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:

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

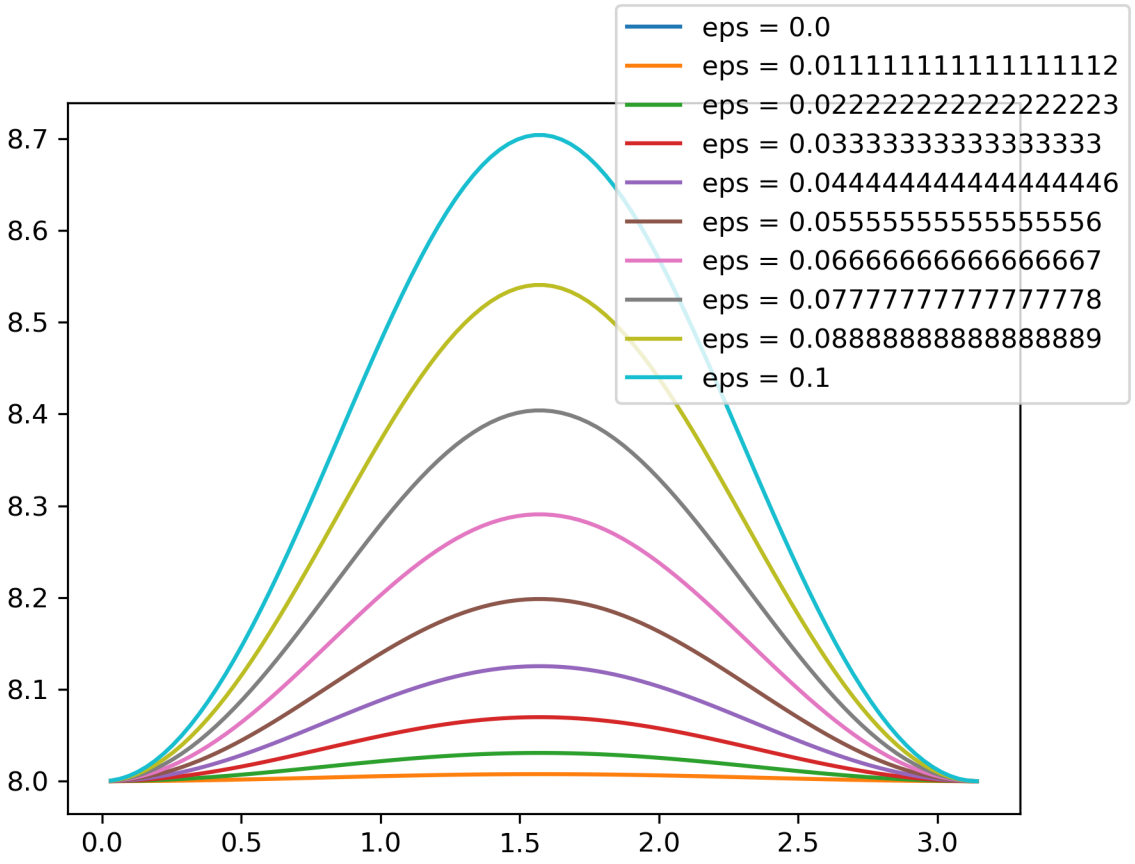
so that the time-constant of decay is given by:

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

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



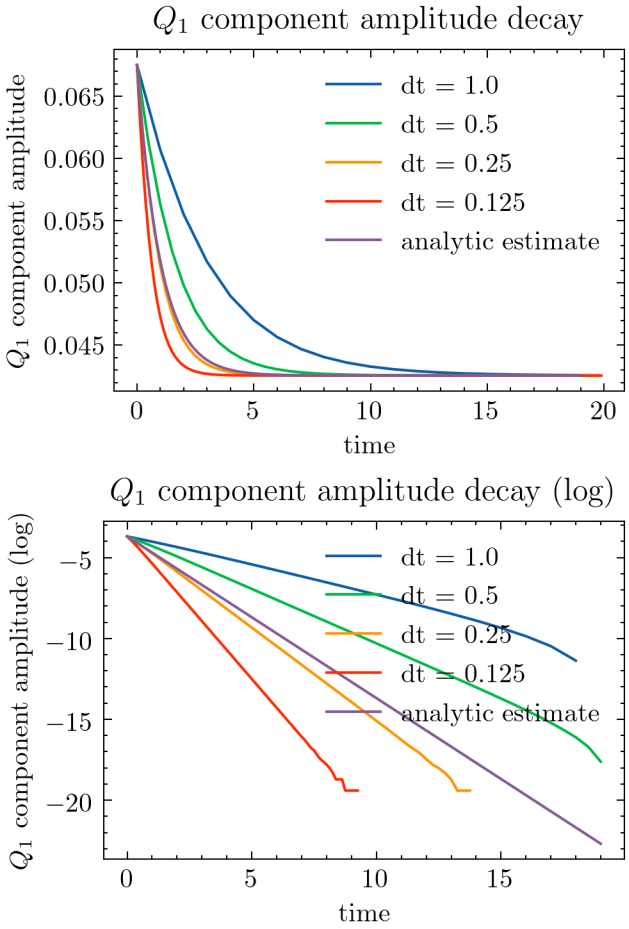
in $\Lambda_2(Q_0+\delta Q)/\delta Q_2$ because Λ is a nonlinear function of Q, but the variation is an order of magnitude less than the slope. Additionally, the slope is around 8 for all values, which coincides with what we calculate for $\partial \Lambda_2/\partial Q_2$:

