

# Energy function for a piecewise linear twist angle field

I will define the piecewise linear twist angle as

$$\psi(r) = \begin{cases} \psi'_c r & 0 \leq r \leq R_c \\ \psi'_s r + \psi_1 & R_c < r \leq R_s \\ \psi'_R r + \psi_2 & R_s < r \leq R. \end{cases} \quad (1)$$

which have two constraints,

$$\psi_1 = (\psi'_c - \psi'_s)R_c, \quad (2a)$$

$$\psi_2 = (\psi'_s - \psi'_R)R_s + (\psi'_c - \psi'_s)R_c, \quad (2b)$$

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

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

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

The resulting equation can be written as

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

which utilizes a derivation shown in the appendix (see eqns 13 and 14, as well as the definitions of the functions  $u$ ,  $v$ ,  $f_\alpha$ , and  $g_\alpha$  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

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

The derivative with respect to the inverse period of density modulations,  $\eta$ , is

$$\begin{aligned}
\frac{\partial E}{\partial \eta} = & \frac{\Lambda \delta^2}{2R^2} ( - 16\pi^2 \eta (g_1(0, R_c, 0, \psi'_c) + g_1(R_c, R_s, \psi_1, \psi'_s) + g_1(R_s, R, \psi_2, \psi'_R)) \\
& + 4\eta^3 (g_2(0, R_c, 0, \psi'_c) + g_2(R_c, R_s, \psi_1, \psi'_s) + g_2(R_s, R, \psi_2, \psi'_R)) ) \tag{6}
\end{aligned}$$

The derivative with respect to the size of the density modulations,  $\delta$ , is

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

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

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

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

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

The derivative with respect to the twist angle gradient in the core,  $\psi'_c$ , is

$$\begin{aligned}
\frac{\partial E}{\partial \psi'_c} = & \frac{2}{R^2} \left( \frac{1}{4} \frac{\partial u(0, R_c, \zeta)}{\partial \zeta} \Big|_{\zeta=\psi'_c} + \frac{1}{8} \left( \frac{\partial f_1(0, R_c, 0, \zeta)}{\partial \zeta} \Big|_{\zeta=\psi'_c} + \frac{\partial f_1(R_c, R_s, \xi, \psi'_s)}{\partial \xi} \Big|_{\xi=\psi_1} \frac{\partial \psi_1}{\partial \psi'_c} \right. \right. \\
& + \frac{\partial f_1(R_s, R, \xi, \psi'_R)}{\partial \xi} \Big|_{\xi=\psi_2} \frac{\partial \psi_2}{\partial \psi'_c} \Big) + \frac{1}{2} K_{33} \left( \frac{\partial f_2(0, R_c, 0, \zeta)}{\partial \zeta} \Big|_{\zeta=\psi'_c} + \frac{\partial f_2(R_c, R_s, \xi, \psi'_s)}{\partial \xi} \Big|_{\xi=\psi_1} \frac{\partial \psi_1}{\partial \psi'_c} \right. \\
& + \frac{\partial f_2(R_s, R, \xi, \psi'_R)}{\partial \xi} \Big|_{\xi=\psi_2} \frac{\partial \psi_2}{\partial \psi'_c} \Big) + \frac{1}{4} \left( \frac{\partial v(0, R_c, 0, \zeta)}{\partial \zeta} \Big|_{\zeta=\psi'_c} + \frac{\partial v(R_c, R_s, \xi, \psi'_s)}{\partial \xi} \Big|_{\xi=\psi_1} \frac{\partial \psi_1}{\partial \psi'_c} \right. \\
& + \frac{\partial v(R_s, R, \xi, \psi'_R)}{\partial \xi} \Big|_{\xi=\psi_2} \frac{\partial \psi_2}{\partial \psi'_c} \Big) + \frac{\Lambda \delta^2}{2R^2} \left( -8\pi^2 \eta^2 \left( \frac{\partial g_1(0, R_c, 0, \zeta)}{\partial \zeta} \Big|_{\zeta=\psi'_c} \right. \right. \\
& + \frac{\partial g_1(R_c, R_s, \xi, \psi'_s)}{\partial \xi} \Big|_{\xi=\psi_1} \frac{\partial \psi_1}{\partial \psi'_c} + \frac{\partial g_1(R_s, R, \xi, \psi'_R)}{\partial \xi} \Big|_{\xi=\psi_2} \frac{\partial \psi_2}{\partial \psi'_c} \Big) \\
& + \eta^4 \left( \frac{\partial g_2(0, R_c, 0, \zeta)}{\partial \zeta} \Big|_{\zeta=\psi'_c} + \frac{\partial g_2(R_c, R_s, \xi, \psi'_s)}{\partial \xi} \Big|_{\xi=\psi_1} \frac{\partial \psi_1}{\partial \psi'_c} \right. \\
& + \left. \left. \frac{\partial g_2(R_s, R, \xi, \psi'_R)}{\partial \xi} \Big|_{\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}. \tag{10}
\end{aligned}$$

