1 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,

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

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 13 and 14, as well as the definitions of the functions u, v, f_α, and g_α in equations 15a, 15b, 15c, and 15d, respectively). I will minimize this equation subject to the constraint equations 2a and 2b to determine the equilibrium configuration of the fibril.

2 Differentiation of the energy

The derivative with respect to the fibril radius, R, is

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

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

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

The derivative with respect to the core radius size, R_c, is

$$
\begin{aligned}
\frac{\partial E}{\partial R_c} = &\\
&\frac{2}{R^2}\left(\frac{1}{4}\left(\left.\frac{\partial u(0,x_2,\psi'_c)}{\partial x_2}\right|_{x_2=R_c} + \left.\frac{\partial u(x_1,R_s,\psi'_s)}{\partial x_1}\right|_{x_1=R_c}\right) + \frac{1}{8}\left(\left.\frac{\partial f_1(0,x_2,0,\psi'_c)}{\partial x_2}\right|_{x_2=R_c}\right.\right.\\
&\left.+\left.\frac{\partial f_1(x_1,R_s,\psi_1,\psi'_c)}{\partial x_1}\right|_{x_1=R_c} + \left.\frac{\partial f_1(R_c,R_s,\xi,\psi'_s)}{\partial \xi}\right|_{\xi=\psi_1}\frac{\partial \psi_1}{\partial R_c} + \left.\frac{\partial f_1(R_s,R,\xi,\psi'_R)}{\partial \xi}\right|_{\xi=\psi_2}\frac{\partial \psi_2}{\partial R_c}\right)\\
&+\frac{1}{2}K_{33}\left(\left.\frac{\partial f_2(0,x_2,0,\psi'_c)}{\partial x_2}\right|_{x_2=R_c} + \left.\frac{\partial f_2(x_1,R_s,\psi_1,\psi'_c)}{\partial x_1}\right|_{x_1=R_c} + \left.\frac{\partial f_2(R_c,R_s,\xi,\psi'_s)}{\partial \xi}\right|_{\xi=\psi_1}\frac{\partial \psi_1}{\partial R_c}\right.\\
&\left.+\left.\frac{\partial f_2(R_s,R,\xi,\psi'_R)}{\partial \xi}\right|_{\xi=\psi_2}\frac{\partial \psi_2}{\partial R_c}\right) + \frac{1}{4}\left(\left.\frac{\partial v(0,x_2,0,\psi'_c)}{\partial x_2}\right|_{x_2=R_c} + \left.\frac{\partial v(x_1,R_s,\psi_1,\psi'_s)}{\partial x_1}\right|_{x_1=R_c}\right.\\
&\left.\left.+\left.\frac{\partial v(R_c,R_s,\xi,\psi'_s)}{\partial \xi}\right|_{\xi=\psi_1}\frac{\partial \psi_1}{\partial R_c} + \left.\frac{\partial v(R_s,R,\xi,\psi'_R)}{\partial \xi}\right|_{\xi=\psi_2}\frac{\partial \psi_2}{\partial R_c}\right)\right)\\
&+\frac{\Lambda\delta^2}{2R^2}\left(16\pi^4\left(\left.\frac{\partial g_2(0,x_2,0,\psi'_c)}{\partial x_2}\right|_{x_2=R_c} + \left.\frac{\partial g_2(x_1,R_s,\psi_1,\psi'_s)}{\partial x_1}\right|_{x_1=R_c}\right.\right.\\
&\left.+\left.\frac{\partial g_2(R_c,R_s,\xi,\psi'_s)}{\partial \xi}\right|_{\xi=\psi_1}\frac{\partial \psi_1}{\partial R_c} + \left.\frac{\partial g_2(R_s,R,\xi,\psi'_R)}{\partial \xi}\right|_{\xi=\psi_2}\frac{\partial \psi_2}{\partial R_c}\right)\\
&-8\pi^2\eta^2\left(\left.\frac{\partial g_1(0,x_2,0,\psi'_c)}{\partial x_2}\right|_{x_2=R_c} + \left.\frac{\partial g_1(x_1,R_s,\psi_1,\psi'_s)}{\partial x_1}\right|_{x_1=R_c} + \left.\frac{\partial g_1(R_c,R_s,\xi,\psi'_s)}{\partial \xi}\right|_{\xi=\psi_1}\frac{\partial \psi_1}{\partial R_c}\right.\\
&\left.\left.+\left.\frac{\partial g_1(R_s,R,\xi,\psi'_R)}{\partial \xi}\right|_{\xi=\psi_2}\frac{\partial \psi_2}{\partial R_c}\right)\right) - \frac{(1+k_{24})}{R^2}\cos(\psi'_R R+\psi_2)\frac{\partial \psi_2}{\partial R_c}. \qquad (8)
\end{aligned}
$$

