Maier-Saupe free energy in weak form

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1 Introduction

Here we will find a PDE describing the time evolution equation of the Q-tensor from thermodynamic effects, according to the Maier-Saupe free energy. Then we will discretize time according to a general finite difference scheme. After this, we will put the resulting space-dependent equations into weak form. The result will be non-linear, so we will have to use Newton's method to compute the solution to the finite difference scheme.

2 Maier-Saupe free energy and equations of motion

2.1 Writing the free energy in terms of Q_{ij}

We begin by defining the tensor order parameter of the nematic system in terms of the probability distribution of the molecular orientation:

$$Q_{ij}(\mathbf{x}) = \int_{S^2} \left(\xi_i \xi_j - \tfrac{1}{3}\delta_{ij}\right) p(\xi; \mathbf{x}) d\xi \tag{1}$$

where $p(\xi; \mathbf{x})$ is the probability distribution of molecular orientation in local equilibrium at some temperature T and position $\mathbf{x}$. Note that this quantity is traceless and symmetric. Then the mean field free energy is given by:

$$F\left[Q_{ij}\right] = H\left[Q_{ij}\right] - T\Delta S \tag{2}$$

where H is the energy of the configuration, and ΔS is the entropy relative to the uniform distribution. We choose H to be:

$$H\left[Q_{ij}\right] = \int_\Omega \left\{-\alpha Q_{ij} Q_{ji} + f_e\left(Q_{ij}, \partial_k Q_{ij}\right)\right\} d\mathbf{x} \tag{3}$$

with α some interaction parameter and f_e the elastic free energy density. The entropy is given by:

$$\Delta S = -n k_B \int_\Omega \left(\int_{S^2} p(\xi; \mathbf{x}) \log\left[4\pi p(\xi; \mathbf{x})\right] d\xi \right) d\mathbf{x} \tag{4}$$

where n is the number density of molecules. Now, in general for a given Q_{ij} there is no unique $p(\xi; \mathbf{x})$ given by (1). Hence, there is no unique ΔS. To find the appropriate ΔS corresponding to some fixed Q_{ij}, we seek to maximize the entropy density for a fixed Q_{ij} via the method of Lagrange multipliers. This goes as follows:

$$\begin{aligned} \mathcal{L}[p] &= \Delta s[p] + \Lambda_{ij}\left[\int_{S^2} \left(\xi_i \xi_j - \tfrac{1}{3}\delta_{ij}\right) p\left(\xi; \mathbf{x}\right) d\xi - Q_{ij}\right] \\ &= \int_{S^2} p(\xi) \bigg(-n k_B \log\left[4\pi p(\xi)\right] + \Lambda_{ij}\left(\xi_i \xi_j - \tfrac{1}{3}\delta_{ij}\right) \bigg) d\xi - \Lambda_{ij} Q_{ij} \end{aligned} \tag{5}$$

where here Q_{ij} is taken to be a constant which defines the constraint. Here we've taken the spatial dependence to be implicit, since each of these are local quantities, and we're minimizing them *locally*. So, define a variation in p given by:

$$p'(\xi) = p(\xi) + \varepsilon \eta(\xi) \tag{6}$$

Then we have that:

$$\begin{aligned}
\frac{\delta \mathcal{L}}{\delta p} &= \frac{d\mathcal{L}[p']}{d\varepsilon}\bigg|_{\varepsilon=0} \\
&= \frac{d\mathcal{L}[p']}{dp'}\frac{dp'}{d\varepsilon}\bigg|_{\varepsilon=0} \\
&= \int_{S^2} \bigg(-nk_B \log\left[4\pi p(\xi)\right] + \Lambda_{ij}\left(\xi_i\xi_j - \tfrac{1}{3}\delta_{ij}\right) - nk_B \bigg) \eta(\xi) d\xi
\end{aligned} \tag{7}$$

Since this is for an arbitrary variation η, we must have that

$$-nk_B \log\left[4\pi p(\xi)\right] + \Lambda_{ij}\left(\xi_i\xi_j - \tfrac{1}{3}\delta_{ij}\right) - nk_B = 0 \tag{8}$$

Solving for $p(\xi)$ yields:

$$p(\xi) = \frac{1}{4\pi}\exp\left[-\tfrac{1}{nk_B}\tfrac{1}{3}\Lambda_{ij}\delta_{ij} - 1\right]\exp\left[\tfrac{1}{nk_B}\Lambda_{ij}\xi_i\xi_j\right] \tag{9}$$

However, $p(\xi)$ is a probability distribution, so we need to normalize it over the domain. When we do this, the constant factors out front cancel. Further, since Λ_{ij} is just an arbitrary factor that we use to calculate $p(\xi)$, we may rescale it by nk_B. Doing all this yields:

$$p(\xi) = \frac{\exp\left[\Lambda_{ij}\xi_i\xi_j\right]}{Z\left[\Lambda\right]} \tag{10}$$

$$Z\left[\Lambda\right] = \int_{S^2} \exp[\Lambda_{ij}\xi_i\xi_j] d\xi \tag{11}$$

Now p is uniquely defined in terms of the Lagrange multipliers Λ_{ij}. Plugging this back into the constraint equation (1) we get:

$$\begin{aligned}
Q_{ij} &= \frac{1}{Z[\Lambda]}\left(\int_{S^2}\left(\xi_i\xi_j \exp[\Lambda_{kl}\xi_k\xi_l] - \tfrac{1}{3}\delta_{ij}\exp[\Lambda_{kl}\xi_k\xi_l]\right) d\xi\right) \\
&= \frac{1}{Z[\Lambda]}\left(\frac{\partial Z[\Lambda]}{\partial \Lambda_{ij}} - \tfrac{1}{3}\delta_{ij} Z[\Lambda]\right) \\
&= \frac{\partial \log Z}{\partial \Lambda_{ij}} - \tfrac{1}{3}\delta_{ij}
\end{aligned} \tag{12}$$