The derivative with respect to the twist angle gradient in the shelf,  $\psi'_s$ , is

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

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

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

## 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

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

and

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

where I have defined the functions

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

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

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

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

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

$$\begin{aligned}
v(x_1, x_2, \xi, \zeta) = & -2 \sin(2\xi)(x_2 - x_1) + 2(\sin(2\xi)(x_2 - x_1) - \cos(2\xi)(x_2^2 - x_1^2))\zeta \\
& + \frac{2}{3}(3 \cos(2\xi)(x_2^2 - x_1^2) + 2 \sin(2\xi)(x_2^3 - x_1^3))\zeta^2 \\
& + \frac{2}{3}(-2 \sin(2\xi)(x_2^3 - x_1^3) + \cos(2\xi)(x_2^4 - x_1^4))\zeta^3,
\end{aligned} \tag{16a}$$

$$\begin{aligned}
f_1(x_1, x_2, \xi, \zeta) = & \sin^2(2\xi) \ln \frac{x_2}{x_1} + 4\zeta(x_2 - x_1) \cos(2\xi) \sin(2\xi) \\
& + 2\zeta^2(x_2^2 - x_1^2) (\cos^2(2\xi) - \sin^2(2\xi)) - \frac{32}{9}\zeta^3(x_2^3 - x_1^3) \sin(2\xi) \cos(2\xi)
\end{aligned} \tag{16b}$$

$$\begin{aligned}
f_2(x_1, x_2, \xi, \zeta) = & \sin^4 \xi \ln \frac{x_2}{x_1} + 4\zeta(x_2 - x_1) \sin^3 \xi \cos \xi + \zeta^2(x_2^2 - x_1^2) \sin^2 \xi (3 \cos^2 \xi - \sin^2 \xi) \\
& + \frac{4}{3}\zeta^3(x_2^3 - x_1^3) \sin \xi \cos \xi (\cos^2 \xi - 5 \sin^2 \xi)
\end{aligned} \tag{16c}$$

$$\begin{aligned}
g_1(x_1, x_2, \xi, \zeta) = & \frac{(x_2^2 - x_1^2) \cos^2 \xi}{2} - \frac{2(x_2^3 - x_1^3) \cos \xi \sin \xi}{3} \zeta - \frac{(x_2^4 - x_1^4) (\cos^2 \xi - \sin^2 \xi)}{4} \zeta^2 \\
& + \frac{4(x_2^5 - x_1^5) \cos \xi \sin \xi}{15} \zeta^3 \\
g_2(x_1, x_2, \xi, \zeta) = & \frac{(x_2^2 - x_1^2) \cos^4 \xi}{2} - \frac{4(x_2^3 - x_1^3) \cos^3 \xi \sin \xi}{3} \zeta - \frac{(x_2^4 - x_1^4) \cos^2 \xi (\cos^2 \xi - 3 \sin^2 \xi)}{2} \zeta^2 \\
& - \frac{(x_2^5 - x_1^5) \cos \xi (5 \cos^3 \xi - 12 \sin^3 \xi)}{15} \zeta^3
\end{aligned} \tag{16d}$$

The derivatives of these functions are listed below:

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

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

$$\frac{\partial u}{\partial \xi} = 0 \tag{17c}$$

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



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

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

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

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

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

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

$$\frac{\partial f_\alpha}{\partial \xi} = \begin{cases} \infty, & x_1 = 0, \xi \neq 0, \\ 4 \sin(2\xi) \cos(2\xi) \ln \frac{x_2}{x_1} + 8(x_2 - x_1)(\cos^2(2\xi) - \sin^2(2\xi))\zeta, & \zeta = 0, \alpha = 1, \\ 4 \sin^3 \xi \cos \xi \ln \frac{x_2}{x_1} + 4(x_2 - x_1) \sin^2 \xi (3 \cos^2 \xi - \sin^2 \xi)\zeta, & \zeta = 0, \alpha = 2, \\ \int_{x_1}^{x_2} du \frac{4 \sin^{2\alpha-1}\left(\frac{2}{\alpha}(\zeta u + \xi)\right) \cos\left(\frac{2}{\alpha}(\zeta u + \xi)\right)}{u}, & x_1 \neq 0 \end{cases} \quad (19c)$$

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

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

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

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

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