The derivative with respect to the shelf radius size, R_s, is

$$
\begin{aligned}
&\frac{\partial E}{\partial R_s} = \\
&\quad \frac{2}{R^2}\left(\frac{1}{4}\left(\left.\frac{\partial u(R_c,x_2,\psi_s')}{\partial x_2}\right|_{x_2=R_s} + \left.\frac{\partial u(x_1,R,\psi_R')}{\partial x_1}\right|_{x_1=R_s}\right) + \frac{1}{8}\left(\left.\frac{\partial f_1(R_c,x_2,\psi_1,\psi_s')}{\partial x_2}\right|_{x_2=R_s}\right.\right. \\
&\quad \left. + \left.\frac{\partial f_1(x_1,R,\psi_2,\psi_R')}{\partial x_1}\right|_{x_1=R_s} + \left.\frac{\partial f_1(R_s,R,\xi,\psi_R')}{\partial \xi}\right|_{\xi=\psi_2}\frac{\partial \psi_2}{\partial R_s}\right) \\
&\quad + \frac{1}{2}K_{33}\left(\left.\frac{\partial f_2(R_c,x_2,\psi_1,\psi_s')}{\partial x_2}\right|_{x_2=R_s} + \left.\frac{\partial f_2(x_1,R,\psi_2,\psi_R')}{\partial x_1}\right|_{x_1=R_s} + \left.\frac{\partial f_2(R_s,R,\xi,\psi_R')}{\partial \xi}\right|_{\xi=\psi_2}\frac{\partial \psi_2}{\partial R_s}\right) \\
&\quad \left. + \frac{1}{4}\left(\left.\frac{\partial v(R_c,x_2,\psi_1,\psi_s')}{\partial x_2}\right|_{x_2=R_s} + \left.\frac{\partial v(x_1,R,\psi_2,\psi_R')}{\partial x_1}\right|_{x_1=R_2} + \left.\frac{\partial v(R_s,R,\xi,\psi_R')}{\partial \xi}\right|_{\xi=\psi_2}\frac{\partial \psi_2}{\partial R_s}\right)\right) \\
&\quad + \frac{\Lambda\delta^2}{2R^2}\left(16\pi^4\left(\left.\frac{\partial g_2(R_c,x_2,\psi_1,\psi_s')}{\partial x_2}\right|_{x_2=R_s} + \left.\frac{\partial g_2(x_1,R,\psi_2,\psi_R')}{\partial x_1}\right|_{x_1=R_s} + \left.\frac{\partial g_2(R_s,R,\xi,\psi_R')}{\partial \xi}\right|_{\xi=\psi_2}\frac{\partial \psi_2}{\partial R_s}\right)\right. \\
&\quad \left. - 8\pi^2\eta^2\left(\left.\frac{\partial g_1(R_c,x_2,\psi_1,\psi_s')}{\partial x_2}\right|_{x_2=R_s} + \left.\frac{g_1(x_1,R,\psi_2,\psi_R')}{\partial x_1}\right|_{x_1=R_s} + \left.\frac{\partial g_1(R_s,R,\xi,\psi_R')}{\partial \xi}\right|_{\xi=\psi_2}\frac{\partial \psi_2}{\partial R_s}\right)\right) \\
&\quad - \frac{(1+k_{24})}{R^2}\cos(\psi_R' R + \psi_2)\frac{\partial \psi_2}{\partial R_s}.
\end{aligned} \tag{9}
$$