This set of equations uniquely defines Λ_{ij} in terms of Q_{ij}, although the equation is not algebraically solvable. We may also plug (10) into (4) to get ΔS as a function of Λ_{ij} (and therefore implicitly of Q_{ij}):

$$\begin{aligned}
\Delta S &= -nk_B \int_\Omega \frac{1}{Z[\Lambda]}\left(\int_{S^2}\exp[\Lambda_{ij}\xi_i\xi_j]\left(\log(4\pi) + \log(1/Z[\Lambda]) + \Lambda_{ij}\xi_i\xi_j\right) d\xi\right) d\mathbf{x} \\
&= -nk_B \int_\Omega \left(\log(4\pi) - \log(Z[\Lambda]) + \Lambda_{ij}\frac{\partial \log Z[\Lambda]}{\partial \lambda_{ij}}\right) \\
&= -nk_B \int_\Omega \left(\log(4\pi) - \log(Z[\Lambda]) + \Lambda_{ij}\left(Q_{ij} + \tfrac{1}{3}\delta_{ij}\right)\right)
\end{aligned} \tag{13}$$

Further, we may explicitly write out the elastic free energy as:

$$f_e(Q_{ij}, \partial_k Q_{ij}) = L_1\left(\partial_k Q_{ij}\right)\left(\partial_k Q_{ij}\right) + L_2\left(\partial_j Q_{ij}\right)\left(\partial_k Q_{ik}\right) + L_3 Q_{kl}\left(\partial_k Q_{ij}\right)\left(\partial_l Q_{ij}\right) \tag{14}$$

2.2 Finding the equations of motion

Now, since Q_{ij} is traceless and symmetric, we need to use a Lagrange multiplier scheme so that there is an extra piece in our free energy:

$$f_l = -\lambda Q_{ii} - \lambda_i \epsilon_{ijk} Q_{jk} \tag{15}$$

To get a time evolution equation for Q, we just take the negative variation of the free energy density f with respect to each of them:

$$\partial_t Q_{ij} = -\frac{\partial f}{\partial Q_{ij}} + \partial_k \frac{\partial f}{\partial(\partial_k Q_{ij})} \tag{16}$$

Let's write out these terms explicitly. We start with the Maier-Saupe interaction term:

$$\begin{aligned} -\frac{\partial}{\partial Q_{ij}} \left(-\alpha Q_{kl} Q_{lk}\right) &= \alpha \delta_{ik}\delta_{jl} Q_{lk} + \alpha \delta_{il}\delta_{jk} Q_{kl} \\ &= 2\alpha Q_{ij} \end{aligned} \tag{17}$$

Now elastic energy:

$$\begin{aligned} -\frac{\partial}{\partial Q_{ij}} \left(L_3 Q_{kl} (\partial_k Q_{nm})(\partial_l Q_{nm})\right) &= -L_3 \delta_{ik}\delta_{jl} (\partial_k Q_{nm})(\partial_l Q_{nm}) \\ &= -L_3 (\partial_i Q_{nm})(\partial_j Q_{nm}) \end{aligned} \tag{18}$$

And the Lagrange multiplier terms:

$$\begin{aligned} -\frac{\partial}{\partial Q_{ij}} \left(-\lambda Q_{kk} - \lambda_k \epsilon_{klm} Q_{lm}\right) &= \lambda \delta_{ik}\delta_{jk} + \lambda_k \epsilon_{klm} \delta_{il}\delta_{jm} \\ &= \lambda \delta_{ij} + \lambda_k \epsilon_{kij} \end{aligned} \tag{19}$$

Now for the other elastic energy terms:

$$\begin{aligned} \partial_k \frac{\partial f}{\partial(\partial_k Q_{ij})} L_1 (\partial_l Q_{nm})(\partial_l Q_{nm}) &= L_1 \partial_k \left(\delta_{kl}\delta_{in}\delta_{jm} \partial_l Q_{nm} + \partial_l Q_{nm} \delta_{kl}\delta_{ik}\delta_{jm}\right) \\ &= 2L_1 \partial_k \partial_k Q_{ij} \end{aligned} \tag{20}$$

And the L_2 term:

$$\begin{aligned} \partial_k \frac{\partial f}{\partial(\partial_k Q_{ij})} L_2 (\partial_m Q_{lm})(\partial_n Q_{ln}) &= L_2 \partial_k \left(\delta_{km}\delta_{il}\delta_{jm} (\partial_n Q_{ln}) + (\partial_m Q_{lm}) \delta_{kn}\delta_{il}\delta_{jn}\right) \\ &= L_2 \partial_k \left(\delta_{kj} (\partial_n Q_{in}) + \delta_{kj} (\partial_m Q_{im})\right) \\ &= 2L_2 \partial_j (\partial_m Q_{im}) \end{aligned} \tag{21}$$

And finally the L_3 term:

$$\begin{aligned} \partial_k \frac{\partial f}{\partial(\partial_k Q_{ij})} L_3 Q_{np} (\partial_n Q_{lm})(\partial_p Q_{lm}) &= L_3 \partial_k Q_{np} \left(\delta_{kn}\delta_{il}\delta_{jm} (\partial_p Q_{lm}) + (\partial_n Q_{lm}) \delta_{kp}\delta_{il}\delta_{jm}\right) \\ &= L_3 \partial_k \left(Q_{kp} (\partial_p Q_{ij}) + Q_{nk} (\partial_n Q_{ij})\right) \\ &= 2L_3 \partial_k \big(Q_{kn} (\partial_n Q_{ij})\big) \end{aligned} \tag{22}$$