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

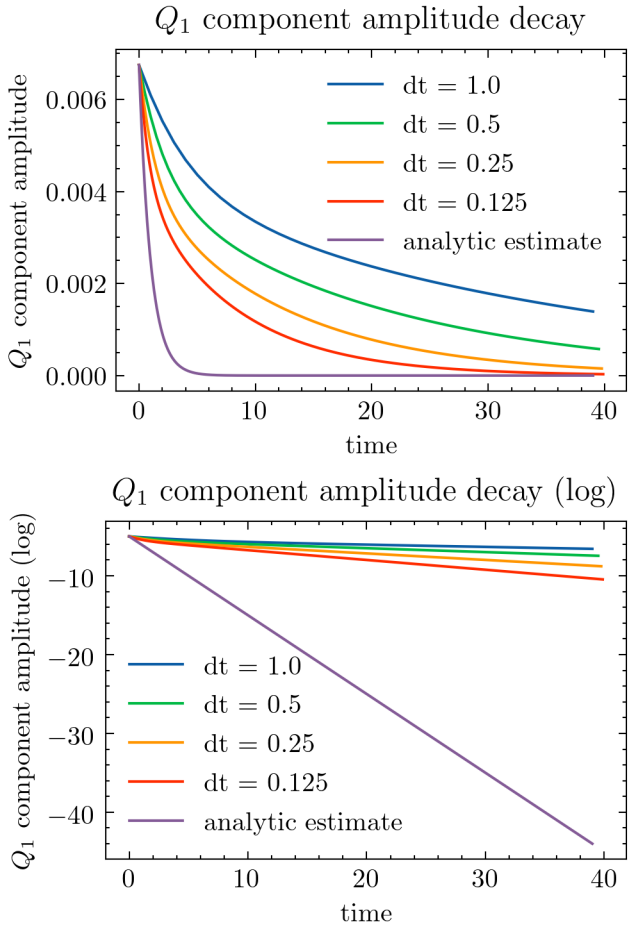
Given these values and taking $\alpha = 8.0$ we get:

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

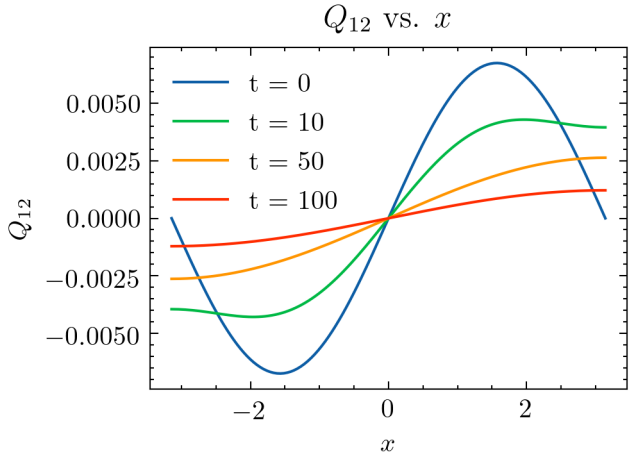
If we run a simulation with domain $[0, \pi] \times [0, \pi]$ and then look at the perturbed Q-component for various Δt-values (that is, different time-discretizations) we get:



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 Checking time evolution equation

The discrete time evolution equation for an isotropic system reads:

$$\frac{Q - Q_0}{\delta t} = \alpha Q_0 - \Lambda(Q) + \nabla^2 Q \tag{28}$$

The right side should be (for a small enough time step) approximately a sinusoid with amplitude $\left(\alpha - \partial\Lambda_2/\partial Q_2 - k^2\right)$ for the Q_2 (perturbed) component. The left side should be that as well, once the implicit equation for Q is solved. Hence, we may output a finite element projection of each of these terms to see whether anything goes wrong during the time evolution. Clearly delineating each of the right-hand side terms:

$$\begin{aligned} f_{\text{lhs}} &= \frac{Q - Q_0}{\delta t} \\ f_{\text{mean field}} &= \alpha Q_0 \\ f_{\text{entropy}} &= -\Lambda(Q) \\ f_{\text{elastic}} &= \nabla^2 Q \end{aligned} \tag{29}$$

Then to calculate the finite element projections of each of these quantities, we assume that they may be written as a sum of basis elements:

$$f = \sum_j \Phi_j f_j \tag{30}$$

and take the inner product with each of the basis functions. Solving the corresponding linear equation gives each of the components of each f.

