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,

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

The resulting equation can be written as

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

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.

Differentiation of the energy

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

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

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

$$
\begin{aligned}
\frac{\partial E}{\partial \eta} =& \frac{\Lambda\delta^2}{2R^2}\big(-16\pi^2\eta(g_1(0,R_c,0,\psi'_c)+g_1(R_c,R_s,\psi_1,\psi'_s)+g_1(R_s,R,\psi_2,\psi'_R)) \\
& + 2\eta^3(g_2(0,R_c,0,\psi'_c)+g_2(R_c,R_s,\psi_1,\psi'_s)+g_2(R_s,R,\psi_2,\psi'_R))\big) \qquad (6)
\end{aligned}
$$

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

$$
\begin{aligned}
\frac{\partial E}{\partial \delta} =& \frac{\Lambda\delta}{R^2}\big(8\pi^4R^2-8\pi^2\eta^2(g_1(0,R_c,0,\psi'_c)+g_1(R_c,R_s,\psi_1,\psi'_s)+g_1(R_s,R,\psi_2,\psi'_R)) \\
& + \eta^4(g_2(0,R_c,0,\psi'_c)+g_2(R_c,R_s,\psi_1,\psi'_s)+g_2(R_s,R,\psi_2,\psi'_R))\big)+\omega\delta\left(\frac{3}{2}\delta^2-1\right). \qquad (7)
\end{aligned}
$$

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

$$
\begin{aligned}
\frac{\partial E}{\partial R_c} &= \\
&\frac{2}{R^2}\Bigg(\frac{1}{4}\Bigg(\frac{\partial u(0,x_2,\psi_c')}{\partial x_2}\bigg|_{x_2=R_c} + \frac{\partial u(x_1,R_s,\psi_s')}{\partial x_1}\bigg|_{x_1=R_c}\Bigg) + \frac{1}{8}\Bigg(\frac{\partial f_1(0,x_2,0,\psi_c')}{\partial x_2}\bigg|_{x_2=R_c} \\
&+ \frac{\partial f_1(x_1,R_s,\psi_1,\psi_c')}{\partial x_1}\bigg|_{x_1=R_c} + \frac{\partial f_1(R_c,R_s,\xi,\psi_s')}{\partial \xi}\bigg|_{\xi=\psi_1}\frac{\partial \psi_1}{\partial R_c} + \frac{\partial f_1(R_s,R,\xi,\psi_R')}{\partial \xi}\bigg|_{\xi=\psi_2}\frac{\partial \psi_2}{\partial R_c}\Bigg) \\
&+ \frac{1}{2}K_{33}\Bigg(\frac{\partial f_2(0,x_2,0,\psi_c')}{\partial x_2}\bigg|_{x_2=R_c} + \frac{\partial f_2(x_1,R_s,\psi_1,\psi_c')}{\partial x_1}\bigg|_{x_1=R_c} + \frac{\partial f_2(R_c,R_s,\xi,\psi_s')}{\partial \xi}\bigg|_{\xi=\psi_1}\frac{\partial \psi_1}{\partial R_c} \\
&+ \frac{\partial f_2(R_s,R,\xi,\psi_R')}{\partial \xi}\bigg|_{\xi=\psi_2}\frac{\partial \psi_2}{\partial R_c}\Bigg) + \frac{1}{4}\Bigg(\frac{\partial v(0,x_2,0,\psi_c')}{\partial x_2}\bigg|_{x_2=R_c} + \frac{\partial v(x_1,R_s,\psi_1,\psi_s')}{\partial x_1}\bigg|_{x_1=R_c} \\
&+ \frac{\partial v(R_c,R_s,\xi,\psi_s')}{\partial \xi}\bigg|_{\xi=\psi_1}\frac{\partial \psi_1}{\partial R_c} + \frac{\partial v(R_s,R,\xi,\psi_R')}{\partial \xi}\bigg|_{\xi=\psi_2}\frac{\partial \psi_2}{\partial R_c}\Bigg)\Bigg) \\
&+ \frac{\Lambda\delta^2}{2R^2}\Bigg(-8\pi^2\eta^2\Bigg(\frac{\partial g_1(0,x_2,0,\psi_c')}{\partial x_2}\bigg|_{x_2=R_c} + \frac{\partial g_1(x_1,R_s,\psi_1,\psi_s')}{\partial x_1}\bigg|_{x_1=R_c} \\
&+ \frac{\partial g_1(R_c,R_s,\xi,\psi_s')}{\partial \xi}\bigg|_{\xi=\psi_1}\frac{\partial \psi_1}{\partial R_c} + \frac{\partial g_1(R_s,R,\xi,\psi_R')}{\partial \xi}\bigg|_{\xi=\psi_2}\frac{\partial \psi_2}{\partial R_c}\Bigg) \\
&+ \eta^4\Bigg(\frac{\partial g_2(0,x_2,0,\psi_c')}{\partial x_2}\bigg|_{x_2=R_c} + \frac{\partial g_2(x_1,R_s,\psi_1,\psi_s')}{\partial x_1}\bigg|_{x_1=R_c} \\
&+ \frac{\partial g_2(R_c,R_s,\xi,\psi_s')}{\partial \xi}\bigg|_{\xi=\psi_1}\frac{\partial \psi_1}{\partial R_c} + \frac{\partial g_2(R_s,R,\xi,\psi_R')}{\partial \xi}\bigg|_{\xi=\psi_2}\frac{\partial \psi_2}{\partial R_c}\Bigg)\Bigg) \\
&- \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

