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,

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

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

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

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

$$\tag{5}$$

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

$$\tag{6}$$

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,

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

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

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

and

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

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

$$\begin{aligned}
v(x_1,x_2,\xi,\zeta) &= -2(1-\zeta)\sin(2\xi)(x_2-x_1) - 2(1-\zeta)\cos(2\xi)(x_2^2-x_1^2)\zeta \\
&\quad + \frac{4}{3}(1-\zeta)\sin(2\xi)(x_2^3-x_1^3)\zeta^2 + \frac{2}{3}\cos(2\xi)(x_2^4-x_1^4)\zeta^3, \qquad (11a)\\
f_1(x_1,x_2,\xi,\zeta) &= \sin^2\left(\frac{2\xi}{\alpha}\right)\ln\frac{x_2}{x_1} + 4\zeta(x_2-x_1)\cos(2\xi)\sin(2\xi) \\
&\quad + 2\zeta^2(x_2^2-x_1^2)\left(\cos^2(2\xi)-\sin^2(2\xi)\right) - \frac{32}{9}\zeta^3(x_2^3-x_1^3)\sin(2\xi)\cos(2\xi) \qquad (11b)\\
f_2(x_1,x_2,\xi,\zeta) &= \sin^4\xi\ln\frac{x_2}{x_1} + 4\zeta(x_2-x_1)\sin^3\xi\cos\xi + \zeta^2(x_2^2-x_1^2)\sin^2\xi(\cos^2\xi-\sin^2\xi) \\
&\quad + \frac{4}{3}\zeta^3(x_2^3-x_1^3)\sin\xi\cos\xi\left(\cos^2\xi-5\sin^2\xi\right) \qquad (11c)\\
g_1(x_1,x_2,\xi,\zeta) &= \frac{1}{\cos^2\xi}\left(\frac{x_2^2-x_1^2}{2} + \frac{2\zeta(x_2^3-x_1^2)}{3}\tan\xi + \frac{\zeta^2(x_2^4-x_1^4)(3\tan^2\xi+1)}{4}\right. \\
&\quad \left. + \frac{4\zeta^3(x_2^5-x_1^5)(4+3\tan^2\xi)\tan\xi}{15}\right) \qquad (11d)\\
g_2(x_1,x_2,\xi,\zeta) &= \frac{1}{\cos^4\xi}\left(\frac{x_2^2-x_1^2}{2} + \frac{4\zeta(x_2^3-x_1^3)\tan\xi}{3} + \frac{\zeta^2(x_2^4-x_1^4)(1+5\tan^2\xi)}{2}\right. \\
&\quad \left. + \frac{\zeta^3(x_2^5-x_1^5)(60\tan^2\xi+28)\tan\xi}{15}\right) \qquad (11e)
\end{aligned}$$

3 References