x)dx$ together with $\int_0^{2\pi}\cos^2(x)+\sin^2(x)dx = 2\pi$ yields $\int_0^{2\pi}\cos^2(x)dx = \int_0^{2\pi}\sin^2(x)dx = \pi$ and we obtain

$$\begin{aligned} \frac{1}{2\pi}\int_0^{2\pi}\widehat{K}(\Omega)\mathrm{d}\Omega &= \mathrm{diag}\left\{\bar{K}_\delta^{-1}, \bar{K}_\delta^{-1}, \frac{K_2}{D}\right\}, \\ \bar{K}_\delta^{-1} &= \frac{1}{2}(K_1^{-1} + K_2^{-1}(1-\delta)), \quad \delta \;=\; (K_{23})^2/(K_2K_3). \end{aligned}$$

Thus, the averaged Hamiltonian is given by

$$\begin{aligned} \overline{H} &= \overline{W}^*(M,s) \;+\; \hat{U}_1 M_1 \;+\; \hat{U}_2 M_2 \;+\; \boldsymbol{n}\cdot\boldsymbol{D}_3, \\ \overline{W}^*(M,s) &= \frac{1}{2} M \cdot \mathrm{diag}\left\{\bar{K}_\delta^{-1}, \bar{K}_\delta^{-1}, \frac{K_2}{D}\right\} M. \end{aligned}$$

Note that $\overline{W}^*$ is not the Legendre transform of the average of $W(\boldsymbol{R}^T(\Omega)U, s)$ since the averaging operator and the Legendre transform do not commute. Using Problem 1 we know that the effective strain energy function can be computed as the Legendre transform of the averaged Legendre transform $\overline{W}^*$ and thus we obtain

$$\overline{W}(U,s) \;=\; \frac{1}{2} U \cdot \overline{K} U, \qquad \overline{K} \;=\; \begin{pmatrix} \bar{K}_\delta & 0 & 0 \\ 0 & \bar{K}_\delta & 0 \\ 0 & 0 & D/K_2 \end{pmatrix}.$$