Dimensional vs dimensionless model

I will denote all unscaled variables with a hat over top of them,and all scaled variables without (i.e. $\hat{R}$ has units, R does not).

In its most general form, the unscaled model is

$$\begin{aligned}
\hat{E}(\hat{R},\hat{L};\hat{\psi}(\hat{r}),\hat{\rho}_\delta(\hat{z})) &= \frac{2\pi}{\pi\hat{R}^2\hat{L}}\int_0^{\hat{L}} d\hat{z}\int_0^{\hat{R}}\hat{r}d\hat{r}\left[\frac{1}{2}\hat{K}_{22}\left(\hat{\psi}'+\frac{\sin 2\hat{\psi}}{2\hat{r}}-\hat{q}\right)^2+\frac{1}{2}\hat{K}_{33}\frac{\sin^4\hat{\psi}}{\hat{r}^2}\right]\\
&\quad+\frac{\hat{\Lambda}}{2}\frac{2\pi}{\pi\hat{R}^2\hat{L}}\int_0^{\hat{L}} d\hat{z}\int_0^{\hat{R}}\hat{r}d\hat{r}\hat{\rho}_\delta\left(\frac{4\pi^2}{\hat{d}_0^2\cos^2\hat{\psi}}+\frac{\partial^2}{\partial\hat{z}^2}\right)^2\hat{\rho}_\delta\\
&\quad+\hat{\omega}\frac{\pi\hat{R}^2}{\pi\hat{R}^2\hat{L}}\int_0^{\hat{L}} d\hat{z}\hat{\rho}_\delta^2\left(\hat{\rho}_\delta^2-\hat{\chi}^2\right)-\frac{(\hat{K}_{22}+\hat{k}_{24})}{\hat{R}^2}\sin\hat{\psi}(\hat{R})+\frac{2\hat{\gamma}}{\hat{R}}\\
&=\frac{2}{\hat{R}^2}\int_0^{\hat{R}}\hat{r}d\hat{r}\left[\frac{1}{2}\hat{K}_{22}\left(\hat{\psi}'+\frac{\sin 2\hat{\psi}}{2\hat{r}}-\hat{q}\right)^2+\frac{1}{2}\hat{K}_{33}\frac{\sin^4\hat{\psi}}{\hat{r}^2}\right]\\
&\quad+\frac{\hat{\Lambda}\hat{\chi}^2}{\hat{R}^2\hat{L}}\int_0^{\hat{L}} d\hat{z}\int_0^{\hat{R}}\hat{r}d\hat{r}\left(\frac{\hat{\rho}_\delta}{\hat{\chi}}\right)\left(\frac{4\pi^2}{\hat{d}_0^2\cos^2\hat{\psi}}+\frac{\partial^2}{\partial\hat{z}^2}\right)^2\left(\frac{\hat{\rho}_\delta}{\hat{\chi}}\right)\\
&\quad+\frac{\hat{\omega}\hat{\chi}^4}{\hat{L}}\int_0^{\hat{L}} d\hat{z}\left(\frac{\hat{\rho}_\delta}{\hat{\chi}}\right)^2\left[\left(\frac{\hat{\rho}_\delta}{\hat{\chi}}\right)^2-1\right]-\frac{(\hat{K}_{22}+\hat{k}_{24})}{\hat{R}^2}\sin\hat{\psi}(\hat{R})+\frac{2\hat{\gamma}}{\hat{R}}
\end{aligned}\tag{1}$$

where I have ignored any surface contributions from the ends of the fibril, and $\hat{L}$ is some multiple of the periodic structure along the $\hat{z}$ axis. I have assumed that $\hat{\chi}^2>0$, as the density amplitude term (pre-factor $\hat{\omega}$) would be positive definite if not, meaning no density modulations would occur. The units of $\hat{\Lambda}$ are $\mathrm{pN}\cdot\mathrm{\mu m}^8$, the units of $\hat{\omega}$ are $\mathrm{pN}\cdot\mathrm{\mu m}^{10}$, and the units of $\hat{\chi}^2$ are $\mathrm{\mu m}^{-6}$. If I divide both side of eqn 1 by $\hat{K}_{22}\hat{q}^2$, I can make the system dimensionless and reduce to the form

