Energy function for a piecewise linear twist angle field

I will define the piecewise linear twist angle as

$$\psi(r) = \begin{cases} \psi_c' r & 0 \leq r \leq R_c \\ \psi_s' r + \psi_1 & R_c < r \leq R_s \\ \psi_R' r + \psi_2 & R_s < r \leq R. \end{cases} \tag{1}$$

which have two constraints,

$$\psi_1 = (\psi_c' - \psi_s')R_c, \tag{2a}$$

$$\psi_2 = (\psi_s' - \psi_R')R_s + (\psi_c' - \psi_s')R_c, \tag{2b}$$

to ensure continuity of $\psi(r)$.

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

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

The resulting equation can be written as

$$
\begin{aligned}
&E(R,\eta,\delta,R_c,R_s,\psi_c',\psi_s',\psi_R') = \\
&\qquad \frac{2}{R^2}\left(\frac{1}{4}(u(0,R_c,\psi_c') + u(R_c,R_s,\psi_s') + u(R_s,R,\psi_R')) + \frac{1}{8}(f_1(0,R_c,0,\psi_c')\right. \\
&\qquad + f_1(R_c,R_s,\psi_1,\psi_s') + f_1(R_s,R,\psi_2,\psi_R')) + \frac{1}{2}K_{33}(f_2(0,R_c,0,\psi_c') + f_2(R_c,R_s,\psi_1,\psi_s') \\
&\qquad \left. + f_2(R_s,R,\psi_2,\psi_R')) + \frac{1}{4}(v(0,R_c,0,\psi_c') + v(R_c,R_s,\psi_1,\psi_s') + v(R_s,R,\psi_2,\psi_R'))\right) \\
&\qquad + \frac{\Lambda\delta^2}{2R^2}\left(16\pi^4(g_2(0,R_c,0,\psi_c') + g_2(R_c,R_s,\psi_1,\psi_s') + g_2(R_s,R,\psi_2,\psi_R'))\right. \\
&\qquad \left. -8\pi^2\eta^2(g_1(0,R_c,0,\psi_c') + g_1(R_c,R_s,\psi_1,\psi_s') + g_1(R_s,R,\psi_2,\psi_R')) + \frac{\eta^4}{2}R^2\right) \\
&\qquad + \frac{\omega\delta^2}{2}\left(\frac{3}{4}\delta^2 - 1\right) - \frac{(1+k_{24})}{R^2}\sin(\psi_R' R + \psi_2) + \frac{2\gamma}{R}
\end{aligned} \tag{4}
$$

which utilizes a derivation shown in the appendix (see eqns 8 and 9, as well as the definitions of the functions u, v, f_α, and g_α in equations 10a, 10b, 10c, and 10d, respectively). I will minimize this equation subject to the constraint equations 2a and 2b to determine the equilibrium configuration of the fibril.

