

Debugging time evolution

Lucas Myers

November 16, 2022

1 Checking periodically perturbed free energy

To check that the configuration force matches with the energy, we check the energy for a uniform configuration first, and then for a small perturbation. The latter check gives an estimate for the configuration force by the functional Taylor series expansion:

$$F(Q + \delta Q) = F(Q) + \left. \frac{\delta F}{\delta Q} \right|_Q : \delta Q + \mathcal{O}(|\delta Q|^2) \quad (1)$$

with

$$\frac{\delta F}{\delta Q} = \frac{\partial F}{\partial Q} - \nabla \cdot \frac{\partial F}{\partial (\nabla Q)} \quad (2)$$

Here Q is given by:

$$Q = S_0 \begin{bmatrix} \frac{2}{3} & 0 & 0 \\ 0 & -\frac{1}{3} & 0 \\ 0 & 0 & -\frac{1}{3} \end{bmatrix} \quad (3)$$

with

$$\delta Q = S_0 \begin{bmatrix} 0 & \epsilon \sin kx & 0 \\ \epsilon \sin kx & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad (4)$$

This corresponds (to first order) to a perturbation of the director so that the total configuration $(Q + \delta Q)$ is a uniform- S configuration with director $\mathbf{n} = (1, \epsilon \sin kx, 0)$.

Here, the nondimensional free energy is given by:

$$F = \int_{\Omega} \left(-\frac{1}{2} \alpha Q : Q + (\log 4\pi - \log Z + \Lambda : (Q + \frac{1}{3} I)) + \frac{1}{2} |\nabla Q|^2 \right) dV \quad (5)$$