

Nematohydrodynamics, Quasi-2D and Linear Approximations

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Assumptions

We will consider a coupled nematic liquid crystal and hydrodynamic system on a flat substrate. Given this, we will assume a quasi-2D system – that is, the nematic crystal director field will only lie in the x-y plane. Additionally, we assume the fluid velocity and Q-tensor magnitude are small so we neglect terms higher than order-1 in Q_{ij} and v_i . Finally, we assume no acceleration so that $\partial v_i / \partial t = 0$ always. From the first assumption, we may assume the director field takes the form $\mathbf{n} = (\cos \phi, \sin \phi, 0)$ so that the Q-tensor, given by $Q_{ij} = S/2(3n_i n_j - \delta_{ij})$ takes the form:

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

Computing homogenous and elastic generalized force in terms of S and ϕ

From Svendsen and Zumer, the free energy density is given by

$$f = \phi(Q) + \frac{1}{2} L \partial_i Q_{jk} \partial_i Q_{jk}$$

so that the homogeneous elastic part of the generalized force is given by:

$$h_{ij}^{he} = L \partial_k^2 Q_{ij} - \frac{\partial \phi}{\partial Q_{ij}} + \lambda \delta_{ij} + \lambda_k \epsilon_{kij}$$

where ϕ is the Landau de Gennes bulk free energy:

$$\phi(Q) = \frac{1}{2} A Q_{ij} Q_{ji} + \frac{1}{3} B Q_{ij} Q_{jk} Q_{ki} + \frac{1}{4} C (Q_{ij} Q_{ji})^2$$

Note that, by our assumptions on Q_{ij} it will always be traceless and symmetric, so we may omit the Lagrange multiplier terms. We begin by explicitly calculating the second term in terms of Q_{ij} , one term at a time in ϕ :

$$\begin{aligned} \frac{\partial}{\partial Q_{mn}} \left(\frac{1}{2} A Q_{ij} Q_{ji} \right) &= \frac{1}{2} A (\delta_{im} \delta_{jn} Q_{ji} + Q_{ij} \delta_{jm} \delta_{in}) \\ &= \frac{1}{2} A (Q_{nm} + Q_{nm}) \\ &= A Q_{mn} \end{aligned}$$

where in the last step we've used symmetry of Q_{ij} .

$$\begin{aligned}\frac{\partial}{\partial Q_{mn}} \left(\frac{1}{3} B Q_{ij} Q_{jk} Q_{ki} \right) &= \frac{1}{3} B (\delta_{im} \delta_{jn} Q_{jk} Q_{ki} + Q_{ij} \delta_{jm} \delta_{kn} Q_{ki} + Q_{ij} Q_{jk} \delta_{mk} \delta_{ni}) \\ &= \frac{1}{3} B (Q_{nk} Q_{km} + Q_{im} Q_{ni} + Q_{nj} Q_{jm}) \\ &= B Q_{ni} Q_{im}\end{aligned}$$

And the final term gives:

$$\begin{aligned}\frac{\partial}{\partial Q_{mn}} \left(\frac{1}{4} C (Q_{ij} Q_{ji})^2 \right) &= \frac{1}{4} C \cdot 2 (Q_{ij} Q_{ji}) \frac{\partial (Q_{kl} Q_{lk})}{\partial Q_{mn}} \\ &= \frac{1}{4} C \cdot 2 (Q_{ij} Q_{ji}) \cdot (\delta_{mk} \delta_{nl} Q_{lk} + Q_{kl} \delta_{lm} \delta_{kn}) \\ &= \frac{1}{4} C \cdot 2 (Q_{ij} Q_{ji}) \cdot (Q_{nm} + Q_{nm}) \\ &= C Q_{mn} (Q_{ij} Q_{ji})\end{aligned}$$

We may explicitly calculate the matrices corresponding to these contractions later. Now we calculate the isotropic elastic term. Note that Q is a function of S and φ , and we would like to write the spatial derivatives in terms of those two parameters.