Differentiation of the energy

The derivative with respect to the fibril radius is

$$
\begin{aligned}
\frac{\partial E}{\partial R} = & \\
& -\frac{4}{R^3}\left(\frac{1}{4}(u(0,R_c,\psi_c') + u(R_c,R_s,\psi_s') + u(R_s,R,\psi_R')) + \frac{1}{8}(f_1(0,R_c,0,\psi_c')\right. \\
& + f_1(R_c,R_s,\psi_1,\psi_s') + f_1(R_s,R,\psi_2,\psi_R')) + \frac{1}{2}K_{33}(f_2(0,R_c,0,\psi_c') + f_2(R_c,R_s,\psi_1,\psi_s') \\
& \left. + f_2(R_s,R,\psi_2,\psi_R')) + \frac{1}{4}(v(0,R_c,0,\psi_c') + v(R_c,R_s,\psi_1,\psi_s') + v(R_s,R,\psi_2,\psi_R'))\right) \\
& + \frac{2}{R^2}\left(\frac{1}{4}\left.\frac{\partial u(R_s,x_2,\psi_R')}{\partial x_2}\right|_{x_2=R} + \frac{1}{8}\left.\frac{\partial f_1(R_s,x_2,\psi_2,\psi_R')}{\partial x_2}\right|_{x_2=R} + \frac{1}{2}K_{33}\left.\frac{\partial f_2(R_s,x_2,\psi_2,\psi_R')}{\partial x_2}\right|_{x_2=R}\right. \\
& \left. + \frac{1}{4}\left.\frac{\partial v(R_s,x_2,\psi_2,\psi_R')}{\partial x_2}\right|_{x_2=R}\right) \\
& - \frac{\Lambda\delta^2}{R^3}\left(16\pi^4(g_2(0,R_c,0,\psi_c') + g_2(R_c,R_s,\psi_1,\psi_s') + g_2(R_s,R,\psi_2,\psi_R'))\right. \\
& \left. -8\pi^2\eta^2(g_1(0,R_c,0,\psi_c') + g_1(R_c,R_s,\psi_1,\psi_s') + g_1(R_s,R,\psi_2,\psi_R')) + \frac{\eta^4}{2}R^2\right) \\
& + \frac{\Lambda\delta^2}{2R^2}\left(16\pi^4\left.\frac{\partial g_2(R_s,x_2,\psi_2,\psi_R')}{\partial x_2}\right|_{x_2=R} - 8\pi^2\eta^2\left.\frac{\partial g_1(R_s,x_2,\psi_2,\psi_R')}{\partial x_2}\right|_{x_2=R} + \eta^4 R\right) \\
& + \frac{2(1+k_{24})}{R^3}\sin(\psi_R' R + \psi_2) - \frac{\psi_R'(1+k_{24})}{R^2}\cos(\psi_R' R + \psi_2) - \frac{2\gamma}{R^2}.
\end{aligned}
\tag{5}
$$

The derivative with respect to the inverse period of density modulations, η, is

$$
\frac{\partial E}{\partial \eta} = \frac{\Lambda\delta^2}{2R^2}\left(-16\pi^2\eta(g_1(0,R_c,0,\psi_c') + g_1(R_c,R_s,\psi_1,\psi_s') + g_1(R_s,R,\psi_2,\psi_R')) + 2\eta^3R^2\right) \tag{6}
$$

The derivative with respect to the size of the density modulations, δ, is

$$
\begin{aligned}
\frac{\partial E}{\partial \delta} = & \frac{\Lambda\delta}{R^2}\left(16\pi^4(g_2(0,R_c,0,\psi_c') + g_2(R_c,R_s,\psi_1,\psi_s') + g_2(R_s,R,\psi_2,\psi_R'))\right. \\
& \left. -8\pi^2\eta^2(g_1(0,R_c,0,\psi_c') + g_1(R_c,R_s,\psi_1,\psi_s') + g_1(R_s,R,\psi_2,\psi_R')) + \frac{\eta^4}{2}R^2\right) + \omega\delta\left(\frac{3}{2}\delta^2 - 1\right).
\end{aligned}
\tag{7}
$$

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 3 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

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

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

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

The derivatives of these functions are listed below:

$$
\begin{aligned}
\frac{\partial u}{\partial x_1} &= -2(1-\zeta)^2 x_1 && \text{(12a)}\\
\frac{\partial u}{\partial x_2} &= 2(1-\zeta)^2 x_2 && \text{(12b)}\\
\frac{\partial u}{\partial \xi} &= 0 && \text{(12c)}\\
\frac{\partial u}{\partial \zeta} &= -2\zeta(1-\zeta)(x_2^2 - x_1^2) && \text{(12d)}
\end{aligned}
$$

$$\frac{\partial v}{\partial x_1} = 2(1-\zeta)\sin(2(\zeta x_1+\xi)) \tag{13a}$$

$$\frac{\partial v}{\partial x_2} = -2(1-\zeta)\sin(2(\zeta x_1+\xi)) \tag{13b}$$

$$\frac{\partial v}{\partial \xi} = \begin{cases} -4\cos(2\xi)(x_2-x_1) + (4\cos(2\xi)(x_2-x_1) + 4\sin(2\xi)(x_2^3-x_1^3))\zeta, & \zeta = 0 \\ -2\frac{(1-\zeta)}{\zeta}(\sin(2(\zeta x_2+\xi)) - \sin(2(\zeta x_1+\xi))), & \zeta \neq 0 \end{cases} \tag{13c}$$

