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

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

Since this holds for an arbitrary functional F, and also for an arbitrary (small) perturbation δQ, it's probably true that:

$$f(Q+\delta Q) = f(Q) + \left(\frac{\partial f}{\partial Q} - \nabla \cdot \frac{\partial f}{\partial (\nabla Q)} \right) : \delta Q + \mathcal{O}\left(|\delta Q|^2\right) \tag{3}$$

for each component of the free energy f. For the example we test, we take Q to be:

$$Q = S_0 \begin{bmatrix} \frac{2}{3} & 0 & 0 \\ 0 & -\frac{1}{3} & 0 \\ 0 & 0 & -\frac{1}{3} \end{bmatrix} \tag{4}$$

with

$$\delta Q = S_0 \begin{bmatrix} 0 & \epsilon \sin kx & 0 \\ \epsilon \sin kx & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{5}$$

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:

$$F = \int_\Omega \left(-\tfrac{1}{2}\alpha Q : Q + \left(\log 4\pi - \log Z + \Lambda : \left(Q + \tfrac{1}{3} I \right) \right) + \tfrac{1}{2} |\nabla Q|^2 \right) dV \tag{6}$$

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

$$-\tfrac{1}{2}\alpha Q : Q = -S_0^2 \frac{\alpha}{3} = -1.2153600266666669 \tag{7}$$

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 $S_0 = 0.6751$:

$$\begin{aligned} Z &= 3.87017170996747 \\ \Lambda &= \begin{bmatrix} 3.6005952163635766 & 0 & 0 \\ 0 & -1.8002976081817883 & 0 \\ 0 & 0 & -1.8002976081817883 \end{bmatrix} \end{aligned} \tag{8}$$

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:

$$f_{\text{entropy}} = 3.60848720197831 \tag{9}$$

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

$$F_{\text{mean field}} = -11.99497833 \tag{10}$$

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

$$F_{\text{entropy}} = 35.61419603 \tag{11}$$

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

We may also consider a configuration with a different S_0-value, just to be sure. Running a similar calculation with $S_0 = 0.5$, we get the following values for Λ and Z:

$$\begin{aligned} Z &= 1.8088523960817302 \\ \Lambda &= \begin{bmatrix} 2.323990879382531 & 0 & 0 \\ 0 & -1.1619954396912653 & 0 \\ 0 & 0 & 0 \end{bmatrix} \end{aligned} \tag{12}$$

Then the entropy and mean field part of the free energy density is given by:

$$\begin{aligned} f_{\text{entropy}} &= 3.100327077782174 \\ f_{\text{mean field}} &= -\frac{2}{3} \end{aligned} \tag{13}$$

Both of these corresopnd with the energy densities written to the vtu file.

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

$$\frac{\delta F}{\delta Q} = -\alpha Q + \Lambda - \nabla^2 Q \tag{14}$$

We need to evaluate this with the unperturbed Q-tensor – since this is just a uniform configuration, the elastic term will be zero. However, if we explicitly calculate it we find that:

$$\left.\frac{\delta F}{\delta Q}\right|_Q : \delta Q = 0 \tag{15}$$

Hence, we actually can't get any information out of this particular perturbation.

2 S-value perturbation

To actually test this, we need to take:

$$\delta Q = \frac{\epsilon}{S_0} \sin kx Q \tag{16}$$

Taking $k = 1$ and $\epsilon = 0.1$, we may explicitly calculate (using values previously stated):

$$\left.\frac{\delta F_{\text{mean field}}}{\delta Q}\right|_Q : \delta Q = -\tfrac{2}{3} S_0 \alpha \epsilon \sin kx = (-0.36005333333333334) \sin kx \tag{17}$$

and

$$\left.\frac{\delta F_{\text{entropy}}}{\delta Q}\right|_Q : \delta Q = \epsilon \sin kx \left(\tfrac{2}{3}\Lambda_1 - \tfrac{1}{3}\Lambda_4 + \tfrac{1}{3}(\Lambda_1 + \Lambda_4)\right) = (0.3600595216363576) \sin kx \tag{18}$$

Since we have chosen the equilibrium S_0-value for the given temperature (α value), it makes sense that these are equal and opposite. However, of course we have perturbed an equilibrium perturbation, so the perturbation should decay, and $F(Q + \delta Q) - F(Q)$ for the total configuration should *not* be zero. When we actually calculate $F(Q + \delta Q) - F(Q)$ numerically, we find that the values at the peaks of the perturbation are:

$$f_{\text{mean field}}(Q + \delta Q) - f_{\text{mean field}}(Q) = -0.386595 \tag{19}$$

$$f_{\text{entropy}}(Q + \delta Q) - f_{\text{entropy}}(Q) = 0.420529 \tag{20}$$

These are the correct signs, and the correct order of magnitude as far as the Taylor expansion above is concerned. However, these values are not the same as predicted by the Taylor expansion, which makes sense because the configuration at the peak of the perturbation takes on a different S_0-value than the equilibrium value dictated by the temperature.