The derivative with respect to the twist angle gradient in the core, ψ_c', is

$$
\begin{aligned}
&\frac{\partial E}{\partial \psi_c'} = \\
&\quad \frac{2}{R^2}\left(\frac{1}{4}\left.\frac{\partial u(0,R_c,\zeta)}{\partial \zeta}\right|_{\zeta=\psi_c'} + \frac{1}{8}\left(\left.\frac{\partial f_1(0,R_c,0,\zeta)}{\partial \zeta}\right|_{\zeta=\psi_c'} + \left.\frac{\partial f_1(R_c,R_s,\xi,\psi_s')}{\partial \xi}\right|_{\xi=\psi_1}\frac{\partial \psi_1}{\partial \psi_c'}\right.\right. \\
&\quad \left. + \left.\frac{\partial f_1(R_s,R,\xi,\psi_R')}{\partial \xi}\right|_{\xi=\psi_2}\frac{\partial \psi_2}{\partial \psi_c'}\right) + \frac{1}{2}K_{33}\left(\left.\frac{\partial f_2(0,R_c,0,\zeta)}{\partial \zeta}\right|_{\zeta=\psi_c'} + \left.\frac{\partial f_2(R_c,R_s,\xi,\psi_s')}{\partial \xi}\right|_{\xi=\psi_1}\frac{\partial \psi_1}{\partial \psi_c'}\right. \\
&\quad \left. + \left.\frac{\partial f_2(R_s,R,\xi,\psi_R')}{\partial \xi}\right|_{\xi=\psi_2}\frac{\partial \psi_2}{\partial \psi_c'}\right) + \frac{1}{4}\left(\left.\frac{\partial v(0,R_c,0,\zeta)}{\partial \zeta}\right|_{\zeta=\psi_c'} + \left.\frac{\partial v(R_c,R_s,\xi,\psi_s')}{\partial \xi}\right|_{\xi=\psi_1}\frac{\partial \psi_1}{\partial \psi_c'}\right. \\
&\quad \left.\left. + \left.\frac{\partial v(R_s,R,\xi,\psi_R')}{\partial \xi}\right|_{\xi=\psi_2}\frac{\partial \psi_2}{\partial \psi_c'}\right)\right) + \frac{\Lambda\delta^2}{2R^2}\left(16\pi^4\left(\left.\frac{\partial g_2(0,R_c,0,\zeta)}{\partial \zeta}\right|_{\zeta=\psi_c'} + \left.\frac{\partial g_2(R_c,R_s,\xi,\psi_s')}{\partial \xi}\right|_{\xi=\psi_1}\frac{\partial \psi_1}{\partial \psi_c'}\right.\right. \\
&\quad \left. + \left.\frac{\partial g_2(R_s,R,\xi,\psi_R')}{\partial \xi}\right|_{\xi=\psi_2}\frac{\partial \psi_2}{\partial \psi_c'}\right) - 8\pi^2\eta^2\left(\left.\frac{\partial g_1(0,R_c,0,\zeta)}{\partial \zeta}\right|_{\zeta=\psi_c'} + \left.\frac{\partial g_1(R_c,R_s,\xi,\psi_s')}{\partial \xi}\right|_{\xi=\psi_1}\frac{\partial \psi_1}{\partial \psi_c'}\right. \\
&\quad \left.\left. + \left.\frac{\partial g_1(R_s,R,\xi,\psi_R')}{\partial \xi}\right|_{\xi=\psi_2}\frac{\partial \psi_2}{\partial \psi_c'}\right)\right) - \frac{(1+k_{24})}{R^2}\cos(\psi_R' R + \psi_2)\frac{\partial \psi_2}{\partial \psi_c'}.
\end{aligned} \tag{10}
$$

