LC Flow Velocity Eqs

Lucas Myers

August 31, 2020

1 Elastic generalized force

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

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

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

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

where ϕ is the Landau de Gennes bulk free energy:

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

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

$$\frac{\partial}{\partial Q_{mn}} \left(\frac{1}{2} A Q_{ij} Q_{ji} \right) = \frac{1}{2} A \left(\delta_{im} \delta_{jn} Q_{ji} + Q_{ij} \delta_{jm} \delta_{in} \right)
= \frac{1}{2} A (Q_{nm} + Q_{nm})
= A Q_{mn}$$
(4)

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

$$\frac{\partial}{\partial Q_{mn}} \left(\frac{1}{3} B Q_{ij} Q_{jk} Q_{ki} \right) = \frac{1}{3} B \left(\delta_{im} \delta_{jn} Q_{jk} Q_{ki} + Q_{ij} \delta_{jm} \delta_{kn} Q_{ki} + Q_{ij} Q_{jk} \delta_{mk} \delta_{ni} \right)
= \frac{1}{3} B \left(Q_{nk} Q_{km} + Q_{im} Q_{ni} + Q_{nj} Q_{jm} \right)
= B Q_{ni} Q_{im}$$
(5)

And the final term gives:

$$\frac{\partial}{\partial Q_{mn}} \left(\frac{1}{4} C (Q_{ij} Q_{ji})^2 \right) = \frac{1}{4} C \cdot 2 (Q_{ij} Q_{ji}) \frac{\partial (Q_{kl} Q_{lk})}{\partial Q_{mn}}$$

$$= \frac{1}{4} C \cdot 2 (Q_{ij} Q_{ji}) \cdot (\delta_{mk} \delta_{nl} Q_{lk} + Q_{kl} \delta_{lm} \delta_{kn})$$

$$= \frac{1}{4} C \cdot 2 (Q_{ij} Q_{ji}) \cdot (Q_{nm} + Q_{nm})$$

$$= C Q_{mn} (Q_{ij} Q_{ji})$$
(6)

Thus, the total homogeneous and elastic force reads:

$$h_{ij}^{he} = L\partial^2 Q_{ij} - AQ_{ij} - BQ_{ik}Q_{kj} - CQ_{ij}(Q_{kl}Q_{lk}) + \lambda \delta_{ij} + \lambda_k \epsilon_{kij}$$
(7)

2 Viscous generalized force

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

$$-h_{ij}^{v} = \frac{1}{2}\mu_2 A_{ij} + \mu_1 N_{ij} \tag{8}$$

with

$$N_{ij} = \frac{dQ_{ij}}{dt} + W_{ik}Q_{kj} - Q_{ik}W_{kj} \tag{9}$$

and

$$\frac{dQ_{ij}}{dt} = \frac{\partial Q_{ij}}{\partial t} + (v \cdot \nabla)Q_{ij} \tag{10}$$

where

$$W_{ij} = \frac{1}{2} \left(\partial_i v_j - \partial_j v_i \right) \tag{11}$$

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

$$N_{ij} \approx \frac{\partial Q_{ij}}{\partial t} \tag{12}$$

We also have the definition

$$A_{ij} = (\partial_i v_j + \partial_j v_i) \tag{13}$$

Plugging this into the viscous force yields:

$$-h_{ij}^{v} = \frac{1}{2}\mu_2(\partial_i v_j + \partial_j v_i) + \mu_1 \frac{\partial Q_{ij}}{\partial t}$$
(14)

Balancing the forces gives the equation:

$$h_{ij}^e = -h_{ij}^v \tag{15}$$

Which yields:

$$\mu_1 \frac{\partial Q_{ij}}{\partial t} = L \partial^2 Q_{ij} - AQ_{ij} - BQ_{ik}Q_{kj} - CQ_{ij} \left(Q_{kl}Q_{lk} \right) - \frac{1}{2}\mu_2 \left(\partial_i v_j + \partial_j v_i \right) \tag{16}$$

(here we have dropped the Lagrange multipliers because we are going to explicitly ensure that Q_{ij} is traceless and symmetric).