Finally, we consider the entropy term:

$$\begin{aligned} -\frac{\partial}{\partial Q_{ij}} (-T\Delta s) &= -\frac{\partial}{\partial Q_{ij}} \left[(-T)(-nk_B)\left(\log(4\pi) - \log(Z[\Lambda]) + \Lambda_{kl}(Q_{kl} + \tfrac{1}{3}\delta_{kl}\right)\right] \\ &= nk_B T \left(\frac{\partial \log Z}{\partial \Lambda_{kl}} \frac{\partial \Lambda_{kl}}{\partial Q_{ij}} - \frac{\partial \Lambda_{kl}}{\partial Q_{ij}} \left(Q_{kl} + \tfrac{1}{3}\delta_{kl}\right) - \Lambda_{kl}\delta_{ik}\delta_{jl}\right) \\ &= nk_B T \left(\left(Q_{kl} + \tfrac{1}{3}\delta_{kl}\right) \frac{\partial \Lambda_{kl}}{\partial Q_{ij}} - \frac{\partial \Lambda_{kl}}{\partial Q_{ij}} \left(Q_{kl} + \tfrac{1}{3}\delta_{kl}\right) - \Lambda_{ij}\right) \\ &= -nk_B T \Lambda_{ij} \end{aligned} \tag{23}$$

Finally, we need to write down the Lagrange multipliers in terms of Q and its spatial derivatives. To do this, note that Q_{ij} is traceless and symmetric so that $\partial_t Q_{ij}$ is also traceless and symmetric. Hence, to find λ we just take negative $\frac{1}{3}$ the trace of the source term. This gives:

$$\begin{aligned} \lambda &= -\tfrac{1}{3}\left(-L_3(\partial_i Q_{nm})(\partial_i Q_{nm}) + 2L_2 \partial_i(\partial_m Q_{im})\right) \\ &= \tfrac{1}{3}\left(L_3(\partial_i Q_{nm})(\partial_i Q_{nm}) - 2L_2 \partial_i(\partial_m Q_{im})\right) \end{aligned} \tag{24}$$

where the rest of the terms are traceless. Now to find λ_k, we know that the anti-symmetric piece of any matrix can be given by:

$$\tfrac{1}{2}\left(A_{ij} - A_{ji}\right) \tag{25}$$

Further, the Lagrange multiplier term needs to cancel out the anti-symmetric piece:

$$\lambda_k \epsilon_{kij} = -\tfrac{1}{2}\left(A_{ij} - A_{ji}\right) \tag{26}$$

To solve for λ_k explicitly, we may calculate:

$$\begin{aligned} -\tfrac{1}{2}\epsilon_{lij}\left(A_{ij} - A_{ji}\right) &= \lambda_k \epsilon_{kij}\epsilon_{lij} \\ &= \lambda_k\left(\delta_{kl}\delta_{ii} - \delta_{ki}\delta_{il}\right) \\ &= 2\lambda_l \end{aligned} \tag{27}$$

Hence:

$$\begin{aligned} \lambda_l &= -\tfrac{1}{2}L_2\epsilon_{lij}\left(\partial_j(\partial_m Q_{im}) - \partial_i(\partial_m Q_{jm})\right) \\ &= \tfrac{1}{2}L_2\epsilon_{lij}\left(\partial_i(\partial_m Q_{jm}) - \partial_j(\partial_m Q_{im})\right) \end{aligned} \tag{28}$$

since the L_2 term is the only one that's anti-symmetric. The source term corresponding to this Lagrange multiplier piece is then given by:

$$\begin{aligned} \tfrac{1}{2}L_2\big((\partial_k\partial_n Q_{mn}) - (\partial_m\partial_n Q_{kn})\big)\epsilon_{lkm}\epsilon_{lij} &= \tfrac{1}{2}L_2\big((\partial_k\partial_n Q_{mn}) - (\partial_m\partial_n Q_{kn})\big)\left(\delta_{ki}\delta_{mj} - \delta_{kj}\delta_{mi}\right) \\ &= \tfrac{1}{2}L_2\big((\partial_i\partial_n Q_{jn}) - (\partial_j\partial_n Q_{in})\big) - \tfrac{1}{2}L_2\big((\partial_j\partial_n Q_{in}) - (\partial_i\partial_n Q_{jn})\big) \\ &= L_2\big((\partial_i\partial_n Q_{jn}) - (\partial_j\partial_n Q_{in})\big) \end{aligned} \tag{29}$$

Hence, the total equation of motion is:

$$\begin{aligned} \partial_t Q_{ij} &= 2\alpha Q_{ij} - L_3(\partial_i Q_{nm})(\partial_j Q_{nm}) + \tfrac{1}{3}\left(L_3(\partial_k Q_{nm})(\partial_k Q_{nm}) - 2L_2(\partial_k\partial_m Q_{km})\right)\delta_{ij} \\ &\quad + L_2\big((\partial_i\partial_n Q_{jn}) - (\partial_j\partial_n Q_{in})\big) - nk_B T\Lambda_{ij} \\ &\quad + 2L_1\partial_k\partial_k Q_{ij} + 2L_2(\partial_j\partial_m Q_{im}) + 2L_3\partial_k\big(Q_{kn}(\partial_n Q_{ij})\big) \\ &= 2\alpha Q_{ij} - L_3(\partial_i Q_{nm})(\partial_j Q_{nm}) - nk_B T\Lambda_{ij} \\ &\quad + 2L_1\partial_k\partial_k Q_{ij} + L_2\left((\partial_j\partial_m Q_{im}) + (\partial_i\partial_m Q_{jm})\right) + 2L_3\partial_k\big(Q_{kn}(\partial_n Q_{ij})\big) \\ &\quad + \tfrac{1}{3}\left(L_3(\partial_k Q_{nm})(\partial_k Q_{nm}) - 2L_2(\partial_k\partial_m Q_{km})\right)\delta_{ij} \\ &= F_{ij}\left(Q_{ij}; \partial_k Q_{ij}; \partial_l\partial_k Q_{ij}\right) \end{aligned} \tag{30}$$

One can see that F_{ij} is both symmetric and traceless by virtue of Q_{ij} being traceless and symmetric.

