1 Piecewise linear definition

I will define the piecewise linear twist angle as

$$\psi(r) = \begin{cases} \psi_c' r & 0 \leq r \leq R_c \\ \psi_s' r + (\psi_c' - \psi_s') R_c & R_c < r \leq R_s \\ \psi_R' r + (\psi_s' - \psi_R') R_s + (\psi_c' - \psi_s') R_c & R_s < r \leq R. \end{cases} \tag{1}$$

Next, I will insert this into the free energy per unit volume,

$$\begin{aligned} E(R, \eta, \delta; \psi(r)) = & \frac{2}{R^2} \int_0^R r dr \left[\frac{1}{2} \left(\psi' + \frac{\sin 2\psi}{2r} - 1 \right)^2 + \frac{1}{2} K_{33} \frac{\sin^4 \psi}{r^2} \right] \\ & + \frac{\Lambda \delta^2}{2R^2} \int_0^R r dr \left(\frac{4\pi^2}{\cos^2 \psi} - \eta^2 \right)^2 \\ & + \frac{\omega \delta^2}{2} \left(\frac{3}{4} \delta^2 - 1 \right) - \frac{(1 + k_{24})}{R^2} \sin \psi(R) + \frac{2\gamma}{R}. \end{aligned} \tag{2}$$

Inserting the form of $\psi(r)$ from eqn 1 I get the free energy as function of 8 variables,

$$E(R, \eta, \delta, R_c, R_s, \psi_c', \psi_s', \psi_R') = \frac{2}{R^2} \left[q(\eta, \delta, 0, 0, R_c, 0, 0, \psi_c') + q(\eta, \delta, 0, R_c, R_s, 0, \psi_c', \psi_s') + q(\eta, \delta, R_c, R_s, R, \psi_c', \psi_s', \right. \tag{3}$$

I will look first only at the two integral terms in eqn 2, as that is where the piecewise linear function enters the calcution. Starting with the region $0 \leq r \leq R_c$, I get

$$\begin{aligned} & \frac{2}{R^2} \int_0^{R_c} r dr \left[\frac{1}{2} \left(\psi_0' + \frac{\sin(2\psi_0' r)}{2r} - 1 \right)^2 + \frac{1}{2} K_{33} \frac{\sin^4(\psi_0' r)}{r^2} \right] + \frac{\Lambda \delta^2}{2R^2} \int_0^{R_c} r dr \left(\frac{4\pi^2}{\cos^2(\psi_0' r)} - \eta^2 \right)^2 \\ = & \frac{2}{R^2} \left(\frac{(\psi_0' - 1)^2}{4} R_c^2 + \frac{\psi_0'}{4} f_1(2\psi_0' R_c) + \frac{(\psi_0' - 1)}{4\psi_0'} (1 - \cos(2\psi_0' R_c)) + \frac{\psi_0'}{2} K_{33} f_2(\psi_0' R_c) \right) \\ & + \frac{\Lambda \delta^2}{2R^2} \left(\frac{16\pi^4}{\psi_0'} g_2(\psi_0' R_c) - \frac{8\pi^2 \eta^2}{\psi_0'} g_1(\psi_0' R_c) + \frac{\eta^4}{2} R_c^2 \right) \end{aligned} \tag{4}$$

Next, looking at the shelf region $R_c \leq r < R_s$, I get

(5)

Finally, in the outer region $R_s \leq r < R$, I get

(6)

Adding all of this together, I end up with the free energy per unit volume of the d-banded fibril which is a function of 8 variables,

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\begin{aligned}
E(R, \eta, \delta, &R_c, R_s, \psi_0', \psi_c, \psi_R') \\
=&\frac{2}{R^2}\left(\frac{(\psi_0'-1)^2}{4}R_c^2 + \frac{\psi_0'}{4}f_1(2\psi_0' R_c) + \frac{(\psi_0'-1)}{4\psi_0'}(1-\cos(2\psi_0' R_c)) + \frac{\psi_0'}{2}K_{33}f_2(\psi_0' R_c)\right) \\
&+ \frac{\Lambda\delta^2}{2R^2}\left(\frac{16\pi^4}{\psi_0'}g_2(\psi_0' R_c) - \frac{8\pi^2\eta^2}{\psi_0'}g_1(\psi_0' R_c) + \frac{\eta^4}{2}R_c^2\right) \\
&\frac{\sin^2(2\psi_c)}{4R^2}\ln\left(\frac{R_s}{R_c}\right) - \frac{\sin(2\psi_c)}{R^2}(R_s - R_c) + \frac{R_s^2 - R_c^2}{2R^2}\left(1 + \frac{\Lambda\delta^2}{2}\left(\frac{4\pi^2}{\cos^2\psi_c} - \eta^2\right)^2\right) \\
=&\frac{2}{R^2}\left(\frac{(\psi_R'-1)^2}{4}(R^2 - R_s^2) + \frac{\psi_R'}{4}(f_1(2\psi_R' R) - f_1(2\psi_R' R_s)) + \frac{(\psi_R'-1)}{4\psi_R'}(\cos(2\psi_R' R_s) - \cos(2\psi_R' R))\right. \\
&\left. + \frac{\psi_R'}{2}K_{33}(f_2(\psi_R' R) - f_2(\psi_R' R))\right) \\
&+ \frac{\Lambda\delta^2}{2R^2}\left(\frac{16\pi^4}{\psi_R'}(g_2(\psi_R' R) - g_2(\psi_R' R_s)) - \frac{8\pi^2\eta^2}{\psi_R'}(g_1(\psi_R' R) - g_1(\psi_R' R_s)) + \frac{\eta^4}{2}(R^2 - R_s^2)\right)
\end{aligned}
\tag{7}
$$