The derivative with respect to the twist angle gradient in the shelf, ψ'_s, is

$$
\begin{aligned}
&\frac{\partial E}{\partial \psi'_s} = \\
&\quad \frac{2}{R^2}\left(\frac{1}{4}\frac{\partial u(R_c,R_s,\zeta)}{\partial \zeta}\bigg|_{\zeta=\psi'_s} + \frac{1}{8}\left(\frac{\partial f_1(R_c,R_s,\psi_1,\zeta)}{\partial \zeta}\bigg|_{\zeta=\psi'_s} + \frac{\partial f_1(R_s,R,\xi,\psi'_R)}{\partial \xi}\bigg|_{\xi=\psi_2}\frac{\partial \psi_2}{\partial \psi'_s}\right)\right. \\
&\quad + \frac{1}{2}K_{33}\left(\frac{\partial f_2(R_c,R_s,\psi_1,\zeta)}{\partial \zeta}\bigg|_{\zeta=\psi'_s} + \frac{\partial f_2(R_s,R,\xi,\psi'_R)}{\partial \xi}\bigg|_{\xi=\psi_2}\frac{\partial \psi_2}{\partial \psi'_s}\right) \\
&\quad \left. + \frac{1}{4}\left(\frac{\partial v(R_c,R_s,\psi_1,\zeta)}{\partial \zeta}\bigg|_{\zeta=\psi'_s} + \frac{\partial v(R_s,R,\xi,\psi'_R)}{\partial \xi}\bigg|_{\xi=\psi_2}\frac{\partial \psi_2}{\partial \psi'_s}\right)\right) \\
&\quad + \frac{\Lambda\delta^2}{2R^2}\left(16\pi^4\left(\frac{\partial g_2(R_c,R_s,\psi_1,\zeta)}{\partial \zeta}\bigg|_{\zeta=\psi'_s} + \frac{\partial g_2(R_s,R,\xi,\psi'_R)}{\partial \xi}\bigg|_{\xi=\psi_2}\frac{\partial \psi_2}{\partial \psi'_s}\right)\right. \\
&\quad \left. - 8\pi^2\eta^2\left(\frac{\partial g_1(R_c,R_s,\psi_1,\zeta)}{\partial \zeta}\bigg|_{\zeta=\psi'_s} + \frac{\partial g_1(R_s,R,\xi,\psi'_R)}{\partial \xi}\bigg|_{\xi=\psi_2}\frac{\partial \psi_2}{\partial \psi'_s}\right)\right) \\
&\quad - \frac{(1+k_{24})}{R^2}\cos(\psi'_R R + \psi_2)\frac{\partial \psi_2}{\partial \psi'_s}.
\end{aligned} \tag{11}
$$

Finally, the derivative with respect to the twist angle gradient in surface reconstruction region, ψ'_R, is

$$
\begin{aligned}
&\frac{\partial E}{\partial \psi'_R} = \\
&\quad \frac{2}{R^2}\left(\frac{1}{4}\frac{\partial u(R_s,R,\zeta)}{\partial \zeta}\bigg|_{\zeta=\psi'_R} + \frac{1}{8}\frac{\partial f_1(R_s,R,\psi_2,\zeta)}{\partial \zeta}\bigg|_{\zeta=\psi'_R} + \frac{1}{2}K_{33}\frac{\partial f_2(R_s,R,\psi_2,\zeta)}{\partial \zeta}\bigg|_{\zeta=\psi'_R}\right. \\
&\quad \left. + \frac{1}{4}\frac{\partial v(R_s,R,\psi_2,\zeta)}{\partial \zeta}\bigg|_{\zeta=\psi'_R}\right) + \frac{\Lambda\delta^2}{2R^2}\left(16\pi^4\frac{\partial g_2(R_s,R,\psi_2,\zeta)}{\partial \zeta}\bigg|_{zeta=\psi'_R}\right. \\
&\quad \left. - 8\pi^2\eta^2\frac{\partial g_1(R_s,R,\psi_2,\zeta)}{\partial \zeta}\bigg|_{\zeta=\psi'_R}\right) - \frac{(1+k_{24})}{R}\cos(\psi'_R R + \psi_2).
\end{aligned} \tag{12}
$$

3 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

$$\int_a^b rdr \left[\frac{1}{2} \left(\psi'_{ab} + \frac{\sin(2(\psi'_{ab}r + \psi_0))}{2r} - 1 \right)^2 + \frac{1}{2} K_{33} \frac{\sin^4(\psi'_{ab}r + \psi_0)}{r^2} \right]$$

$$= \int_a^b dr \left(\frac{(1-\psi'_{ab})^2}{2} r + \frac{1}{8} \frac{\sin^2(2(\psi'_{ab}r + \psi_0))}{r} - \frac{(1-\psi'_{ab})}{2} \sin(2(\psi'_{ab}r + \psi_0)) + \frac{1}{2} K_{33} \frac{\sin^4(\psi'_{ab}r + \psi_0)}{r} \right)$$

$$= \left(\frac{1}{4} u(a, b, \psi'_{ab}) + \frac{1}{8} f_1(a, b, \psi_0, \psi'_{ab}) + \frac{1}{2} K_{33} f_2(a, b, \psi_0, \psi'_{ab}) + \frac{1}{4} v(a, b, \psi_0, \psi'_{ab}) \right) \tag{13}$$

and

$$\int_a^b rdr \left(\frac{4\pi^2}{\cos^2(\psi'_{ab}r + \psi_0)} - \eta^2 \right)^2$$