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

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}\Bigg(\frac{1}{4}\frac{\partial u(0,R_c,\zeta)}{\partial \zeta}\Bigg|_{\zeta=\psi_c'} + \frac{1}{8}\Bigg(\frac{\partial f_1(0,R_c,0,\zeta)}{\partial \zeta}\Bigg|_{\zeta=\psi_c'} + \frac{\partial f_1(R_c,R_s,\xi,\psi_s')}{\partial \xi}\Bigg|_{\xi=\psi_1}\frac{\partial \psi_1}{\partial \psi_c'} \\
&\quad + \frac{\partial f_1(R_s,R,\xi,\psi_R')}{\partial \xi}\Bigg|_{\xi=\psi_2}\frac{\partial \psi_2}{\partial \psi_c'}\Bigg) + \frac{1}{2}K_{33}\Bigg(\frac{\partial f_2(0,R_c,0,\zeta)}{\partial \zeta}\Bigg|_{\zeta=\psi_c'} + \frac{\partial f_2(R_c,R_s,\xi,\psi_s')}{\partial \xi}\Bigg|_{\xi=\psi_1}\frac{\partial \psi_1}{\partial \psi_c'} \\
&\quad + \frac{\partial f_2(R_s,R,\xi,\psi_R')}{\partial \xi}\Bigg|_{\xi=\psi_2}\frac{\partial \psi_2}{\partial \psi_c'}\Bigg) + \frac{1}{4}\Bigg(\frac{\partial v(0,R_c,0,\zeta)}{\partial \zeta}\Bigg|_{\zeta=\psi_c'} + \frac{\partial v(R_c,R_s,\xi,\psi_s')}{\partial \xi}\Bigg|_{\xi=\psi_1}\frac{\partial \psi_1}{\partial \psi_c'} \\
&\quad + \frac{\partial v(R_s,R,\xi,\psi_R')}{\partial \xi}\Bigg|_{\xi=\psi_2}\frac{\partial \psi_2}{\partial \psi_c'}\Bigg)\Bigg) + \frac{\Lambda\delta^2}{2R^2}\Bigg(-8\pi^2\eta^2\Bigg(\frac{\partial g_1(0,R_c,0,\zeta)}{\partial \zeta}\Bigg|_{\zeta=\psi_c'} \\
&\quad + \frac{\partial g_1(R_c,R_s,\xi,\psi_s')}{\partial \xi}\Bigg|_{\xi=\psi_1}\frac{\partial \psi_1}{\partial \psi_c'} + \frac{\partial g_1(R_s,R,\xi,\psi_R')}{\partial \xi}\Bigg|_{\xi=\psi_2}\frac{\partial \psi_2}{\partial \psi_c'}\Bigg) \\
&\quad \eta^4\Bigg(\frac{\partial g_2(0,R_c,0,\zeta)}{\partial \zeta}\Bigg|_{\zeta=\psi_c'} + \frac{\partial g_2(R_c,R_s,\xi,\psi_s')}{\partial \xi}\Bigg|_{\xi=\psi_1}\frac{\partial \psi_1}{\partial \psi_c'} \\
&\quad + \frac{\partial g_2(R_s,R,\xi,\psi_R')}{\partial \xi}\Bigg|_{\xi=\psi_2}\frac{\partial \psi_2}{\partial \psi_c'}\Bigg)\Bigg) - \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