3 Decay of periodic perturbation as an exponential

For a perturbation of the form:

$$\delta Q = S \begin{bmatrix} 0 & \epsilon \cos kx & 0 \\ \epsilon \cos kx & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{21}$$

We may compute:

$$\begin{aligned} \frac{\partial (Q_0 + \delta Q)}{\partial Q} &= \alpha(Q_0 + \delta Q) - \Lambda(Q_0 + \delta Q) + \nabla^2 (Q_0 + \delta Q) \\ &\approx \alpha Q_0 - \Lambda(Q_0) + \nabla^2 Q_0 + \alpha \delta Q - \left.\frac{\partial \Lambda}{\partial Q}\right|_{Q_0} : \delta Q + \nabla^2 \delta Q \\ &= \alpha \delta Q - \left.\frac{\partial \Lambda}{\partial Q}\right|_{Q_0} : \delta Q + \nabla^2 \delta Q \end{aligned} \tag{22}$$

by definition of Q_0 as the equilibrium value. If we consider the above equation just for the degrees of freedom of Q, then there is only one nonzero entry so that:

$$\frac{\partial \epsilon(t)}{\partial t} = \alpha \epsilon(t) - \frac{\partial \Lambda_2}{\partial Q_2} \epsilon(t) - k^2 \epsilon(t) = \left(\alpha - \frac{\partial \Lambda_2}{\partial Q_2} - k^2\right) \epsilon(t) \tag{23}$$

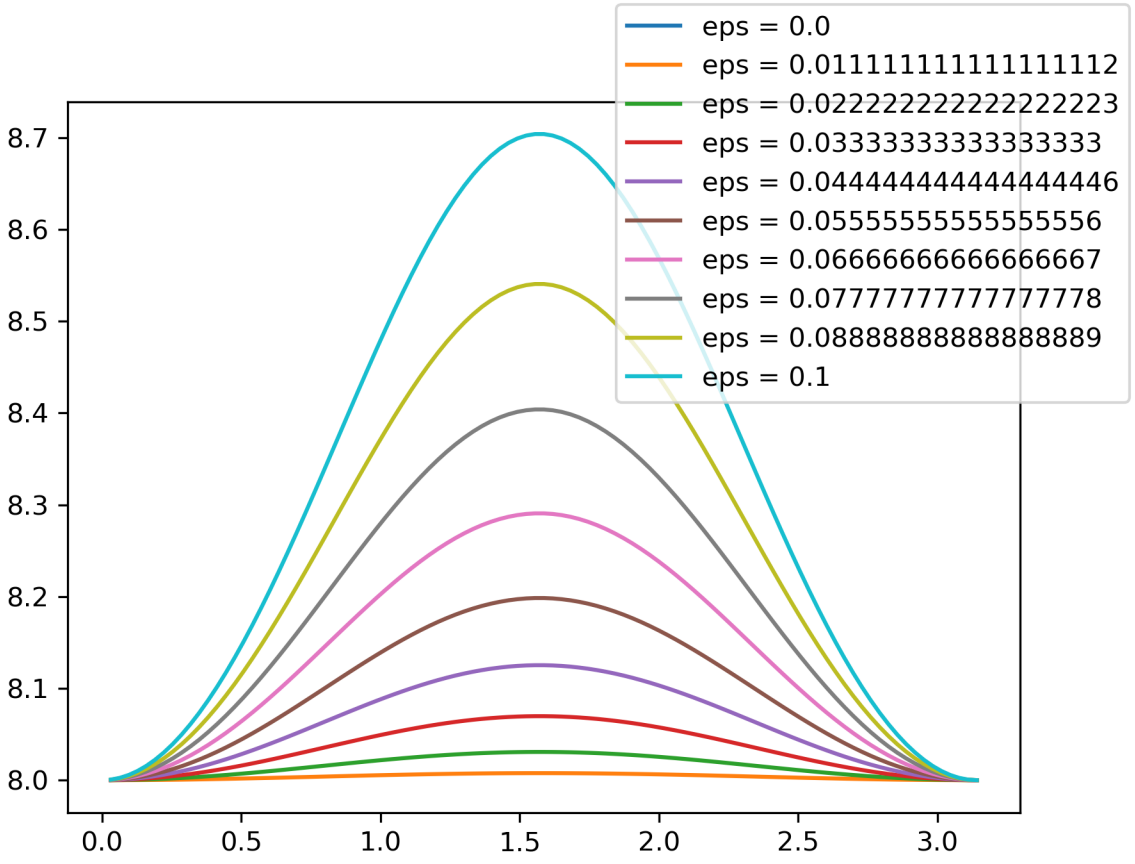
so that the time-constant of decay is given by:

$$\tau_{\text{decay}} = -\left(\alpha - \frac{\partial \Lambda_2}{\partial Q_2} - k^2\right) \tag{24}$$