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

$$= \left(16\pi^4 g_2(a, b, \psi_0, \psi'_{ab}) - 8\pi^2 \eta^2 g_1(a, b, \psi_0, \psi'_{ab}) + \frac{\eta^4}{2}(b^2 - a^2) \right) \tag{14}$$

where I have defined the functions

$$u(x_1, x_2, \zeta) = (1-\zeta)^2 (x_2^2 - x_1^2), \tag{15a}$$

$$v(x_1, x_2, \xi, \zeta) = \frac{(1-\zeta)}{\zeta} (\cos(2(\zeta x_2 + \xi)) - \cos(2(\zeta x_1 + \xi))), \tag{15b}$$

$$f_\alpha(x_1, x_2, \xi, \zeta) = \int_{x_1}^{x_2} du \frac{\sin^{2\alpha}\left(\frac{2}{\alpha}(\zeta u + \xi)\right)}{u}, \tag{15c}$$

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

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

$$\begin{aligned} v(x_1,x_2,\xi,\zeta) &= -2(1-\zeta)\sin(2\xi)(x_2-x_1) - 2(1-\zeta)\cos(2\xi)(x_2^2-x_1^2)\zeta \\ &\quad + \frac{4}{3}(1-\zeta)\sin(2\xi)(x_2^3-x_1^3)\zeta^2 + \frac{2}{3}\cos(2\xi)(x_2^4-x_1^4)\zeta^3, \qquad (16a) \\ f_1(x_1,x_2,\xi,\zeta) &= \sin^2(2\xi)\ln\frac{x_2}{x_1} + 4\zeta(x_2-x_1)\cos(2\xi)\sin(2\xi) \\ &\quad + 2\zeta^2(x_2^2-x_1^2)\left(\cos^2(2\xi)-\sin^2(2\xi)\right) - \frac{32}{9}\zeta^3(x_2^3-x_1^3)\sin(2\xi)\cos(2\xi) \qquad (16b) \\ f_2(x_1,x_2,\xi,\zeta) &= \sin^4\xi\ln\frac{x_2}{x_1} + 4\zeta(x_2-x_1)\sin^3\xi\cos\xi + \zeta^2(x_2^2-x_1^2)\sin^2\xi(\cos^2\xi-\sin^2\xi) \\ &\quad + \frac{4}{3}\zeta^3(x_2^3-x_1^3)\sin\xi\cos\xi\left(\cos^2\xi-5\sin^2\xi\right) \qquad (16c) \\ g_1(x_1,x_2,\xi,\zeta) &= \frac{1}{\cos^2\xi}\left(\frac{x_2^2-x_1^2}{2} + \frac{2\zeta(x_2^3-x_1^2)}{3}\tan\xi + \frac{\zeta^2(x_2^4-x_1^4)(3\tan^2\xi+1)}{4}\right. \\ &\quad \left. + \frac{4\zeta^3(x_2^5-x_1^5)(4+3\tan^2\xi)\tan\xi}{15}\right) \qquad (16d) \\ g_2(x_1,x_2,\xi,\zeta) &= \frac{1}{\cos^4\xi}\left(\frac{x_2^2-x_1^2}{2} + \frac{4\zeta(x_2^3-x_1^3)\tan\xi}{3} + \frac{\zeta^2(x_2^4-x_1^4)(1+5\tan^2\xi)}{2}\right. \\ &\quad \left. + \frac{\zeta^3(x_2^5-x_1^5)(60\tan^2\xi+28)\tan\xi}{15}\right) \qquad (16e) \end{aligned}$$

The derivatives of these functions are listed below:

$$\frac{\partial u}{\partial x_1} = -2(1-\zeta)^2 x_1 \qquad (17a)$$

$$\frac{\partial u}{\partial x_2} = 2(1-\zeta)^2 x_2 \qquad (17b)$$

$$\frac{\partial u}{\partial \xi} = 0 \qquad (17c)$$

$$\frac{\partial u}{\partial \zeta} = -2\zeta(1-\zeta)(x_2^2-x_1^2) \qquad (17d)$$

$$\frac{\partial v}{\partial x_1} = 2(1-\zeta)\sin(2(\zeta x_1+\xi)) \tag{18a}$$

$$\frac{\partial v}{\partial x_2} = -2(1-\zeta)\sin(2(\zeta x_2+\xi)) \tag{18b}$$

