1 Piecewise linear definition

I will define the piecewise linear twist angle as

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

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 $0 \le r \le R_c$, 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,

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

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

$$
\begin{aligned}
&\frac{2}{R^2}\int_a^b rdr\left[\frac{1}{2}\left(\psi'_{ab}+\frac{\sin(2(\psi'_{ab}r+\psi_0))}{2r}-1\right)^2+\frac{1}{2}K_{33}\frac{\sin^4(\psi'_{ab}r+\psi_0)}{r^2}\right] \\
&+\frac{\Lambda\delta^2}{2R^2}\int_a^b rdr\left(\frac{4\pi^2}{\cos^2(\psi'_{ab}r+\psi_0)}-\eta^2\right)^2 \\
=&\frac{2}{R^2}\int_a^b dr\left(\frac{(\psi'_{ab}-1)^2}{2}r+\frac{1}{8}\frac{\sin^2(2(\psi'_{ab}r+\psi_0))}{r}+\frac{(\psi'_{ab}-1)}{2}\sin(2(\psi'_{ab}r+\psi_0))+\frac{1}{2}K_{33}\frac{\sin^4(\psi'_{ab}r+\psi_0)}{r}\right) \\
&+\frac{\Lambda\delta^2}{2R^2}\int_a^b dr\left(\frac{16\pi^4 r}{\cos^4(\psi'_{ab}r+\psi_0)}-\frac{8\pi^2 r}{\cos^2(\psi'_{ab}r+\psi_0)}\eta^2+\eta^4 r\right) \\
=&\frac{2}{R^2}\left(\frac{(\psi'_{ab}-1)^2}{2}\left.\frac{r^2}{2}\right|_{r=a}^{b}+\frac{2\psi'_{ab}}{8}f_1(2(\psi'_{ab}r+\psi_0))\Big|_{r=a}^{b}+\frac{(\psi'_{ab}-1)}{2}\left.\frac{-\cos(2(\psi'_{ab}r+\psi_0))}{2\psi'_{ab}}\right|_{r=a}^{b}\right. \\
&\left.+\frac{\psi'_{ab}}{2}K_{33}f_2(\psi'_{ab}r+\psi_0)\Big|_{r=a}^{b}\right) \\
&+\frac{\Lambda\delta^2}{2R^2}\left(\frac{16\pi^4}{\psi'_{ab}}g_2(\psi'_{ab}r+\psi_0)\Big|_{r=a}^{b}-\frac{8\pi^2\eta^2}{\psi'_{ab}}g_1(\psi'_{ab}r+\psi_0)\Big|_{r=a}^{b}+\eta^4\left.\frac{r^2}{2}\right|_{r=a}^{b}\right) \\
=&\frac{2}{R^2}\left(\frac{(\psi'_{ab}-1)^2}{4}(b^2-a^2)+\frac{2\psi'_{ab}}{8}(f_1(2(\psi'_{ab}b+\psi_0))-f_1(2(\psi'_{ab}a+\psi_0)))\right. \\
&\left.+\frac{(\psi'_{ab}-1)}{4\psi'_{ab}}(\cos(2(\psi'_{ab}a+\psi_0))-\cos(2(\psi'_{ab}b+\psi_0)))+\frac{\psi'_{ab}}{2}K_{33}(f_2(\psi'_{ab}b+\psi_0)-f_2(\psi'_{ab}a+\psi_0))\right) \\
&+\frac{\Lambda\delta^2}{2R^2}\left(\frac{16\pi^4}{\psi'_{ab}}(g_2(\psi'_{ab}b+\psi_0)-g_2(\psi'_{ab}a+\psi_0))-\frac{8\pi^2\eta^2}{\psi'_{ab}}(g_1(\psi'_{ab}b+\psi_0)-g_1(\psi'_{ab}a+\psi_0))+\frac{\eta^4}{2}(b^2-a^2)\right)
\end{aligned}
\tag{8}
$$

where I have defined the functions

$$f_\alpha(x,\beta) = \int_0^{2(x+\beta)} du\frac{sin^{2\alpha}u}{u-2\beta}, \tag{9a}$$

$$g_\alpha(x,\beta) = \int_0^{x+\beta} du\frac{u-\beta}{cos^{2\alpha}u}. \tag{9b}$$

3 References