2 Detailed calculations

For a general linear function of the form $\psi(r) = \psi'_{ab} r + \psi_0$ in the region $a < r < b$, the two integrals in eqn 2 become

$$\int_a^b r dr \left[\frac{1}{2} \left(\psi'_{ab} + \frac{\sin(2(\psi'_{ab} r + \psi_0))}{2r} - 1 \right)^2 + \frac{1}{2} K_{33} \frac{\sin^4(\psi'_{ab} r + \psi_0)}{r^2} \right]$$
$$= \int_a^b dr \left(\frac{(1-\psi'_{ab})^2}{2} r + \frac{1}{8} \frac{\sin^2(2(\psi'_{ab} r + \psi_0))}{r} - \frac{(1-\psi'_{ab})}{2} \sin(2(\psi'_{ab} r + \psi_0)) + \frac{1}{2} K_{33} \frac{\sin^4(\psi'_{ab} r + \psi_0)}{r} \right)$$
$$= \left(\frac{1}{4} u(a, b, \psi'_{ab}) + \frac{1}{8} f_1(a, b, \psi_0, \psi'_{ab}) + \frac{1}{2} K_{33} f_2(a, b, \psi_0, \psi'_{ab}) + \frac{1}{4} v(a, b, \psi_0, \psi'_{ab}) \right) \tag{8}$$

and

$$\int_a^b r dr \left(\frac{4\pi^2}{\cos^2(\psi'_{ab} r + \psi_0)} - \eta^2 \right)^2$$
$$= \int_a^b dr \left(\frac{16\pi^4 r}{\cos^4(\psi'_{ab} r + \psi_0)} - \frac{8\pi^2 r}{\cos^2(\psi'_{ab} r + \psi_0)} \eta^2 + \eta^4 r \right)$$
$$= \left(16\pi^4 g_2(a, b, \psi_0, \psi'_{ab}) - 8\pi^2 \eta^2 g_1(a, b, \psi_0, \psi'_{ab}) + \frac{\eta^4}{2}(b^2 - a^2) \right) \tag{9}$$

where I have defined the functions

$$u(x_1, x_2, \zeta) = (1-\zeta)^2 (x_2^2 - x_1^2), \tag{10a}$$
$$v(x_1, x_2, \xi, \zeta) = \frac{(1-\zeta)}{\zeta} (\cos(2(\zeta x_2 + \xi)) - \cos(2(\zeta x_1 + \xi))), \tag{10b}$$
$$f_\alpha(x_1, x_2, \xi, \zeta) = \int_{x_1}^{x_2} du \frac{sin^{2\alpha}\left(\frac{2}{\alpha}(\zeta u + \xi)\right)}{u}, \tag{10c}$$
$$g_\alpha(x_1, x_2, \xi, \zeta) = \int_{x_1}^{x_2} du \frac{u}{cos^{2\alpha}(\zeta u + \xi)}. \tag{10d}$$

$$\tag{10e}$$

For $\zeta \ll 1$, I can expand the final three of these equations up to $\mathcal{O}(\zeta^4)$ using trigonometric identities to get

$$v(x_1, x_2, \xi, \zeta) = -2(1-\zeta)\sin(2\xi)(x_2 - x_1) - 2(1-\zeta)\cos(2\xi)(x_2^2 - x_1^2)\zeta + \frac{4}{3}(1-\zeta)\sin(2\xi)(x_2^3 - x_1^3)\zeta^2 + \frac{2}{3}\cos(2\xi)(x_2^4 - x_1^4)\zeta^3, \tag{11a}$$

$$f_1(x_1, x_2, \xi, \zeta) = \sin^2\left(\frac{2\xi}{\alpha}\right)\ln\frac{x_2}{x_1} + 4\zeta(x_2 - x_1)\cos(2\xi)\sin(2\xi) + 2\zeta^2(x_2^2 - x_1^2)\left(\cos^2(2\xi) - \sin^2(2\xi)\right) - \frac{32}{9}\zeta^3(x_2^3 - x_1^3)\sin(2\xi)\cos(2\xi) \tag{11b}$$

$$f_2(x_1, x_2, \xi, \zeta) = \sin^4\xi\ln\frac{x_2}{x_1} + 4\zeta(x_2 - x_1)\sin^3\xi\cos\xi + \zeta^2(x_2^2 - x_1^2)\sin^2\xi(\cos^2\xi - \sin^2\xi) + \frac{4}{3}\zeta^3(x_2^3 - x_1^3)\sin\xi\cos\xi\left(\cos^2\xi - 5\sin^2\xi\right) \tag{11c}$$

3 References