$$\begin{aligned}
E(R,L;\psi(r),\rho_\delta(z)) &= \frac{2}{R^2}\int_0^R rdr\left[\frac{1}{2}\left(\psi'+\frac{\sin 2\psi}{2r}-1\right)^2+\frac{1}{2}K_{33}\frac{\sin^4\psi}{r^2}\right]\\
&\quad+\frac{\Lambda}{R^2L}\int_0^L dz\int_0^R rdr\rho_\delta\left(\frac{4\pi^2}{d_0^2\cos^2\psi}+\frac{\partial^2}{\partial z^2}\right)^2\rho_\delta\\
&\quad+\frac{\omega}{L}\int_0^L dz\rho_\delta^2\left(\rho_\delta^2-1\right)-\frac{(1+k_{24})}{R^2}\sin\psi(R)+\frac{2\gamma}{R}.
\end{aligned}\tag{2}$$

In general, the liquid crystal elastic constants $\hat{K}_{ii}$, $\hat{q}=\hat{k}_2/\hat{K}_{22}$, and $\hat{k}_{24}$ depend on the density of the system [?]. Therefore, any density modulations $\hat{\rho}_\delta$ from some reference density $\hat{\rho}_0$ must be small. For systems with periodicity in only a single axis, it is reasonable to take a single mode approximation to the density modulations of the form

$$\hat{\rho}_\delta = \delta \cos(\hat{\eta}\hat{z}), \quad \hat{\delta} \ll \hat{\rho}_0. \tag{3}$$

For collagen fibrils, $\hat{\delta} \sim 0.1\hat{\rho}_0$. Inserting the eqn 3 in dimensionless form into eqn 2 and noting that the period of this structure will be $L = 2\pi/\eta$, I get

$$\begin{aligned}
E(R,\eta,\delta;\psi(r)) = {} & \frac{2}{R^2}\int_0^R rdr\left[\frac{1}{2}\left(\psi' + \frac{\sin 2\psi}{2r} - 1\right)^2 + \frac{1}{2}K_{33}\frac{\sin^4\psi}{r^2}\right] \\
& + \frac{\Lambda}{R^2\frac{2\pi}{\eta}}\int_0^{\frac{2\pi}{\eta}} dz \int_0^R rdr\delta^2\cos^2(\eta z)\left(\frac{4\pi^2}{d_0^2\cos^2\psi} - \eta^2\right)^2 \\
& + \frac{\omega}{\frac{2\pi}{\eta}}\int_0^{\frac{2\pi}{\eta}} dz\delta^2\cos^2(\eta z)\left(\delta^2\cos^2(\eta z) - 1\right) - \frac{(1+k_{24})}{R^2}\sin\psi(R) + \frac{2\gamma}{R} \\
= {} & \frac{2}{R^2}\int_0^R rdr\left[\frac{1}{2}\left(\psi' + \frac{\sin 2\psi}{2r} - 1\right)^2 + \frac{1}{2}K_{33}\frac{\sin^4\psi}{r^2}\right] \\
& + \frac{\Lambda\delta^2}{2R^2}\int_0^R rdr\left(\frac{4\pi^2}{d_0^2\cos^2\psi} - \eta^2\right)^2 \\
& + \frac{\omega\delta^2}{2}\left(\frac{3}{4}\delta^2 - 1\right) - \frac{(1+k_{24})}{R^2}\sin\psi(R) + \frac{2\gamma}{R}.
\end{aligned} \tag{4}$$