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

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

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

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

$$
\begin{aligned}
&\int_a^b r dr \left[\frac{1}{2} \left(\psi'_{ab} + \frac{\sin(2(\psi'_{ab} r + \psi_0))}{2r} - 1 \right)^2 + \frac{1}{2} K_{33} \frac{\sin^4(\psi'_{ab} r + \psi_0)}{r^2} \right] \\
&\quad = \int_a^b dr \left(\frac{(1-\psi'_{ab})^2}{2} r + \frac{1}{8} \frac{\sin^2(2(\psi'_{ab} r + \psi_0))}{r} - \frac{(1-\psi'_{ab})}{2} \sin(2(\psi'_{ab} r + \psi_0)) + \frac{1}{2} K_{33} \frac{\sin^4(\psi'_{ab} r + \psi_0)}{r} \right) \\
&\quad = \left(\frac{1}{4} u(a, b, \psi'_{ab}) + \frac{1}{8} f_1(a, b, \psi_0, \psi'_{ab}) + \frac{1}{2} K_{33} f_2(a, b, \psi_0, \psi'_{ab}) + \frac{1}{4} v(a, b, \psi_0, \psi'_{ab}) \right) \qquad (13)
\end{aligned}
$$

and

$$
\begin{aligned}
&\int_a^b r dr \big(4\pi^2 - \eta^2 \cos^2(\psi'_{ab} r + \psi_0) \big)^2 \\
&\quad = \int_a^b dr \big(16\pi^4 r - 8\pi^2 r \cos^2(\psi'_{ab} r + \psi_0) \eta^2 + \eta^4 r \cos^4(\psi'_{ab} r + \psi_0) \big) \\
&\quad = \big(8\pi^4 (b^2 - a^2) - 8\pi^2 \eta^2 g_1(a, b, \psi_0, \psi'_{ab}) + \eta^4 g_2(a, b, \psi_0, \psi'_{ab}) \big) \qquad (14)
\end{aligned}
$$

where I have defined the functions

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

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

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

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

Note that eqn 15d can be integrated analytically, and will be in the computation, but it's form is not very illuminating and so I have left it in integral form.