$$\frac{\partial v}{\partial \zeta} = \begin{cases} 2\sin(2\xi)(x_2-x_1) - 2\cos(2\xi)(x_2^2-x_1^2) + 4(\cos(2\xi)(x_2^2-x_1^2) + \frac{2}{3}\sin(2\xi)(x_2^3-x_1^3))\zeta, & \zeta = 0 \\ \frac{-2(1-\zeta)}{\zeta}(x_2\sin(2(\zeta x_2+\xi)) - x_1\sin(2(\zeta x_1+\xi))) - \frac{1}{\zeta^2}(\cos(2(\zeta x_2+\xi)) - \cos(2(\zeta x_1+\xi))), & \zeta \neq 0 \end{cases} \tag{13d}$$

$$\frac{\partial f_\alpha}{\partial x_1} = \begin{cases} \infty, & x_1 = 0, \xi \neq 0 \\ -\left(\frac{2\zeta}{\alpha}\right)^{2\alpha} x_1^{2\alpha-1}, & x_1 = 0, \xi = 0 \\ -\frac{\sin^{2\alpha}\left(\frac{2}{\alpha}(\zeta x_1+\xi)\right)}{x_1}, & x_1 \neq 0 \end{cases} \tag{14a}$$

$$\frac{\partial f_\alpha}{\partial x_2} = \begin{cases} \infty, & x_1 = 0, \xi \neq 0 \\ \left(\frac{2\zeta}{\alpha}\right)^{2\alpha} x_2^{2\alpha-1}, & x_1 = 0, \xi = 0 \\ \frac{\sin^{2\alpha}\left(\frac{2}{\alpha}(\zeta x_1+\xi)\right)}{x_1}, & x_1 \neq 0 \end{cases} \tag{14b}$$

$$\frac{\partial f_\alpha}{\partial \xi} = \begin{cases} \infty, & x_1 = 0, \xi \neq 0 \\ \int_{x_1}^{x_2} du \frac{4\sin\left(\frac{2}{\alpha}(\zeta u+\xi)\right)\cos\left(\frac{2}{\alpha}(\zeta u+\xi)\right)}{u}, & x_1 \neq 0 \end{cases} \tag{14c}$$

$$\frac{\partial f_\alpha}{\partial \zeta} = \begin{cases} 4(x_2-x_1)\cos(2\xi)\sin(2\xi) + 4(x_2^2-x_1^2)(\cos^2(2\xi) - \sin^2(2\xi))\zeta, & \zeta = 0, \alpha = 1 \\ 4(x_2-x_1)\sin^3(\xi)\cos(\xi) + 2(x_2^2-x_1^2)\sin^2(\xi)(3\cos^2(\xi) - \sin^2(\xi))\zeta, & \zeta = 0, \alpha = 2 \\ \frac{1}{4\zeta}\left(\sin\left(\frac{2}{\alpha}(\zeta x_2+\xi)\right) - \sin\left(\frac{2}{\alpha}(\zeta x_1+\xi)\right)\right), & \zeta \neq 0 \end{cases} \tag{14d}$$

$$\frac{\partial g_\alpha}{\partial x_1} = \frac{-x_1}{\cos^{2\alpha}(\zeta x_1 + \xi)} \tag{15a}$$

$$\frac{\partial g_\alpha}{\partial x_2} = \frac{x_2}{\cos^{2\alpha}(\zeta x_2 + \xi)} \tag{15b}$$

$$\frac{\partial g_\alpha}{\partial \xi} = \int_{x_1}^{x_2} du \frac{2\alpha u \sin(\zeta u + \xi)}{\cos^{2\alpha+1}(\zeta u + \xi)} \tag{15c}$$

$$\frac{\partial g_\alpha}{\partial \zeta} = \int_{x_1}^{x_2} du \frac{2\alpha u^2 \sin(\zeta u + \xi)}{\cos^{2\alpha+1}(\zeta u + \xi)} \tag{15d}$$

References