The following is a list of the redefined, dimensionless quantites:

$$E = \frac{\hat{E}}{\hat{K}_{22}\hat{q}^2}, \tag{5}$$

$$R = \hat{R}\hat{q}, \tag{6}$$

$$r = \hat{r}\hat{q}, \tag{7}$$

$$\psi(r) = \hat{\psi}(\hat{r}), \tag{8}$$

$$K_{33} = \frac{\hat{K}_{33}}{\hat{K}_{22}}, \tag{9}$$

$$L = \hat{L}\hat{q}, \tag{10}$$

$$\Lambda = \frac{\hat{\Lambda}\hat{\chi}^2\hat{q}^2}{\hat{K}_{22}}, \tag{11}$$

$$\rho_\delta = \frac{\hat{\rho}_\delta}{\hat{\chi}}, \tag{12}$$

$$\delta = \frac{\hat{\delta}}{\hat{\chi}}, \tag{13}$$

$$\eta = \frac{\hat{\eta}}{\hat{q}}, \tag{14}$$

$$d_0 = \hat{d}_0\hat{q}, \tag{15}$$

$$\omega = \frac{\hat{\omega}\hat{\chi}^4}{\hat{K}_{22}\hat{q}^2}, \tag{16}$$

$$\gamma = \frac{\hat{\gamma}}{\hat{K}_{22}\hat{q}}. \tag{17}$$

Approximating coefficients

Approximating $\hat{\chi}$

To begin with, I will determine the value of $\hat{\chi}$ with two assumptions:

1. The standard d-band model holds, where gap regions have 4/5 the density of filled regions and so $\hat{\delta} = 0.1\hat{\rho}_0$.

2. As the d-banding strength increases, our model is consistent with the standard d-band model, i.e. the dimensional version of $\delta(\omega \to \infty) = \sqrt{2/3}$ is always $0.1\hat{\rho}_0$.

Taking a hexagonal packing of collagen molecules within the fibril with intermolecular spacings of 1.53 nm (cross section) and $\sim$ 35 nm (axial), the primitive unit cell of a fibril has lattice vectors $\boldsymbol{a} = 1.53\,\mathrm{nm}\,\hat{\boldsymbol{x}}$, $\boldsymbol{b} = 1.53\,\mathrm{nm}(0.5\,\hat{\boldsymbol{x}} + 0.866\,\hat{\boldsymbol{y}})$, and $\boldsymbol{c} \sim 330\,\mathrm{nm}\,\hat{\boldsymbol{z}}$, giving a molecular number density $\hat{\rho}_0 \sim 1.67 \times 10^6\,\mu\mathrm{m}^{-3}$, and so $\hat{\delta} \sim 1.67 \times 10^5\,\mu\mathrm{m}^{-3}$ using assumption 1. above. By assumption 2, this implies

$$\hat{\chi} = \sqrt{\frac{3}{2}}\hat{\delta} \sim 2 \times 10^5\,\mu\mathrm{m}^{-3}. \tag{18}$$

Approximating ω

In approximating ω, we can utilize experimental work [?] which measures the Gibbs free energy of type I collagen molecules polymerizing into fibrils as $13\,\mathrm{kcal\,mol}^{-1} \sim 2 \times 10^5\,\mathrm{pN}\,\mu\mathrm{m}^{-2}$. If we assume that most of this energy comes from formation of the d-band, then we can take this value as an estimate for $\hat{\omega}\hat{\chi}^4$. From there, the approximation relies on the estimates of $\hat{K}_{22}$ and $\hat{q}$, which have been estimated in our previous work [?]. If we choose $\hat{K}_{22} = 6\,\mathrm{pN}$ and $\hat{q} = 10\,\mu\mathrm{m}^{-1}$, our estimate of ω is

$$\omega = \frac{2 \times 10^5\,\mathrm{pN}\,\mu\mathrm{m}^{-2}}{6\,\mathrm{pN}\,(10\,\mu\mathrm{m}^{-1})^2} \sim 300. \tag{19}$$

Approximating Λ

In order to approximate Λ, we can look at how our model will respond to a small strain on the periodic spacing (i.e. the d-band), a method that has been applied in determining the bulk modulus of contribution in phase field crystal models [?]. If I define $\eta = 2\pi/d$, with d being the perturbed d-band spacing, then expanding our free energy in terms of the applied strain $u = (d - d_0)/d_0$ will provide a dimensionless bulk modulus, $K = 1/2\partial^2 E/\partial u^2$, from the definition

$$E(u) = E(0) + \frac{1}{2}\left.\frac{\partial^2 E}{\partial u^2}\right|_{u=0} u^2 + \mathcal{O}(u^3). \tag{20}$$

References