$$\begin{aligned}L \partial_k^2 Q_{ij} &= L \partial_k \left[\frac{\partial S}{\partial x_k} \frac{\partial Q_{ij}}{\partial S} + \frac{\partial \varphi}{\partial x_k} \frac{\partial Q_{ij}}{\partial \varphi} \right] \\ &= L \left[\frac{\partial^2 S}{\partial x_k^2} \frac{\partial Q_{ij}}{\partial S} + \frac{\partial S}{\partial x_k} \frac{\partial}{\partial x_k} \left(\frac{\partial Q_{ij}}{\partial S} \right) + \frac{\partial^2 \varphi}{\partial x_k^2} \frac{\partial Q_{ij}}{\partial \varphi} + \frac{\partial \varphi}{\partial x_k} \frac{\partial}{\partial x_k} \left(\frac{\partial Q_{ij}}{\partial \varphi} \right) \right] \\ &= L \left[\frac{\partial^2 S}{\partial x_k^2} \frac{\partial Q_{ij}}{\partial S} + \frac{\partial^2 \varphi}{\partial x_k^2} \frac{\partial Q_{ij}}{\partial \varphi} + \frac{\partial S}{\partial x_k} \left(\frac{\partial S}{\partial x_k} \frac{\partial^2 Q_{ij}}{\partial S^2} + \frac{\partial \varphi}{\partial x_k} \frac{\partial^2 Q_{ij}}{\partial \varphi \partial S} \right) + \frac{\partial \varphi}{\partial x_k} \left(\frac{\partial \varphi}{\partial x_k} \frac{\partial^2 Q_{ij}}{\partial \varphi^2} + \frac{\partial S}{\partial x_k} \frac{\partial^2 Q_{ij}}{\partial S \partial \varphi} \right) \right] \\ &= L \left[\frac{\partial^2 S}{\partial x_k^2} \frac{\partial Q_{ij}}{\partial S} + \frac{\partial^2 \varphi}{\partial x_k^2} \frac{\partial Q_{ij}}{\partial \varphi} + 2 \frac{\partial S}{\partial x_k} \frac{\partial \varphi}{\partial x_k} \frac{\partial^2 Q_{ij}}{\partial S \partial \varphi} + \left(\frac{\partial S}{\partial x_k} \right)^2 \frac{\partial^2 Q_{ij}}{\partial S^2} + \left(\frac{\partial \varphi}{\partial x_k} \right)^2 \frac{\partial^2 Q_{ij}}{\partial \varphi^2} \right]\end{aligned}$$

Thus, the total homogeneous and elastic force reads:

$$\begin{aligned}h_{ij}^{he} &= L \left[\frac{\partial^2 S}{\partial x_k^2} \frac{\partial Q_{ij}}{\partial S} + \frac{\partial^2 \varphi}{\partial x_k^2} \frac{\partial Q_{ij}}{\partial \varphi} + 2 \frac{\partial S}{\partial x_k} \frac{\partial \varphi}{\partial x_k} \frac{\partial^2 Q_{ij}}{\partial S \partial \varphi} + \left(\frac{\partial S}{\partial x_k} \right)^2 \frac{\partial^2 Q_{ij}}{\partial S^2} + \left(\frac{\partial \varphi}{\partial x_k} \right)^2 \frac{\partial^2 Q_{ij}}{\partial \varphi^2} \right] \\ &\quad - A Q_{mn} - B Q_{ni} Q_{im} - C Q_{mn} (Q_{ij} Q_{ji})\end{aligned}$$

Computing viscous force in terms of S , ϕ and ψ_i

Alrighty then, now we need the viscous force on the liquid crystals. From Svnsek and Zumer, the viscous force is given by:

$$-h_{ij}^v = \frac{1}{2} \mu_2 A_{ij} + \mu_1 N_{ij}$$

with

$$N_{ij} = \frac{dQ_{ij}}{dt} + W_{ik} Q_{kj} - Q_{ik} W_{kj}$$

and

$$\frac{dQ_{ij}}{dt} = \frac{\partial Q_{ij}}{\partial t} + (v \cdot \nabla) Q_{ij}$$

The second two terms in the expression for N_{ij} are quadratic in v_i and Q_{ij} so we may drop them, and $(v \cdot \nabla) Q_{ij}$ is clearly quadratic. Hence, we make the approximation

$$N_{ij} \approx \frac{\partial Q_{ij}}{\partial t}$$

We also have the definition

$$A_{ij} = (\partial_i v_j + \partial_j v_i)$$

Note that we want to restrict our analysis to an incompressible fluid, so we must have the restriction that

$$\partial_i v_i = 0$$

It turns out that, on any simply-connected domain (I think we will be using a square here so we're good), one may express such a vector field as the curl of another vector field. Hence we define ψ_k by

$$v_i = \epsilon_{ijk} \partial_j \psi_k$$

Hence, we may plug this into our expression for A_{ij} to get

$$\begin{aligned} A_{ij} &= (\partial_i v_j + \partial_j v_i) \\ &= \partial_i \epsilon_{jkl} \partial_k \psi_l + \partial_j \epsilon_{ikl} \partial_k \psi_l \\ &= (\epsilon_{ikl} \partial_j + \epsilon_{jkl} \partial_i) \partial_k \psi_l \end{aligned}$$