3 Elastic stress tensor

The elastic stress tensor is obtained via

$$\sigma_{ij}^e = -\frac{\partial f}{\partial(\partial_i Q_{kl})} \partial_j Q_{kl} \tag{17}$$

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

$$\frac{\partial f}{\partial(\partial_{i}Q_{kl})} = \frac{\partial}{\partial(\partial_{i}Q_{kl})} \frac{1}{2} L \partial_{j} Q_{mn} \partial_{j} Q_{mn}
= \frac{1}{2} L (\delta_{ij}\delta_{km}\delta_{ln}\partial_{j}Q_{mn} + \partial_{j}Q_{mn}\delta_{ij}\delta_{km}\delta_{ln})
= \frac{1}{2} L (\partial_{i}Q_{kl} + \partial_{i}Q_{kl})
= L \partial_{i}Q_{kl}$$
(18)

Then the elastic stress tensor is given by

$$\sigma_{ij}^e = -L\partial_i Q_{kl}\partial_j Q_{kl} \tag{19}$$

4 Viscous stress tensor

The viscous stress tensor is given by

$$\sigma_{ij}^{v} = \beta_1 Q_{ij} Q_{kl} A_{kl} + \beta_4 A_{ij} + \beta_5 Q_{ik} A_{ki} + \frac{1}{2} \mu_2 N_{ij} - \mu_1 Q_{ik} N_{kj} + \mu_1 Q_{jk} N_{ki}$$
 (20)

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

$$\sigma_{ij}^v \approx \beta_4 A_{ij} + \frac{1}{2} \mu_2 N_{ij} \tag{21}$$

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

$$\sigma_{ij}^{v} \approx \beta_4 (\partial_i v_j + \partial_j v_i) + \frac{1}{2} \mu_2 \frac{\partial Q_{ij}}{\partial t}$$
 (22)

Plugging in for the time evolution of Q_{ij} gives:

$$\sigma_{ij}^{v} \approx \beta_4 \left(\partial_i v_j + \partial_j v_i\right) + \frac{1}{2} \frac{\mu_2}{\mu_1} \left[L \partial^2 Q_{ij} - A Q_{ij} - B Q_{ik} Q_{kj} - C Q_{ij} \left(Q_{kl} Q_{lk}\right) - \frac{1}{2} \mu_2 \left(\partial_i v_j + \partial_j v_i\right) \right]$$
(23)

5 Fluid equation of motion

The equation of motion for the fluid is given by

$$\rho \frac{\partial v_i}{\partial t} = -\partial_i p + \partial_j (\sigma^v_{ji} + \sigma^e_{ji}) \tag{24}$$

We can make the assumption that $\partial v_i/\partial t \approx 0$. Using this and plugging in for σ_{ji}^v and σ_{ji}^e , we get:

$$\partial_{i}p = \left(\beta_{4} - \frac{1}{4}\frac{\mu_{2}^{2}}{\mu_{1}}\right)\left(\partial_{i}\partial_{j}v_{j} + \partial^{2}v_{i}\right) + \frac{1}{2}\frac{\mu_{2}}{\mu_{1}}\left[L\partial^{2}\partial_{j}Q_{ij} - A\partial_{j}Q_{ij} - B\partial_{j}\left(Q_{ik}Q_{kj}\right) - C\partial_{j}\left[Q_{ij}\left(Q_{kl}Q_{lk}\right)\right]\right] - L\partial_{j}\left(\partial_{i}Q_{kl}\partial_{j}Q_{kl}\right) \quad (25)$$

Note that, by incompressibility, $\partial_i v_i = 0$ so a term in parentheses goes away. Now define:

$$f_{\mu_2,i}(Q) = L\partial^2\partial_j Q_{ij} - A\partial_j Q_{ij} - B\partial_j \left(Q_{ik} Q_{kj} \right) - C\partial_j \left[Q_{ij} \left(Q_{kl} Q_{lk} \right) \right]$$
 (26)

$$f_{L,i}(Q) = \partial_j \left(\partial_i Q_{kl} \partial_j Q_{kl} \right) \tag{27}$$

$$f_i(Q) = -\frac{1}{2} \frac{\mu_2}{\mu_1} f_{\mu_2,i}(Q) + L f_{L,i}(Q)$$
(28)

$$\alpha = \left(\beta_4 - \frac{1}{4} \frac{\mu_2^2}{\mu_1}\right)^{-1} \tag{29}$$