2.3 Reducing degrees of freedom

Since Q_{ij} is traceless and symmetric, we only have five independent degrees of freedom. We label as follows:

$$Q_{ij} = \begin{bmatrix} Q_1 & Q_2 & Q_3 \\ Q_2 & Q_4 & Q_5 \\ Q_3 & Q_5 & -(Q_1 + Q_4) \end{bmatrix} \tag{31}$$

We can define similarly for F_{ij}. In this case, we just get a five-component vector equation:

$$\partial_t Q_i = F_i \left(Q_i; \partial_j Q_i; \partial_k \partial_j Q_i\right) \tag{32}$$

where, we may write F_i as a function of the vector components Q_i (and spatial derivatives thereof) by just explicitly carrying out the sums over the tensor indices. This observation reduces the number of equations from 9 down to 5.

3 Numerically inverting $Q_{ij}(\Lambda)$

3.1 Newton's method scheme

In all variations of investigating the behavior of nematic-state liquid crystals using a Maier-Saupe free energy, we will need to numerically invert $Q_{ij}(\Lambda)$. Hence, we describe the method for doing that first, and implement it as a practice for working with numerical libraries. To begin, we have the following explicit expression for Q_{ij} in terms of Λ_{ij}:

$$Q_{ij}(\Lambda) = \frac{\int_{S^2} \xi_i \xi_j \exp\left[\Lambda_{kl} \xi_k \xi_l\right] d\xi}{\int_{S^2} \exp\left[\Lambda_{kl} \xi'_k \xi'_l\right] d\xi'} - \tfrac{1}{3}\delta_{ij} \tag{33}$$

For this we use Newton's method to find the values for Λ given fixed values for the components of Q_{ij}. Note that, during these calculations, we use Lebedev quadrature to do the integrations over the sphere.

To actually implement Newton's method, we do as follows. For any fixed Q_{ij} define a vector residual R_m such that:

$$R_m(\Lambda) = \frac{\int_{S^2} \xi_{i(m)} \xi_{j(m)} \exp\left[\Lambda_{kl} \xi_k \xi_l\right] d\xi}{\int_{S^2} \exp\left[\Lambda_{kl} \xi'_k \xi'_l\right] d\xi'} - \tfrac{1}{3}\delta_{i(m)j(m)} - Q_{i(m)j(m)} \tag{34}$$

where m refers to the index of the distinct degrees of freedom of Q, and $(i(m), j(m))$ denotes the location in the matrix. We see values of Λ_m which will be a zero of this quantity. Hence, we must find the Jacobian, which is just:

$$R'(\Lambda) = \frac{\partial R_m}{\partial \Lambda_n} \tag{35}$$

This will be a 5×5 matrix. This needs to be done in a non-uniform way because the elements corresponding to diagonals on the Λ matrix (that is, $n = 1, 4$) show up differently than the elements corresponding to off-diagonal elements (i.e. $n = 2, 3, 5$). For the off-diagonal elements we get:

$$\begin{aligned} R'_{mn} = &\frac{\int_{S^2} 2\xi_{i(m)} \xi_{i(n)} \xi_{j(m)} \xi_{j(n)} \exp\left[\Lambda_{kl} \xi_k \xi_l\right] d\xi}{\int_{S^2} \exp\left[\Lambda_{kl} \xi_k \xi_l\right] d\xi} \\ &- \frac{\int_{S^2} \xi_{i(m)} \xi_{j(m)} \exp\left[\Lambda_{kl} \xi_k \xi_l\right] \int_{S^2} 2\xi_{i(n)} \xi_{j(n)} \exp\left[\Lambda_{kl} \xi_k \xi_l\right]}{\left(\int_{S^2} \exp\left[\Lambda_{kl} \xi_k \xi_l\right]\right)^2} \end{aligned} \tag{36}$$

where the factor of 2 in each term comes from the fact that, for off-diagonal elements, each entry in Λ_n appears twice in the Λ_{kl} tensor, and the ξ coefficients turn out to be the same (because the expression is symmetric in k and l within the exponent). For the diagonal elements, we get:

$$\begin{aligned} R'_{mn} = &\frac{\int_{S^2} \xi_{i(m)} \xi_{j(m)} \left(\xi_{i(n)}^2 - \xi_3^2\right) \exp\left[\Lambda_{kl} \xi_k \xi_l\right]}{\int_{S^2} \exp\left[\Lambda_{kl} \xi_k \xi_l\right] d\xi} \\ &- \frac{\int_{S^2} \xi_{i(m)} \xi_{j(m)} \exp\left[\Lambda_{kl} \xi_k \xi_l\right] \int_{S^2} \left(\xi_{i(n)}^2 - \xi_3^2\right) \exp\left[\Lambda_{kl} \xi_k \xi_l\right]}{\left(\int_{S^2} \exp\left[\Lambda_{kl} \xi_k \xi_l\right]\right)^2} \end{aligned} \tag{37}$$

where here the expression in parentheses comes from the fact that the $(3, 3)$ must be such that the tensor is traceless. Given these expressions for the Jacobian, we must solve:

$$R'_{ij}(\Lambda^n)\delta\Lambda_j^n = -R_m(\Lambda^n) \tag{38}$$

$$\Lambda_i^{n+1} = \Lambda_i^n + \delta\Lambda_i^n \tag{39}$$

iteratively until $|R_m(\Lambda^n)| < \epsilon$ for some small error ϵ.

