Debugging time evolution

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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:

$$F(Q+\delta Q) = F(Q) + \int_\Omega \left(\frac{\delta F}{\delta Q}\Big|_Q : \delta Q \right) dV + \mathcal{O}\left(|\delta Q|^2\right) \tag{1}$$

with

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

Here Q is given by:

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

with

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

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:

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

Then we can calculate $F(Q)$ partially analytically and partially numerically. Of course the elastic part is zero, and we calculate:

$$-\tfrac{1}{2}\alpha Q : Q = -S_0^2 \frac{\alpha}{3} = -1.2153600266666669 \tag{6}$$

with $S_0 = 0.6751$ and $\alpha = 8.0$. Further, we can calculate numerically (see `calc_lambda` program with `generate_periodic_Q_tensors.py`) Λ and Z for $S_0 = 0.6751$:

$$\begin{aligned} Z &= 3.87017170996747 \\ \Lambda &= \begin{bmatrix} 3.6005952163635766 & 0 & 0 \\ 0 & -1.8002976081817883 & 0 \\ 0 & 0 & -1.8002976081817883 \end{bmatrix} \end{aligned} \tag{7}$$

Then we may calculate F by multiplying this energy density by the size of the domain. The uniform configuration check is then just to compare that number with the energy output from the simulation for a uniform configuration with the same S_0 and α values and domain size. Calculating the energy density from the mean-field interaction gives:

$$f_{\text{entropy}} = 3.60848720197831 \tag{8}$$

Running the simulation and calculating the free energy over the domain gives:

$$F_{\text{mean field}} = -11.99497833 \tag{9}$$

and calculating out the energy density from the entropy term gives:

$$F_{\text{entropy}} = 35.61419603 \tag{10}$$

Comparing these values to the energy density multiplied by $(3.1415926 \times 3.1415926)$ (the domain size) we get similar results.

The configuration force, which is exactly the functional derivative of the free energy, is given by:

$$\frac{\delta F}{\delta Q} = -\alpha Q + \Lambda - \nabla^2 Q \tag{11}$$

Calculating the elastic term explicitly yields:

$$-\nabla^2 Q = S_0 \epsilon k^2 \sin kx \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{12}$$

Further, we may explicitly calculate the inner product of δQ with each of those terms. Because Q and Λ are diagonal, it happens that $Q : \delta Q = \Lambda : \delta Q = 0$. Then we just calculate:

$$-\nabla^2 Q : \delta Q = 2 S_0^2 \epsilon^2 k^2 \sin^2 kx \tag{13}$$