Then the fluid equation of motion becomes:

$$\partial^2 v_i = \alpha \left(\partial_i p + f_i \right) \tag{30}$$

6 Choosing a specific Q_{ij}

Now, we would like to choose f_i to be something which is just a sum of sines. These terminate at the endpoints, so it happens that we will fulfill our no slip condition ($v_i = 0$ at the boundary). Since we need to actually choose Q_{ij} to do that (so that we can use the same scenario for the stream function formulation), we will have to just guess and check. Note that many of the terms involved in f_i have third derivatives, so we will want to choose a cos to be the important term. Recall that, in the uniaxial case:

$$Q_{ij} = \frac{S}{2} \left(3n_i n_j - \delta_{ij} \right) \tag{31}$$

Choose S to be constant. Plugging Q_{ij} into the expression for $f_{\mu_2,i}$ yields:

$$f_{\mu_{2},i}(Q) = \frac{3S}{2}L\partial^{2}\partial_{j}(n_{i}n_{j}) - \frac{3S}{2}A\partial_{j}(n_{i}n_{j}) - \frac{S^{2}}{4}B\partial_{j}(3n_{i}n_{k} - \delta_{ik})(3n_{k}n_{j} - \delta_{kj}) - \frac{S^{3}}{8}C\partial_{j}\left[(3n_{i}n_{j} - \delta_{ij})(3n_{k}n_{l} - \delta_{kl})(3n_{l}n_{k} - \delta_{lk})\right]$$
(32)

This simplifies to:

$$f_{\mu_{2},i}(Q) = \frac{3S}{2}L\partial^{2}\partial_{j}(n_{i}n_{j}) - \frac{3S}{2}A\partial_{j}(n_{i}n_{j}) - \frac{3S^{2}}{2}B\partial_{j}(n_{i}n_{j}) - \frac{9S^{3}}{4}C\partial_{j}(n_{i}n_{j})$$

$$= \frac{3S}{2}\left(L\partial^{2} - A - SB - \frac{3S^{2}}{2}C\right)\partial_{j}(n_{i}n_{j})$$
(33)

Do the same for $f_{L,i}$ to get:

$$f_{L,i}(Q) = \frac{9S^2}{4} \partial_j \left[\partial_i \left(n_k n_l \right) \partial_j \left(n_l n_k \right) \right]$$
(34)

Our first guess will be:

$$\hat{n} = (\cos k_x x, \sin k_x x, 0) \tag{35}$$

Note that this expression is independent of y so that any y-derivatives will be zero by default. We will do pieces at a time:

$$\partial_{j} (n_{x} n_{j}) = \partial_{x} \cos^{2} k_{x} x$$

$$= 2 \cos k_{x} x (-k_{x} \sin k_{x} x)$$

$$= -k_{x} \sin (2k_{x} x)$$
(36)

Great, this still terminates at the endpoints. Now taking the Laplacian of this:

$$\partial^{2} \partial_{j} (n_{x} n_{j}) = \partial_{x}^{2} (-k_{x} \sin(2k_{x}x))$$

$$= -4k_{x}^{2} \partial_{x} \cos(2k_{x}x)$$

$$= 8k_{x}^{3} \sin(2k_{x}x)$$
(37)

Cool, this also terminates at the endpoints. So far so good. Let's look at the y-component:

$$\partial_{j} (n_{y} n_{j}) = \partial_{x} (\cos k_{x} x \sin k_{x} x)$$

$$= \partial_{x} \frac{1}{2} \sin 2k_{x} x$$

$$= -k_{x} \cos 2k_{x} x$$
(38)

This certainly does not go to zero at the endpoints, so we have not met our no-slip condition. Dang. Now for the last term:

$$\partial_{j} \left[\partial_{x} \left(n_{k} n_{l} \right) \partial_{j} \left(n_{l} n_{k} \right) \right] = \partial_{x} \left[\left(\partial_{x} \cos^{2} k_{x} x \right)^{2} + \left(\partial_{x} \cos k_{x} x \sin k_{x} x \right)^{2} + \left(\partial_{x} \cos k_{x} x \sin k_{x} x \right)^{2} + \left(\partial_{x} \sin^{2} k_{x} x \right)^{2} \right]$$

$$= \partial_{x} \left[k_{x}^{2} \sin^{2} \left(2k_{x} x \right) + 2 \left(\partial_{x} \frac{1}{2} \sin 2k_{x} x \right)^{2} + k_{x}^{2} \sin^{2} \left(2k_{x} x \right) \right]$$