3.2 Initialization case

Initially, we set $\Lambda_m = 0$. In this case, we can save some computational power by explicitly calculating the residual and Jacobian given Q_m. For $m = 1$ we get that:

$$R_1(\Lambda) = \frac{\int_{S^2} x^2}{\int_{S^2} 1} - \tfrac{1}{3} - Q_1 = -Q_1 \tag{40}$$

where we have calculated $\int_{S^2} x^2$ by noting that $x^2 + y^2 + z^2 = r^2 = 1$ on the sphere, that the integral of 1 around the sphere is 4π (the surface area of a unit sphere), and that by symmetry $\int_{S^2} x^2 = \int_{S^2} y^2 = \int_{S^2} z^2$. By the same token, we have that:

$$R_4(\Lambda) = -Q_4 \tag{41}$$

For $m = 2$ we have:

$$R_2(\Lambda) = \frac{\int_{S^2} xy}{\int_{S^2} 1} - Q_2 = -Q_2 \tag{42}$$

where we have noted that, for fixed x, y is has matching positive and negative values throughout the integral. This is true for all x values, and so the total integral is zero. By the same token we have that:

$$R_3(\Lambda) = -Q_3 \tag{43}$$

$$R_5(\Lambda) = -Q_5 \tag{44}$$

Now for the Jacobian. Here, for $n = 1$, $m = 1$ we get:

$$\begin{aligned} R'_{11} &= \frac{\int_{S^2} x^2(x^2 - z^2)}{4\pi} - \frac{\int_{S^2} x^2 \int_{S^2}(x^2 - z^2)}{16\pi^2} \\ &= \frac{2}{15} \end{aligned} \tag{45}$$

Similarly, for $n = 4$, $m = 4$:

$$R'_{44} = \frac{2}{15} \tag{46}$$

For $n = 1$, $m = 2$ we get:

$$\begin{aligned} R'_{21} &= \frac{\int_{S^2} xy(x^2 - z^2)}{4\pi} - \frac{(\int_{S^2} xy)(\int_{S^2}(x^2 - z^2)}{16\pi^2} \\ &= 0 \end{aligned} \tag{47}$$

Similarly, we find that

$$R'_{31} = R'_{51} = 0 \tag{48}$$

For $n = 1$, $m = 4$ we get:

$$\begin{aligned} R'_{41} &= \frac{\int_{S^2} y^2(x^2 - z^2)}{4\pi} - \frac{\int_{S^2} y^2 \int_{S^2}(x^2 - z^2)}{16\pi^2} \\ &= \end{aligned} \tag{49}$$

I got lazy and computed the rest with sympy. It turns out to be:

$$
R'_{mn} = \begin{bmatrix} \frac{2}{15} & 0 & 0 & 0 & 0 \\ 0 & \frac{2}{15} & 0 & 0 & 0 \\ 0 & 0 & \frac{2}{15} & 0 & 0 \\ 0 & 0 & 0 & \frac{2}{15} & 0 \\ 0 & 0 & 0 & 0 & \frac{2}{15} \end{bmatrix} \tag{50}
$$

4 Isotropic steady state problem

As a first problem using finite element analysis, we seek to simplify as much as possible. To this end, we only consider the steady-state equation ($\partial_t Q_i = 0$), and we only consider isotropic elasticity ($L_2 = L_3 = 0$). Then the governing equation reads:

$$
0 = 2\alpha Q_i + 2L_1 \partial_k \partial_k Q_i - n k_B T \Lambda_i \tag{51}
$$

We may non-dimensionalize by defining a characteristic length-scale:

$$
\xi = \sqrt{\frac{2L_1}{n k_B T}} \tag{52}
$$

and then define a dimensionless length and interaction parameter:

$$
x = \overline{x}\,\xi \tag{53}
$$

$$
\overline{\alpha} = \frac{2\alpha}{n k_B T} \tag{54}
$$

Dropping the overlines for brevity, our equation of motion reads:

$$
0 = \alpha Q_i + \partial_k \partial_k Q_i - \Lambda_i \tag{55}
$$

4.1 Numerical scheme

Because Λ_i is a nonlinear function of Q_i, this problem is nonlinear. Since the finite element scheme can only handle linear problems, we use Newton's method to solve. To that end, we define a residual as exactly the source term:

$$
F_i(Q) = \alpha Q_i + \partial_k \partial_k Q_i - \Lambda_i \tag{56}
$$

We want this to have magnitude zero, and so we iteratively solve the equations:

$$
F'_{ij}(Q^n) \delta Q_j^n = -F_i(Q^n) \tag{57}
$$

$$
Q_i^{n+1} = Q_i^n + \delta Q_i^n \tag{58}
$$

where n denotes the step in the iteration, and F'_{ij} is the Gateaux derivative of the residual. Writing out this Gateaux derivative gives us:

$$
\begin{aligned}
F'_{ij} \delta Q_j &= \alpha \frac{\partial Q_i}{\partial Q_j} \delta Q_j + \left(\partial_k \partial_k \frac{\partial Q_i}{\partial Q_j} \delta Q_j \right) - \frac{\partial \Lambda_i}{\partial Q_j} \delta Q_j \\
&= \alpha \delta Q_i + \partial_k \partial_k \delta Q_i - \left(\frac{\partial Q_i}{\partial \Lambda_j} \right)^{-1} \delta Q_j \\
&= \alpha \delta Q + \nabla^2 \delta Q - R'^{-1}(Q) \delta Q
\end{aligned} \tag{59}
$$

where in the second to last line we have used the chain rule to rewrite $\partial \Lambda_i / \partial Q_j$ and then in the final line we have written everything in vector notation so that we may use indices to indicate test and basis functions. Note that we have used the same Jacobian from our dicussion of inverting $Q(\Lambda)$.