First want to verify that:

$$\Lambda_2(Q_0 + \delta Q) - \Lambda_2(Q_0) \approx \frac{\partial \Lambda_2}{\partial Q_2}\delta Q_2 \tag{25}$$

Note that $\Lambda_2(Q_0) = 0$ in this case. Since the configuration is periodic, we calculate $\Lambda_2(Q_0+\delta Q)/\delta Q_2$ across the domain for various ϵ values. The resulting plot is given by: Clearly there is some variation



in $\Lambda_2(Q_0+\delta Q)/\delta Q_2$ because Λ is a nonlinear function of Q, but the variation is an order of magnitude less than the slope. Additionally, the slope is around 8 for all values, which coincides with what we calculate for $\partial\Lambda_2/\partial Q_2$:

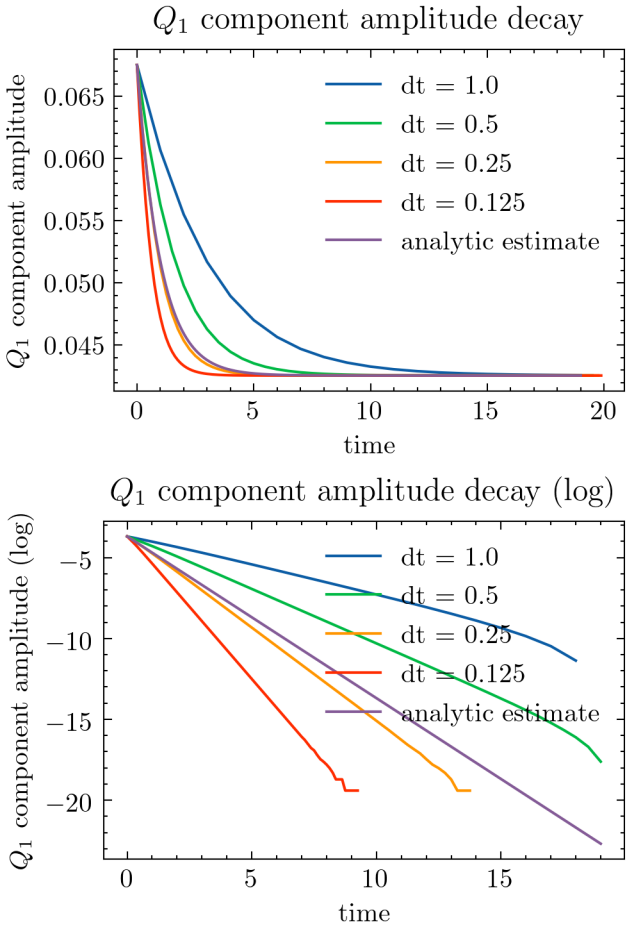
$$\left.\frac{\partial \Lambda_2}{\partial Q_2}\right|_{Q_0} = 8.00013749747499 \tag{26}$$

Given these values and taking $\alpha = 8.0$ we get:

$$\tau_{\text{decay}} \approx k^2 \tag{27}$$

If we run a simulation with domain $[0, \pi] \times [0, \pi]$ and then look at the perturbed Q-component for various Δt-values (that is, different time-discretizations) we get:

One problem with this is that the perturbation proposed does not actually decay to zero – the director actually remains slightly rotated because of the perturbation. Instead, we need to run



the simulation over a whole period so it decays to zero. The plots for this are given by: This is better because, as expected, the analytic result decays much faster than the numerical result. However, what we see when we look at the actual profile of the $(1,2)$ component of Q is that the Neumann boundary conditions severely affect the time evolution: To fix this effect on the problem, we just shift our domain so that the periodic configuration already has zero derivative at the boundary.