4.1 Explicitly solving the convex splitting discrete time evolution equation

With the perturbation analysis, we may actually rewrite the discrete-time equation of motion for Q_2 as:

$$\frac{\epsilon \sin(kx) - \epsilon_0 \sin(kx)}{\delta t} = \alpha \epsilon_0 \sin(kx) - \left.\frac{\partial \Lambda_2}{\partial Q_2}\right|_{Q_{\text{eq}}} \epsilon \sin(kx) - k^2 \epsilon \sin(kx) \tag{31}$$

where ϵ is the perturbation amplitude at the current time step and ϵ_0 is the perturbation amplitude at the previous time step. This gives an algebraic equation for ϵ whose solution reads:

$$\begin{aligned} \epsilon &= \frac{(1 + \alpha \delta t)}{1 + \delta t\, \partial\Lambda_2/\partial Q_2 + \delta t\, k^2} \epsilon_0 \\ &= \epsilon_0 + \frac{\alpha - \partial\Lambda_2/\partial Q_2 - k^2}{1 + \delta t\, \partial\Lambda_2/\partial Q_2 + \delta t\, k^2} \delta t\, \epsilon_0 \end{aligned} \tag{32}$$

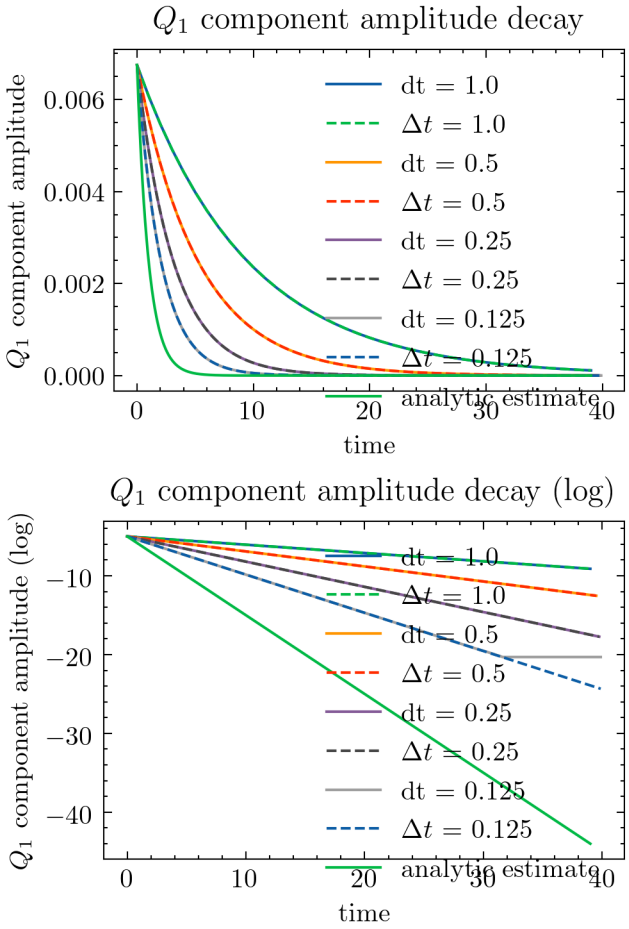
Let us denote a convex-splitting time-discretized time constant as:

$$\tau_{\text{CS}} = -\left(\frac{\alpha - \partial\Lambda_2/\partial Q_2 - k^2}{1 + \delta t\, \partial\Lambda_2/\partial Q_2 + \delta t\, k^2}\right) \tag{33}$$

Then for any n we may calculate the discrete ϵ_n value recursively as:

$$\begin{aligned} \epsilon_n &= (1 - \tau_{\text{CS}}\, \delta t)\, \epsilon_{n-1} \\ &= (1 - \tau_{\text{CS}}\, \delta t)^n\, \epsilon_0 \end{aligned} \tag{34}$$

where here ϵ_0 is the initial perturbation amplitude. We may plot this estimate against each of our numerical simulation runs to see whether the simulation results are in line with the time-discretized estimates.



