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. 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. Additionally, we assume no acceleration so that $\partial v_i / \partial t = 0$ always. We give an initial director field configuration of $\mathbf{n} = (\cos\phi, \sin\phi, 0)$ for some φ (to be specified) so that the Q-tensor, given by $Q_{ij} = S/2(3n_i n_j - \delta_{ij})$ takes the form:

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

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

Computing homoegenous and elastic generalized force

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

$$f = \phi(Q) + \frac{1}{2}L\partial_i Q_{jk}\partial_i Q_{jk} \tag{3}$$

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

$$h_{ij}^{he} = L\partial_k^2 Q_{ij} - \frac{\partial\phi}{\partial Q_{ij}} + \lambda\delta_{ij} + \lambda_k\epsilon_{kij} \tag{4}$$

where ϕ is the Landau de Gennes bulk free energy:

$$\phi(Q) = \frac{1}{2}AQ_{ij}Q_{ji} + \frac{1}{3}BQ_{ij}Q_{jk}Q_{ki} + \frac{1}{4}C(Q_{ij}Q_{ji})^2 \tag{5}$$

We begin by explicitly calculating the second term in terms of Q_{ij}, one term at a time in ϕ:

$$\begin{aligned} \frac{\partial}{\partial Q_{mn}}\left(\frac{1}{2}AQ_{ij}Q_{ji}\right) &= \frac{1}{2}A\left(\delta_{im}\delta_{jn}Q_{ji} + Q_{ij}\delta_{jm}\delta_{in}\right) \\ &= \frac{1}{2}A(Q_{nm} + Q_{nm}) \\ &= AQ_{mn} \end{aligned} \tag{6}$$

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

$$\begin{aligned}
\frac{\partial}{\partial Q_{mn}}\left(\frac{1}{3}BQ_{ij}Q_{jk}Q_{ki}\right) &= \frac{1}{3}B(\delta_{im}\delta_{jn}Q_{jk}Q_{ki} + Q_{ij}\delta_{jm}\delta_{kn}Q_{ki} + Q_{ij}Q_{jk}\delta_{mk}\delta_{ni}) \\
&= \frac{1}{3}B(Q_{nk}Q_{km} + Q_{im}Q_{ni} + Q_{nj}Q_{jm}) \\
&= BQ_{ni}Q_{im}
\end{aligned} \tag{7}$$

And the final term gives:

$$\begin{aligned}
\frac{\partial}{\partial Q_{mn}}\left(\frac{1}{4}C(Q_{ij}Q_{ji})^2\right) &= \frac{1}{4}C\cdot 2(Q_{ij}Q_{ji})\frac{\partial(Q_{kl}Q_{lk})}{\partial Q_{mn}} \\
&= \frac{1}{4}C\cdot 2(Q_{ij}Q_{ji})\cdot(\delta_{mk}\delta_{nl}Q_{lk} + Q_{kl}\delta_{lm}\delta_{kn}) \\
&= \frac{1}{4}C\cdot 2(Q_{ij}Q_{ji})\cdot(Q_{nm} + Q_{nm}) \\
&= CQ_{mn}(Q_{ij}Q_{ji})
\end{aligned} \tag{8}$$

Thus, the total homogeneous and elastic force reads:

$$h_{ij}^{he} = L\partial^2 Q_{ij} - AQ_{mn} - BQ_{ni}Q_{im} - CQ_{mn}(Q_{ij}Q_{ji}) + \lambda\delta_{ij} + \lambda_k\epsilon_{kij} \tag{9}$$

Computing viscous force explicitly

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

$$-h_{ij}^{v} = \frac{1}{2}\mu_2 A_{ij} + \mu_1 N_{ij} \tag{10}$$

with

$$N_{ij} = \frac{dQ_{ij}}{dt} + W_{ik}Q_{kj} - Q_{ik}W_{kj} \tag{11}$$

and

$$\frac{dQ_{ij}}{dt} = \frac{\partial Q_{ij}}{\partial t} + (v\cdot\nabla)Q_{ij} \tag{12}$$

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

$$N_{ij} \approx \frac{\partial Q_{ij}}{\partial t} \tag{13}$$

We also have the definition

$$A_{ij} = (\partial_i v_j + \partial_j v_i) \tag{14}$$

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

$$\partial_i v_i = 0 \tag{15}$$

Then the expression for the complete viscous force is

$$-h_{ij}^{v} = \frac{1}{2}\mu_2(\partial_i v_j + \partial_j v_i) + \mu_1\frac{\partial Q_{ij}}{\partial t} \tag{16}$$