To implement this as a finite element problem, we take (57) and integrate it against some finite number of test functions enumerated by i:

$$\langle \phi_i, \alpha\, \delta Q^n \rangle + \left\langle \phi_i, \nabla^2 \delta Q^n \right\rangle - \left\langle \phi_i, R'^{-1}(Q^n) \delta Q^n \right\rangle = - \langle \phi_i, \alpha Q^n \rangle - \left\langle \phi_i, \nabla^2 Q^n \right\rangle + \langle \phi_i, \Lambda(Q^n) \rangle \tag{60}$$

Integrating by parts using the divergence theorem gives us:

$$\begin{aligned} \langle \phi_i, \alpha\, \delta Q^n \rangle &+ \left\langle \phi_i, \frac{\partial \delta Q^n}{\partial n} \right\rangle_{\partial\Omega} \\ &- \langle \nabla \phi_i, \nabla \delta Q^n \rangle - \left\langle \phi_i, R'^{-1}(Q^n) \delta Q^n \right\rangle = - \langle \phi_i, \alpha Q^n \rangle - \left\langle \phi_i, \frac{\partial Q^n}{\partial n} \right\rangle_{\partial\Omega} \\ &\qquad + \langle \nabla \phi_i, \nabla Q^n \rangle + \langle \phi_i, \Lambda(Q^n) \rangle \end{aligned} \tag{61}$$

and taking into account the Dirichlet conditions so that the test functions go to zero on the boundaries (or zero Neumann conditions), we get:

$$\langle \phi_i, \alpha\, \delta Q^n \rangle - \langle \nabla \phi_i, \nabla \delta Q^n \rangle - \left\langle \phi_i, R'^{-1}(Q^n) \delta Q^n \right\rangle = - \langle \phi_i, \alpha Q^n \rangle + \langle \nabla \phi_i, \nabla Q^n \rangle + \langle \phi_i, \Lambda(Q^n) \rangle \tag{62}$$

Now we approximate δQ^n as a linear combination of some number of basis functions:

$$\delta Q^n = \sum_j \delta Q_j^n \phi_j \tag{63}$$

Substituting this into our equation yields:

$$\sum_j \left[\alpha \langle \phi_i, \phi_j \rangle - \langle \nabla \phi_i, \nabla \phi_j \rangle - \left\langle \phi_i, R'^{-1}(Q^n) \phi_j \right\rangle \right] \delta Q_j^n = - \langle \phi_i, \alpha Q^n \rangle + \langle \nabla \phi_i, \nabla Q^n \rangle + \langle \phi_i, \Lambda(Q^n) \rangle \tag{64}$$

which is the same as the linear problem:

$$A_{ij}^n \delta Q_j^n = b_i^n \tag{65}$$

with the definitions:

$$A_{ij}^n = \alpha \langle \phi_i, \phi_j \rangle - \langle \nabla \phi_i, \nabla \phi_j \rangle - \left\langle \phi_i, R'^{-1}(Q^n) \phi_j \right\rangle \tag{66}$$

and

$$b_i = - \langle \phi_i, \alpha Q^n \rangle + \langle \nabla \phi_i, \nabla Q^n \rangle + \langle \phi_i, \Lambda(Q^n) \rangle \tag{67}$$

5 Checking free energy

Here, we write out the free energy density, and then plot it as a function of temperature. This will help us check the numerical inversion scheme:

$$f_b(Q) = -\alpha Q_{ij} Q_{ji} + n k_B T \left(\log(4\pi) - \log(Z[\Lambda]) + \Lambda_{ij} (Q_{ij} + \tfrac{1}{3} \delta_{ij}) \right) \tag{68}$$

We non-dimensionalize by dividing by $n k_B T$, and defining $\kappa = \alpha / n k_B T$:

$$f_b(Q) = -\kappa Q_{ij} Q_{ji} \left(\log(4\pi) - \log(Z[\Lambda]) + \Lambda_{ij} (Q_{ij} + \tfrac{1}{3} \delta_{ij}) \right) \tag{69}$$

We will plot this for a uniaxial Q_{ij} configuration given different values of S:

$$\begin{aligned} Q_{ij} &= S \begin{bmatrix} \cos^2 \phi - \frac{1}{3} & \cos \phi \sin \phi & 0 \\ \cos \phi \sin \phi & \sin^2 \phi - \frac{1}{3} & 0 \\ 0 & 0 & -\frac{1}{3} \end{bmatrix} \\ &= \frac{S}{2} \begin{bmatrix} \frac{1}{3} + \cos 2\phi & \sin 2\phi & 0 \\ \sin 2\phi & \frac{1}{3} - \cos 2\phi & \\ 0 & 0 & -\frac{2}{3} \end{bmatrix} \end{aligned} \tag{70}$$

Here we just take $\phi = 0$, though the value should not depend on ϕ given rotational invariance.

6 Isotropic time-dependent problem

Here we have to non-dimensionalize again. The original problem is given by:

$$\partial_t Q_i = 2\alpha Q_i + 2L_1 \partial_k^2 Q_i - n k_B T \Lambda_i \tag{71}$$

We may once again use the constants from part 4 to get:

$$\frac{1}{n k_B T} \partial_t Q_i = \alpha Q_i + \partial_k^2 Q_i - \Lambda_i \tag{72}$$