The time at which ϵ_n is evaluated is $t = n\,\delta t$. Making the subsitution for δt gives:

$$\epsilon_{\mathrm{CS}}(t) = \left(1 - \left(\frac{\alpha - \partial\Lambda_2/\partial Q_2 - k^2}{n + t\,\partial\Lambda_2/\partial Q_2 + t\,k^2}\right) t\right)^n \epsilon_0 \tag{35}$$

Taking the limit as $n \to \infty$ gives:

$$\begin{aligned}
\lim_{n\to\infty} \epsilon_{\mathrm{CS}}(t) &= \lim_{n\to\infty} \left(1 + \left(\frac{-\tau_{\mathrm{decay}}}{n + t\,\partial\Lambda_2/\partial Q_2 + t\,k^2}\right) t\right)^n \epsilon_0 \\
&= \lim_{n\to\infty} \left(1 + \left(\frac{-\tau_{\mathrm{decay}}}{n}\right) t\right)^n \epsilon_0 \\
&= \epsilon_0 e^{-\tau_{\mathrm{decay}} t}
\end{aligned} \tag{36}$$

Hence, the perturbation amplitudes that we calculate using the convex splitting algorithm converge pointwise in t to the analytic solution as $\delta t \to 0$.

4.2 Explicitly solving the forward Euler discrete time evolution equation

For the forward Euler (explicit) scheme, we get the following discrete equation for ϵ:

$$\frac{\epsilon - \epsilon_0}{\delta t} = \alpha\epsilon_0 - \frac{\partial\Lambda_2}{\partial Q_2}\epsilon_0 - k^2\epsilon_0 \tag{37}$$

which gives:

$$\begin{aligned}\epsilon &= \left(1 + \delta t\,\alpha - \delta t \frac{\partial \Lambda_2}{\partial Q_2} - \delta t k^2\right)\epsilon_0 \\ &= (1 - \tau_{\text{decay}}\delta t)\,\epsilon_0\end{aligned} \tag{38}$$

Then substituting $\delta t = t/n$ and using the recursion relation to calculate $\epsilon_{\text{FE}}(t)$ we get:

$$\epsilon_{\text{FE}}(t) = \left(1 + \frac{-\tau_{\text{decay}}}{n} t\right)^n \tag{39}$$

The limit is then obviously:

$$\lim_{n\to\infty} \epsilon_{\text{FE}}(t) = e^{-\tau_{\text{decay}} t} \tag{40}$$

5 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:

$$\frac{\partial Q}{\partial t} = -\left(AQ + B(Q\cdot Q) + C(Q:Q)Q\right) + \nabla^2 Q \tag{41}$$

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:

$$Q(x,t) = S(x,t)\left(\mathbf{n}\otimes\mathbf{n} - \tfrac{1}{3}I\right) = S(x,t)\begin{bmatrix}\frac{2}{3} & 0 & 0\\ 0 & -\frac{1}{3} & 0\\ 0 & 0 & -\frac{1}{3}\end{bmatrix} \tag{42}$$

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

$$3\frac{\partial S(x,t)}{\partial t} = -3AS(x,t) + BS^2(x,t) - CS^3(x,t) + 3\frac{\partial^2 S(x,t)}{\partial x^2} \tag{43}$$

Supposing a periodic initial condition:

$$S(x,0) = A_0 \sin kx \tag{44}$$

we take as an ansatz that:

$$S(x,t) = \sum_n A_n(t)\sin nkx \tag{45}$$

So that the time evolution equation becomes:

$$
\begin{aligned}
3\sum_n \sin(nkx)\frac{dA_n(t)}{dt} = & -3A\sum_n A_n(t)\sin(nkx) \\
& + B\sum_{m,n} A_m(t)A_n(t)\sin(nkx)\sin(mkx) \\
& - C\sum_{l,m,n} A_l(t)A_m(t)A_n(t)\sin(lkx)\sin(mkx)\sin(nkx) \\
& - 3\sum_n A_n(t)n^2k^2\sin(nkx) \\
= & -3A\sum_n A_n(t)\sin(nkx) \\
& + B\sum_{m,n} \tfrac{1}{2}A_m(t)A_n(t)\Big[\cos((n-m)kx) - \cos((n+m)kx)\Big] \\
& - C\sum_{l,m,n} \tfrac{1}{4}A_l(t)A_m(t)A_n(t)\Big[\sin((l+n-m)kx) + \sin((l-n+m)kx) \\
& \qquad - \sin((l+n+m)kx) - \sin((l-n-m)kx)\Big] \\
& - 3\sum_n A_n(t)n^2k^2\sin(nkx)
\end{aligned}
\tag{46}
$$