One equation of motion is then given by

$$h_{ij}^{he} + h_{ij}^{v} = 0 \tag{17}$$

or explicitly

$$\mu_1\frac{\partial Q_{ij}}{\partial t} = L\partial^2 Q_{ij} - AQ_{mn} - BQ_{ni}Q_{im} - CQ_{mn}(Q_{ij}Q_{ji}) + \lambda\delta_{ij} + \lambda_k\epsilon_{kij} - \frac{1}{2}\mu_2(\partial_i v_j + \partial_j v_i) \tag{18}$$

Using this, we may update Q_{ij} in time by solving for $\partial Q_{ij}/\partial t$ in terms of Q_{ij} and v_i from the previous iteration.

Computing the elastic stress tensor explicitly

The elastic stress tensor is obtained via

$$\sigma^e_{ij} = -\frac{\partial f}{\partial(\partial_i Q_{kl})}\partial_j Q_{kl} \tag{19}$$

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

$$\begin{aligned}\frac{\partial f}{\partial(\partial_i Q_{kl})} &= \frac{\partial}{\partial(\partial_i Q_{kl})}\frac{1}{2}L\partial_j Q_{mn}\partial_j Q_{mn} \\ &= \frac{1}{2}L(\delta_{ij}\delta_{km}\delta_{ln}\partial_j Q_{mn} + \partial_j Q_{mn}\delta_{ij}\delta_{km}\delta_{ln}) \\ &= \frac{1}{2}L(\partial_i Q_{kl} + \partial_i Q_{kl}) \\ &= L\partial_i Q_{kl}\end{aligned} \tag{20}$$

Then the elastic stress tensor is given by

$$\sigma^e_{ij} = -L\partial_i Q_{kl}\partial_j Q_{kl} \tag{21}$$

Computing viscous stress tensor explicitly

The viscous stress tensor is given by

$$\sigma^v_{ij} = \beta_1 Q_{ij}Q_{kl}A_{kl} + \beta_4 A_{ij} + \beta_5 Q_{ik}A_{ki} + \frac{1}{2}\mu_2 N_{ij} - \mu_1 Q_{ik}N_{kj} + \mu_1 Q_{jk}N_{ki} \tag{22}$$

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

$$\sigma^v_{ij} \approx \beta_4 A_{ij} + \frac{1}{2}\mu_2 N_{ij} \tag{23}$$

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

$$\sigma^v_{ij} \approx \beta_4(\partial_i v_j + \partial_j v_i) + \frac{1}{2}\mu_2\frac{\partial Q_{ij}}{\partial t} \tag{24}$$

Computing the fluid equation of motion

The equation of motion for the fluid is given by

$$\rho\frac{\partial v_i}{\partial t} = -\partial_i p + \partial_j(\sigma^v_{ji} + \sigma^e_{ji}) \tag{25}$$

We've made the assumption that $\partial v_i/\partial t \approx 0$. Plugging in for σ^v_{ji} and σ^e_{ji} yields

$$\begin{aligned}0 &= -\partial_i p + \partial_j\left(-L\partial_j Q_{kl}\partial_i Q_{kl} + \beta_4(\partial_j v_i + \partial_i v_j) + \frac{1}{2}\mu_2\frac{\partial Q_{ji}}{\partial t}\right) \\ &= -\partial_i p - L\left[(\partial^2 Q_{kl})\partial_i Q_{kl} + (\partial_j Q_{kl})\partial_j\partial_i Q_{kl}\right] + \beta_4(\partial^2 v_i + \partial_j\partial_i v_j) + \frac{1}{2}\mu_2\partial_j\frac{\partial Q_{ji}}{\partial t} \\ &= -\partial_i p - L\left[(\partial^2 Q_{kl})\partial_i Q_{kl} + (\partial_j Q_{kl})\partial_j\partial_i Q_{kl}\right] + \beta_4\partial^2 v_i + \frac{1}{2}\mu_2\partial_j\frac{\partial Q_{ji}}{\partial t}\end{aligned} \tag{26}$$

where in the last step we have used the condition that $\partial_j v_j = 0$.