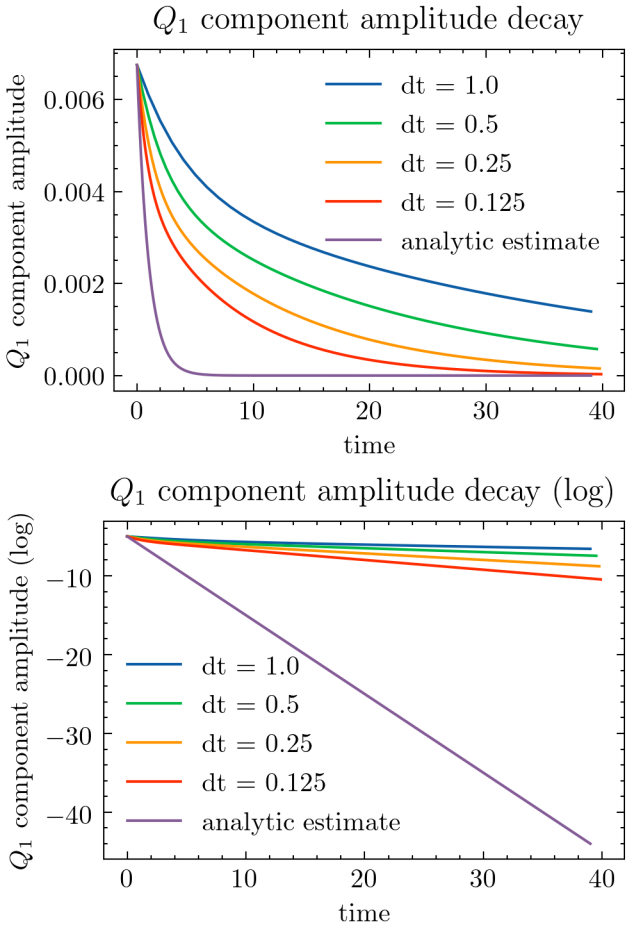
4 Landau-de Gennes time evolution for periodically-perturbed S-value

To check the general scheme, we employ a Landau-de Gennes field theory with elastic isotropy. With this, the time evolution is governed by:

$$\frac{\partial Q}{\partial t} = -\left(AQ + B(Q \cdot Q) + C(Q : Q)Q\right) + \nabla^2 Q \tag{28}$$

First we consider a configuration with director pointing completely in the x-direction so that $\mathbf{n} = (1,0,0)$ and an S-value dependent on time and the x-coordinate. By symmetry, S will not depend on y or z supposing that the initial condition is only a function of x. Then we get:

$$Q(x,t) = S(x,t)\left(\mathbf{n} \otimes \mathbf{n} - \tfrac{1}{3}I\right) = S(x,t)\begin{bmatrix} \frac{2}{3} & 0 & 0 \\ 0 & -\frac{1}{3} & 0 \\ 0 & 0 & -\frac{1}{3} \end{bmatrix} \tag{29}$$



Plugging into the Landau-de Gennes time evolution equation gives:

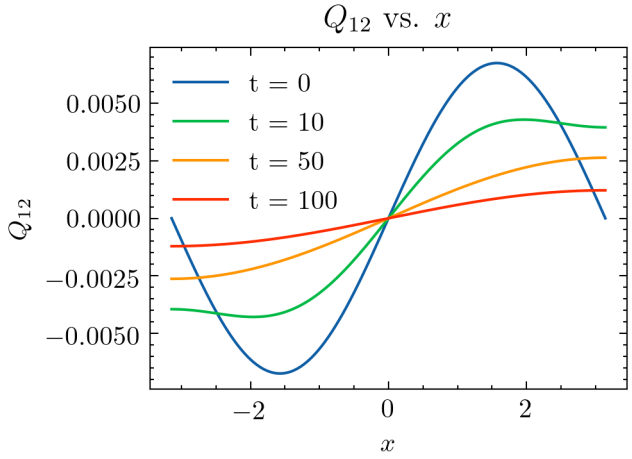
$$3\frac{\partial S(x,t)}{\partial t} = -3AS(x,t) + BS^2(x,t) - CS^3(x,t) + 3\frac{\partial^2 S(x,t)}{\partial x^2} \tag{30}$$

Supposing a periodic initial condition:

$$S(x,0) = A_0 \sin kx \tag{31}$$

we take as an ansatz that:

$$S(x,t) = \sum_n A_n(t) \sin nkx \tag{32}$$



So that the time evolution equation becomes:

$$
\begin{aligned}
3\sum_n \sin(nkx)\frac{dA_n(t)}{dt} = & -3A\sum_n A_n(t)\sin(nkx) \\
& + B\sum_{m,n} A_m(t)A_n(t)\sin(nkx)\sin(mkx) \\
& - C\sum_{l,m,n} A_l(t)A_m(t)A_n(t)\sin(lkx)\sin(mkx)\sin(nkx) \\
& - 3\sum_n A_n(t)n^2k^2\sin(nkx) \\
= & -3A\sum_n A_n(t)\sin(nkx) \\
& + B\sum_{m,n} \tfrac{1}{2}A_m(t)A_n(t)\Big[\cos((n-m)kx) - \cos((n+m)kx)\Big] \\
& - C\sum_{l,m,n} \tfrac{1}{4}A_l(t)A_m(t)A_n(t)\Big[\sin((l+n-m)kx) + \sin((l-n+m)kx) \\
& \qquad - \sin((l+n+m)kx) - \sin((l-n-m)kx)\Big] \\
& - 3\sum_n A_n(t)n^2k^2\sin(nkx)
\end{aligned}
\tag{33}
$$