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

$$
\begin{aligned}
v(x_1,x_2,\xi,\zeta) &= -2(1-\zeta)\sin(2\xi)(x_2-x_1) - 2(1-\zeta)\cos(2\xi)(x_2^2-x_1^2)\zeta \\
&\quad + \frac{4}{3}(1-\zeta)\sin(2\xi)(x_2^3-x_1^3)\zeta^2 + \frac{2}{3}\cos(2\xi)(x_2^4-x_1^4)\zeta^3, && \text{(16a)}\\
f_1(x_1,x_2,\xi,\zeta) &= \sin^2(2\xi)\ln\frac{x_2}{x_1} + 4\zeta(x_2-x_1)\cos(2\xi)\sin(2\xi) \\
&\quad + 2\zeta^2(x_2^2-x_1^2)\left(\cos^2(2\xi)-\sin^2(2\xi)\right) - \frac{32}{9}\zeta^3(x_2^3-x_1^3)\sin(2\xi)\cos(2\xi) && \text{(16b)}\\
f_2(x_1,x_2,\xi,\zeta) &= \sin^4\xi\ln\frac{x_2}{x_1} + 4\zeta(x_2-x_1)\sin^3\xi\cos\xi + \zeta^2(x_2^2-x_1^2)\sin^2\xi(\cos^2\xi-\sin^2\xi) \\
&\quad + \frac{4}{3}\zeta^3(x_2^3-x_1^3)\sin\xi\cos\xi\left(\cos^2\xi-5\sin^2\xi\right) && \text{(16c)}\\
g_1(x_1,x_2,\xi,\zeta) &= \frac{(x_2^2-x_1^2)\cos^2\xi}{2} - \frac{2(x_2^3-x_1^3)\cos\xi\sin\xi}{3}\zeta - \frac{(x_2^4-x_1^4)(\cos^2\xi-\sin^2\xi)}{4}\zeta^2 \\
&\quad + \frac{4(x_2^5-x_1^5)\cos\xi\sin\xi}{15}\zeta^3 \\
g_2(x_1,x_2,\xi,\zeta) &= \frac{(x_2^2-x_1^2)\cos^4\xi}{2} - \frac{4(x_2^3-x_1^3)\cos^3\xi\sin\xi}{3}\zeta - \frac{(x_2^4-x_1^4)\cos^2\xi(\cos^2\xi-3\sin^2\xi)}{2}\zeta^2 \\
&\quad - \frac{(x_2^5-x_1^5)\cos\xi(5\cos^3\xi-12\sin^3\xi)}{15}\zeta^3 && \text{(16d)}
\end{aligned}
$$

The derivatives of these functions are listed below:

$$
\begin{aligned}
\frac{\partial u}{\partial x_1} &= -2(1-\zeta)^2 x_1 && \text{(17a)}\\
\frac{\partial u}{\partial x_2} &= 2(1-\zeta)^2 x_2 && \text{(17b)}\\
\frac{\partial u}{\partial \xi} &= 0 && \text{(17c)}\\
\frac{\partial u}{\partial \zeta} &= -2\zeta(1-\zeta)(x_2^2-x_1^2) && \text{(17d)}
\end{aligned}
$$

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

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

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

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

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

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

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

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

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

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

$$\frac{\partial g_\alpha}{\partial \xi} = \begin{cases} -(x_2^2 - x_1^2)\cos\xi\sin\xi - \frac{2(x_2^3 - x_1^3)(\cos^2\xi - \sin^2\xi)}{3}\zeta, & \zeta = 0, \alpha = 1, \\ -2(x_2^2 - x_1^2)\cos^3\xi\sin\xi - \frac{4(x_2^3 - x_1^3)(\cos^4\xi - 3\cos^2\xi\sin^2\xi)}{3}\zeta, & \zeta = 0, \alpha = 2, \\ -2\alpha\int_{x_1}^{x_2} u\cos^{2\alpha-1}(\zeta u + \xi)\sin(\zeta u + \xi)du & \zeta \neq 0, \end{cases} \tag{20c}$$

$$\frac{\partial g_\alpha}{\partial \zeta} = \begin{cases} \frac{-2(x_2^3 - x_1^3)\cos\xi\sin\xi}{3} - \frac{(x_2^4 - x_1^4)(\cos^2\xi - \sin^2\xi)}{2}\zeta, & \zeta = 0, \alpha = 1, \\ \frac{-4(x_2^3 - x_1^3)\cos^3\xi\sin\xi}{3} - (x_2^4 - x_1^4)\cos^2\xi(\cos^2\xi - \sin^2\xi)\zeta, & \zeta = 0, \alpha = 2, \\ -2\alpha\int_{x_1}^{x_2} u^2\cos^{2\alpha-1}(\zeta u + \xi)\sin(\zeta u + \xi)du, & \zeta \neq 0. \end{cases} \tag{20d}$$