And then for N_{ij} we have

$$\begin{aligned} N_{ij} &\approx \frac{\partial Q_{ij}}{\partial t} \\ &= \frac{\partial S}{\partial t} \frac{\partial Q_{ij}}{\partial S} + \frac{\partial \varphi}{\partial t} \frac{\partial Q_{ij}}{\partial \varphi} \end{aligned}$$

Then the expression for the complete viscous force is

$$-h_{ij}^v = \frac{1}{2} \mu_2 (\epsilon_{ikl} \partial_j + \epsilon_{jkl} \partial_i) \partial_k \psi_l + \mu_1 \frac{\partial S}{\partial t} \frac{\partial Q_{ij}}{\partial S} + \frac{\partial \varphi}{\partial t} \frac{\partial Q_{ij}}{\partial \varphi}$$

One equation of motion is then given by

$$h_{ij}^{he} + h_{ij}^v = 0$$

Computing the elastic stress tensor explicitly

The elastic stress tensor is obtained via

$$\sigma_{ij}^e = - \frac{\partial f}{\partial (\partial_i Q_{kl})} \partial_j Q_{kl}$$

Note that only the elastic part of the free energy make references to derivatives:

$$\begin{aligned} \frac{\partial f}{\partial (\partial_i Q_{kl})} &= \frac{\partial}{\partial (\partial_i Q_{kl})} \frac{1}{2} L \partial_j Q_{mn} \partial_j Q_{mn} \\ &= \frac{1}{2} L (\delta_{ij} \delta_{km} \delta_{ln} \partial_j Q_{mn} + \partial_j Q_{mn} \delta_{ij} \delta_{km} \delta_{ln}) \\ &= \frac{1}{2} L (\partial_i Q_{kl} + \partial_i Q_{kl}) \\ &= L \partial_i Q_{kl} \end{aligned}$$

Then the elastic stress tensor is given by

$$\sigma_{ij}^e = -L \partial_i Q_{kl} \partial_j Q_{kl}$$

Using the chain rule to find this as a function of S and φ

$$\begin{aligned} \sigma_{ij}^e &= -L \left(\frac{\partial S}{\partial x_i} \frac{\partial Q_{kl}}{\partial S} + \frac{\partial \varphi}{\partial x_i} \frac{\partial Q_{kl}}{\partial \varphi} \right) \left(\frac{\partial S}{\partial x_j} \frac{\partial Q_{kl}}{\partial S} + \frac{\partial \varphi}{\partial x_j} \frac{\partial Q_{kl}}{\partial \varphi} \right) \\ &= -L \left[\left(\frac{\partial Q_{kl}}{\partial S} \right)^2 \frac{\partial S}{\partial x_i} \frac{\partial S}{\partial x_j} + \left(\frac{\partial Q_{kl}}{\partial \varphi} \right)^2 \frac{\partial \varphi}{\partial x_i} \frac{\partial \varphi}{\partial x_j} + \frac{\partial Q_{kl}}{\partial S} \frac{\partial Q_{kl}}{\partial \varphi} \left(\frac{\partial S}{\partial x_i} \frac{\partial \varphi}{\partial x_j} + \frac{\partial S}{\partial x_j} \frac{\partial \varphi}{\partial x_i} \right) \right] \end{aligned}$$

Computing viscous stress tensor explicitly

The viscous stress tensor is given by

$$\sigma_{ij}^v = \beta_1 Q_{ij} Q_{kl} A_{kl} + \beta_4 A_{ij} + \beta_5 Q_{ik} A_{kj} + \frac{1}{2} \mu_2 N_{ij} - \mu_1 Q_{ik} N_{kj} + \mu_1 Q_{jk} N_{ki}$$

However, only the β_4 and μ_2 are linear in Q_{ij} and v_i . Hence, this simplifies to

$$\sigma_{ij}^v \approx \beta_4 A_{ij} + \frac{1}{2} \mu_2 N_{ij}$$

Again, plugging in for A_{ij} and N_{ij} as we did for the viscous force, we get

$$\sigma_{ij}^v \approx \beta_4 (\epsilon_{ikl} \partial_j + \epsilon_{jkl} \partial_i) \partial_k \psi_l + \frac{1}{2} \mu_2 \left(\frac{\partial S}{\partial t} \frac{\partial Q_{ij}}{\partial S} + \frac{\partial \varphi}{\partial t} \frac{\partial Q_{ij}}{\partial \varphi} \right)$$

Computing the fluid equation of motion

The equation of motion for the fluid is given by

$$\rho \frac{\partial v_i}{\partial t} = -\partial_i p + \partial_j (\sigma_{ji}^v + \sigma_{ji}^e)$$

We've made the assumption that $\partial v_i / \partial t \approx 0$. Additionally, we would like to get rid of the pressure term. For this, we take the curl of the whole expression to yield:

$$0 = -\epsilon_{ijk} \partial_j \partial_k p + \epsilon_{ijk} \partial_j \partial_l (\sigma_{lk}^v + \sigma_{lk}^e)$$