Then, taking:

$$\begin{aligned} t &= \bar{t}\, t_0 \\ t_0 &= \frac{1}{n k_B T} \end{aligned} \tag{73}$$

our equation of motion becomes:

$$\partial_t Q_i = \alpha Q_i + \partial_k^2 Q_i - \Lambda_i \tag{74}$$

6.1 Time discretization

Here we will again take the elasticity to be isotropic, but we introduce time-dependence into the problem. To that end, we use the convex splitting scheme given by Cody, and define the following terms:

$$\delta t = t_n - t_{n-1} \tag{75}$$

$$\partial_t Q_i \to \frac{Q_i^n - Q_i^{n-1}}{\delta t} \tag{76}$$

where t_n and Q_i^n are the time and order parameter evaluated at timestep n. For the convex splitting scheme, we will evaluate terms at either timestep n or timestep $n+1$ to take advantage of convexity. This gives a time-discretized equation of:

$$\frac{Q_i^n - Q_i^{n-1}}{\delta t} = \alpha Q_i^{n-1} + \partial_k^2 Q_i^n - \Lambda_i(Q^n) \tag{77}$$

Rearranging this gives:

$$Q_i^n - \delta t \left(\partial_k^2 Q_i^n - \Lambda_i^n \right) - (1 + \delta t\, \alpha) Q_i^{n-1} = 0 = F_i(Q^n) \tag{78}$$

This equation is nonlinear in Q^n and so we define the residual F_i to be the left hand side. In order to use Newton's method we need to take the Gateaux derivative of the residual, and then iteratively solve the resulting linear equation:

$$F'_{ij}(Q^{n,m}) \delta_j^{n,m} = -F_i(Q^{n,m}) \tag{79}$$

$$Q_i^{n,m+1} = Q_i^{n,m} + \delta Q_i^{n,m} \tag{80}$$

For sake of simplicity, we use the superscript n to correspond with the particular time-step, and use a superscript m to discuss the mth iteration of the Newton's method scheme. Implicit in the definition of F_i is that it is a function of Q^{n-1}, although when we take a Gateaux derivative we are taking with with respect to Q^n so that Q^{n-1} behaves like a constant. This gives us:

$$\begin{aligned} F'_{ij} \delta Q_j &= \frac{\partial Q_i}{\partial Q_j} \delta Q_j - \delta t \partial_k^2 \left(\frac{\partial Q_i}{\partial Q_j} \delta Q_j \right) + \delta t \frac{\partial \Lambda_i}{\partial Q_j} \delta Q_j \\ &= \delta Q_i - \delta t \partial_k^2 \delta Q_i + \delta t \left(\frac{\partial Q_i}{\Lambda_j} \right)^{-1} \\ &= \delta Q - \delta t \nabla^2 \delta Q + \delta t\, R'^{-1}(Q) \delta Q \end{aligned} \tag{81}$$

This is exactly what we had before, except each term has different coefficients. In this case our linear system will be identical, except for the different coefficients and the fact that we have a constant term in our residual due to the Q^{n-1} term. This yields:

$$A_{ij}^m \delta Q_j^{n,m} = b_i^m \tag{82}$$

with the definitions:

$$A_{ij}^m = \langle \phi_i, \phi_j \rangle + \delta t \langle \nabla \phi_i, \nabla \phi_j \rangle + \delta t \langle \phi_i, R'^{-1}(Q^{n,m}) \phi_j \rangle \tag{83}$$

and

$$b_i^m = -\langle \phi_i, Q^{n,m} \rangle - \delta t \, \langle \nabla \phi_i, \nabla Q^{n,m} \rangle - \delta t \, \langle \phi_i, \Lambda(Q^{n,m}) \rangle + (1 + \delta t \, \alpha) \langle \phi_i, Q^{n-1} \rangle \tag{84}$$

Note that this last term can just be evaluated once per time-step, to save a meager amount of computational resources.

7 Numerical scheme

7.1 Time discretization

To numerically solve this equation, we use Rothe's method to discretize the time dependence before the spatial dependence. To this end, we introduce the following finite difference scheme. For n the number of the current time step, call:

$$k = t_n - t_{n-1} \tag{85}$$

$$\partial_t Q_i \rightarrow \frac{Q_i^n - Q_i^{n-1}}{k} \tag{86}$$

$$F_i \rightarrow \left[\theta F_i^n + (1 - \theta) F_i^{n-1} \right] \tag{87}$$

where F_i^n is just F_i with Q_i evaluated at timestep n. Here $\theta = 0$ corresponds to an explicit Euler method, while $\theta = 1$ corresponds to an implicit Euler method. Also, $\theta = 1/2$ corresponds to a Crank-Nicolson method – we leave it undefined so that we may play with it later. The time-discretized equation is thus:

$$\begin{aligned} G_i \left(Q_i^n; \partial_k Q_i^n; \partial_l \partial_k Q_i^n \right) &= k \left[\theta F_i^n + (1 - \theta) F_i^{n-1} \right] - Q_i^n + Q_i^{n-1} \\ &= 0 \end{aligned} \tag{88}$$

7.2 Space discretization

To turn this into a finite element problem, we introduce a scalar residual function:

$$R \left(Q_i^n; \partial_k Q_i^n; \partial_l \partial_k Q_i^n \right) (\phi_i) = \int_\Omega G_i \phi_i = 0 \tag{89}$$

where ϕ_i is a vector of test functions. Now, we would like to only sum over the 5 free components to keep from making redundant calculations. However, in the explicit definition of F_i there are two floating indices which are, on some terms, located on differential operators. Hence, we consider a tensor test function which is defined in the same way as Q_{ij}:

$$\phi_{ij} = \begin{bmatrix} \phi_1 & \phi_2 & \phi_3 \\ \phi_2 & \phi_4 & \phi_5 \\ \phi_3 & \phi_5 & -(\phi_1 + \phi_4) \end{bmatrix} \tag{90}$$

