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:

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

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

From Svensek 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:

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

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

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

And the final term gives:

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

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:

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

Computing viscous force in terms of S, ϕ and ψ_i

Alrighty then, now we need the viscous force on the liquid crystals. From Svensek 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

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

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

$$\sigma^v_{ij} \approx \beta_4 A_{ij} + \frac{1}{2}\mu_2 N_{ij}$$

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

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

Computing the fluid equation of motion

The equation of motion for the fluid is given by

$$\rho \frac{\partial v_i}{\partial t} = -\partial_i p + \partial_j(\sigma^v_{ji} + \sigma^e_{ji})$$

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:

$$0 = -\epsilon_{ijk}\partial_j\partial_k p + \epsilon_{ijk}\partial_j\partial_l(\sigma^v_{lk} + \sigma^e_{lk})$$

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

$$\epsilon_{ijk}\partial_j\partial_l(\sigma^v_{lk} + \sigma^e_{lk}) = 0$$

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:

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

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):

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