The first term is zero by antisymmetry of the Levi-Civita tensor and commutativity of partial derivatives. Hence, we're left with

$$\epsilon_{ijk} \partial_j \partial_l (\sigma_{lk}^v + \sigma_{lk}^e) = 0$$

Here things get a little out of hand, just because we end up with a ton of derivatives. In any case, we continue to calculate term by term:

$$\partial_l \sigma_{lk}^e = -L \partial_l \left[\frac{\partial Q_{mn}}{\partial S} \frac{\partial Q_{mn}}{\partial S} \frac{\partial S}{\partial x_l} \frac{\partial S}{\partial x_k} + \frac{\partial Q_{mn}}{\partial \varphi} \frac{\partial Q_{mn}}{\partial \varphi} \frac{\partial \varphi}{\partial x_l} \frac{\partial \varphi}{\partial x_k} + \frac{\partial Q_{mn}}{\partial S} \frac{\partial Q_{mn}}{\partial \varphi} \left(\frac{\partial S}{\partial x_l} \frac{\partial \varphi}{\partial x_k} + \frac{\partial S}{\partial x_k} \frac{\partial \varphi}{\partial x_l} \right) \right]$$

First term first:

$$\begin{aligned} \partial_l \left(\frac{\partial Q_{mn}}{\partial S} \frac{\partial Q_{mn}}{\partial S} \frac{\partial S}{\partial x_l} \frac{\partial S}{\partial x_k} \right) &= \left(\frac{\partial S}{\partial x_l} \frac{\partial^2 Q_{mn}}{\partial S^2} + \frac{\partial \varphi}{\partial x_l} \frac{\partial^2 Q_{mn}}{\partial \varphi \partial S} \right) \frac{\partial Q_{mn}}{\partial S} \frac{\partial S}{\partial x_l} \frac{\partial S}{\partial x_k} \\ &\quad + \frac{\partial Q_{mn}}{\partial S} \left(\frac{\partial S}{\partial x_l} \frac{\partial^2 Q_{mn}}{\partial S^2} + \frac{\partial \varphi}{\partial x_l} \frac{\partial^2 Q_{mn}}{\partial \varphi \partial S} \right) \frac{\partial S}{\partial x_l} \frac{\partial S}{\partial x_k} \\ &\quad + \frac{\partial Q_{mn}}{\partial S} \frac{\partial Q_{mn}}{\partial S} \left(\frac{\partial^2 S}{\partial x_l^2} \right) \frac{\partial S}{\partial x_k} \\ &\quad + \frac{\partial Q_{mn}}{\partial S} \frac{\partial Q_{mn}}{\partial S} \frac{\partial S}{\partial x_l} \left(\frac{\partial^2 S}{\partial x_l \partial x_k} \right) \\ &= 2 \left(\frac{\partial S}{\partial x_l} \frac{\partial^2 Q_{mn}}{\partial S^2} + \frac{\partial \varphi}{\partial x_l} \frac{\partial^2 Q_{mn}}{\partial \varphi \partial S} \right) \frac{\partial Q_{mn}}{\partial S} \frac{\partial S}{\partial x_l} \frac{\partial S}{\partial x_k} \\ &\quad + \frac{\partial Q_{mn}}{\partial S} \frac{\partial Q_{mn}}{\partial S} \left(\frac{\partial^2 S}{\partial x_l^2} \frac{\partial S}{\partial x_k} + \frac{\partial S}{\partial x_l} \frac{\partial^2 S}{\partial x_l \partial x_k} \right) \end{aligned}$$

Now for the x_j derivative (one term at a time):

$$\begin{aligned} \partial_k 2 \frac{\partial^2 Q_{mn}}{\partial \varphi \partial S} \frac{\partial Q_{mn}}{\partial S} \frac{\partial S}{\partial x_l} \frac{\partial S}{\partial x_k} \frac{\partial \varphi}{\partial x_l} &= 2 \left(\frac{\partial S}{\partial x_k} \frac{\partial^3 Q_{mn}}{\partial \varphi \partial S^2} + \frac{\partial \varphi}{\partial x_k} \frac{\partial^3 Q_{mn}}{\partial S \partial \varphi^2} \right) \frac{\partial Q_{mn}}{\partial S} \frac{\partial S}{\partial x_l} \frac{\partial S}{\partial x_k} \frac{\partial \varphi}{\partial x_l} \\ &+ 2 \frac{\partial^2 Q_{mn}}{\partial \varphi \partial S} \left(\frac{\partial S}{\partial x_k} \frac{\partial^2 Q_{mn}}{\partial} \right) \end{aligned}$$