We can write the expression for F_i^n out explicitly as follows:

$$
\begin{aligned}
\int_\Omega F_i^n \phi_i = \int_\Omega F_{ij}^n \phi_{ij} \\
= 2\alpha \int_\Omega Q_{ij}^n \phi_{ij} - L_3 \int_\Omega (\partial_i Q_{nm}^n)(\partial_j Q_{nm}^n)\phi_{ij} - n k_B T \int_\Omega \Lambda_{ij}\phi_{ij} \\
+ 2L_1 \int_{\partial\Omega} n_k (\partial_k Q_{ij}^n)\phi_{ij} - 2L_1 \int_\Omega (\partial_k Q_{ij}^n)(\partial_k \phi_{ij}) + L_2 \int_{\partial\Omega} n_m (\partial_j Q_{im}^n)\phi_{ij} \\
- L_2 \int_\Omega (\partial_j Q_{im}^n)(\partial_m \phi_{ij}) + L_2 \int_{\partial\Omega} n_m (\partial_i Q_{jm}^n)\phi_{ij} - L_2 \int_\Omega (\partial_i Q_{jm}^n)(\partial_m \phi_{ij}) \\
+ 2L_3 \int_{\partial\Omega} n_k Q_{kn}^n (\partial_n Q_{ij}^n)\phi_{ij} - 2L_3 \int_\Omega Q_{kn}^n (\partial_n Q_{ij}^n)(\partial_k \phi_{ij}) + \tfrac{1}{3} L_3 \int_\Omega (\partial_k Q_{nm}^n)(\partial_k Q_{nm}^n)\phi_{ii} \\
- \tfrac{2}{3} L_2 \int_{\partial\Omega} n_k (\partial_m Q_{km}^n)\phi_{ii} + \tfrac{2}{3} L_2 \int_\Omega (\partial_m Q_{km}^n)(\partial_k \phi_{ii})
\end{aligned}
\tag{91}
$$

where we understand the sum over (i, j) to be only over those components which are distinct in the test function (i.e. (1, 1), (1, 2), (1, 3), (2, 2), (2, 3)), and where n_i is the vector normal to the boundary. Note that the other sums (e.g. over m) range over all three elements because that is how they appear in the definition of F_i.

At this point, we choose Dirichlet boundary conditions so that ϕ_i comes from the tangent space and thus takes value zero on the boundary. This lets us disregard all of the boundary terms. Further, we use the inner product notation $\langle \cdot, \cdot \rangle$ to denote the integral over the domain. This reduces the expression to:

$$
\begin{aligned}
\langle F_i^n, \phi_i \rangle = 2\alpha \langle Q_i^n, \phi_i \rangle - n k_B T \langle \Lambda_i, \phi_i \rangle - 2L_1 \langle \partial_k Q_i^n, \partial_k \phi_i \rangle \\
- L_2 \Big[\left\langle \partial_j Q_{im}^n + \partial_i Q_{jm}^n, \partial_m \phi_{ij} \right\rangle - \tfrac{2}{3} \langle \partial_m Q_{km}^n, \partial_k \phi_{ij} \delta_{ij} \rangle \Big] \\
- L_3 \Big[\langle (\partial_i Q_{nm}^n)(\partial_j Q_{nm}^n), \phi_{ij} \rangle + 2 \langle Q_{kn}^n (\partial_n Q_i^n), \partial_k \phi_i \rangle \\
- \tfrac{1}{3} \langle (\partial_k Q_{nm}^n)(\partial_k Q_{nm}^n), \phi_{ij} \delta_{ij} \rangle \Big]
\end{aligned}
\tag{92}
$$

With this explicit expression in mind, the residual function is given by:

$$
R(Q^n)(\phi) = k \Big[\theta \langle F_i^n, \phi_i \rangle + (1 - \theta) \left\langle F_i^{n-1}, \phi_i \right\rangle \Big] - \langle Q_i^n, \phi_i \rangle + \left\langle Q_i^{n-1}, \phi_i \right\rangle \tag{93}
$$

For each time step, we will need to iteratively solve for Q^n as a zero of this expression using Newton's method. Using subscripts to denote the number of the iteration in Newton's method, the method reads:

$$
R'(Q_{k-1}^n, \delta Q_{k-1}^n)(\phi) = -R(Q_{k-1}^n)(\phi) \tag{94}
$$

$$
Q_k^n = Q_{k-1}^n + \delta Q_{k-1}^n \tag{95}
$$

To be clear about what objects we're dealing with here, for a fixed test function ϕ, $R(Q_{k-1}^n)$ is a scalar, and $R'(Q_{k-1}^n)$ is a linear operator which acts on δQ_{k-1}^n to produce a scalar. In this case, we can create a linear system by solving this equation simultaneously for some number N of basis functions. Writing δQ_{k-1}^n as a linear combination of these basis elements, we now have a linear equation in those elements which we may solve for the coefficients. Hence, we can find Q^n and thus step forward in time.

7.3 An example to check

Consider a uniaxial, constant S configuration:

$$\hat{n} = (\cos\phi, \sin\phi, 0) \tag{96}$$

$$\begin{aligned} Q_{ij} &= S(n_i n_j - \tfrac{1}{3}\delta_{ij}) \\ &= S \begin{bmatrix} \cos^2\phi - \frac{1}{3} & \cos\phi\sin\phi & 0 \\ \cos\phi\sin\phi & \sin^2\phi - \frac{1}{3} & 0 \\ 0 & 0 & -\frac{1}{3} \end{bmatrix} \end{aligned} \tag{97}$$

Choose a particularly simple configuration with $\phi = 0$ and $S = 1$ so that we get:

$$Q_{ij} = \begin{bmatrix} \frac{2}{3} & 0 & 0 \\ 0 & -\frac{1}{3} & 0 \\ 0 & 0 & -\frac{1}{3} \end{bmatrix} \tag{98}$$

8 A first problem to solve numerically

In order to get our feet wet programming with numerical libraries, we begin by solving the problem of numerically inverting $Q_{ij}(\Lambda)$.