$$\frac{\partial v}{\partial \xi} = \begin{cases} -4\cos(2\xi)(x_2-x_1)+(4\cos(2\xi)(x_2-x_1)+4\sin(2\xi)(x_2^2-x_1^2))\zeta, & \zeta = 0 \\ -2\frac{(1-\zeta)}{\zeta}(\sin(2(\zeta x_2+\xi))-\sin(2(\zeta x_1+\xi))), & \zeta \neq 0 \end{cases} \tag{18c}$$

$$\frac{\partial v}{\partial \zeta} = \begin{cases} 2\sin(2\xi)(x_2-x_1)-2\cos(2\xi)(x_2^2-x_1^2)+4(\cos(2\xi)(x_2^2-x_1^2)+\frac{2}{3}\sin(2\xi)(x_2^3-x_1^3))\zeta, & \zeta = 0 \\ \frac{-2(1-\zeta)}{\zeta}(x_2\sin(2(\zeta x_2+\xi))-x_1\sin(2(\zeta x_1+\xi)))-\frac{1}{\zeta^2}(\cos(2(\zeta x_2+\xi))-\cos(2(\zeta x_1+\xi))), & \zeta \neq 0 \end{cases} \tag{18d}$$

$$\frac{\partial f_\alpha}{\partial x_1} = \begin{cases} \infty, & x_1 = 0, \xi \neq 0 \\ -\left(\frac{2\zeta}{\alpha}\right)^{2\alpha} x_1^{2\alpha-1}, & x_1 = 0, \xi = 0 \\ -\frac{\sin^{2\alpha}\left(\frac{2}{\alpha}(\zeta x_1+\xi)\right)}{x_1}, & x_1 \neq 0 \end{cases} \tag{19a}$$

$$\frac{\partial f_\alpha}{\partial x_2} = \begin{cases} \infty, & x_1 = 0, \xi \neq 0 \\ \left(\frac{2\zeta}{\alpha}\right)^{2\alpha} x_2^{2\alpha-1}, & x_1 = 0, \xi = 0 \\ \frac{\sin^{2\alpha}\left(\frac{2}{\alpha}(\zeta x_1+\xi)\right)}{x_1}, & x_1 \neq 0 \end{cases} \tag{19b}$$

$$\frac{\partial f_\alpha}{\partial \xi} = \begin{cases} \infty, & x_1 = 0, \xi \neq 0 \\ \int_{x_1}^{x_2} du \frac{4\sin^{2\alpha-1}\left(\frac{2}{\alpha}(\zeta u+\xi)\right)\cos\left(\frac{2}{\alpha}(\zeta u+\xi)\right)}{u}, & x_1 \neq 0 \end{cases} \tag{19c}$$

$$\frac{\partial f_\alpha}{\partial \zeta} = \begin{cases} 4(x_2-x_1)\cos(2\xi)\sin(2\xi)+4(x_2^2-x_1^2)(\cos^2(2\xi)-\sin^2(2\xi))\zeta, & \zeta = 0, \alpha = 1 \\ 4(x_2-x_1)\sin^3(\xi)\cos(\xi)+2(x_2^2-x_1^2)\sin^2(\xi)(3\cos^2(\xi)-\sin^2(\xi))\zeta, & \zeta = 0, \alpha = 2 \\ \frac{1}{\zeta}\left(\sin^{2\alpha}\left(\frac{2}{\alpha}(\zeta x_2+\xi)\right)-\sin^{2\alpha}\left(\frac{2}{\alpha}(\zeta x_1+\xi)\right)\right), & \zeta \neq 0 \end{cases} \tag{19d}$$

$$\frac{\partial g_\alpha}{\partial x_1} = \frac{-x_1}{\cos^{2\alpha}(\zeta x_1 + \xi)} \tag{20a}$$

$$\frac{\partial g_\alpha}{\partial x_2} = \frac{x_2}{\cos^{2\alpha}(\zeta x_2 + \xi)} \tag{20b}$$

$$\frac{\partial g_\alpha}{\partial \xi} = \int_{x_1}^{x_2} du \frac{2\alpha u \sin(\zeta u + \xi)}{\cos^{2\alpha+1}(\zeta u + \xi)} \tag{20c}$$

$$\frac{\partial g_\alpha}{\partial \zeta} = \int_{x_1}^{x_2} du \frac{2\alpha u^2 \sin(\zeta u + \xi)}{\cos^{2\alpha+1}(\zeta u + \xi)} \tag{20d}$$

4 References