$$= \partial_{x} \left[2k_{x}^{2} \sin^{2} \left(2k_{x} x \right) + 2k_{x}^{2} \cos^{2} \left(2k_{x} x \right) \right]$$

$$= 0$$

$$(39)$$

Well this is not actually helpful to understanding why the elastic piece is so small – here it is actually zero. However, we can check the rest of the configuration with this scheme. In this case, we get:

$$f_i(x,y) = -\frac{\mu_2}{\mu_1} \frac{3S}{4} \left[8k_x^3 L + \left(A + SB + \frac{3S^2}{2} C \right) k_x \right] \sin(2k_x x) \tag{40}$$

Clearly we have that for all $k_y \neq 0$, we have $\hat{f}_{i,k_xk_y} = 0$ (since there is no y-dependence). Additionally, the only nonzero Fourier term is for $k_x = 4\pi/L_x$, and is completely imaginary since only sine is involved. This comes out to be:

$$f_{x,4\pi/L_x,0} = -i\frac{\mu_2}{\mu_1} \frac{3S}{4} \left[8k_x^3 L + \left(A + SB + \frac{3S^2}{2}C \right) k_x \right]$$
 (41)

Now, we would like to choose f_i to be something which is just a sum of sines. These terminate at the endpoints, so we will fulfill our no slip condition ($v_i = 0$ at the boundaries) if we do that. Since we need to actually choose Q_{ij} to do that (so that we can use the same scenario for the stream function formulation), we will have to just guess and check. Note that many of the terms involved in f_i have third derivatives, so we will want to choose a cos to be the important term. Recall that:

$$Q_{ij} = \frac{S}{2} \left(3n_i n_j - \delta_{ij} \right) \tag{42}$$

Choose S to be constant. Plugging Q_{ij} into the expression for $f_{mu_2,i}$ yields:

$$f_{\mu_{2},i}(Q) = \frac{3S}{2}L\partial^{2}\partial_{j}(n_{i}n_{j}) - \frac{3S}{2}A\partial_{j}(n_{i}n_{j}) - \frac{S^{2}}{4}B\partial_{j}(3n_{i}n_{k} - \delta_{ik})(3n_{k}n_{j} - \delta_{kj}) - \frac{S^{3}}{8}C\partial_{j}\left[(3n_{i}n_{j} - \delta_{ij})(3n_{k}n_{l} - \delta_{kl})(3n_{l}n_{k} - \delta_{lk})\right]$$
(43)

This simplifies to:

$$f_{\mu_{2},i}(Q) = \frac{3S}{2}L\partial^{2}\partial_{j}(n_{i}n_{j}) - \frac{3S}{2}A\partial_{j}(n_{i}n_{j}) - \frac{3S^{2}}{2}B\partial_{j}(n_{i}n_{j}) - \frac{9S^{3}}{4}C\partial_{j}(n_{i}n_{j})$$

$$= \frac{3S}{2}\left(L\partial^{2} - A - SB - \frac{3S^{2}}{2}C\right)\partial_{j}(n_{i}n_{j})$$
(44)

Do the same for $f_{L,i}$ to get:

$$f_{L,i}(Q) = \frac{9S^2}{4} \partial_j \left[\partial_i \left(n_k n_l \right) \partial_j \left(n_l n_k \right) \right] \tag{45}$$

Our first guess will be:

$$\hat{n} = (\cos k_x x, \sin k_x x, 0) \tag{46}$$

Note that this expression is independent of y so that any y-derivatives will be zero by default. We will do pieces at a time:

$$\partial_{j} (n_{x} n_{j}) = \partial_{x} \cos^{2} k_{x} x$$

$$= 2 \cos k_{x} x (-k_{x} \sin k_{x} x)$$

$$= -k_{x} \sin (2k_{x} x)$$
(47)

Great, this still terminates at the endpoints. Now taking the Laplacian of this:

$$\partial^{2} \partial_{j} (n_{x} n_{j}) = \partial_{x}^{2} (-k_{x} \sin(2k_{x} x))$$

$$= -4k_{x}^{2} \partial_{x} \cos(2k_{x} x)$$

$$= 8k_{x}^{3} \sin(2k_{x} x)$$

$$(48)$$

Cool, this also terminates at the endpoints. So far so good. Now for the last term:

$$\partial_{j} \left[\partial_{x} \left(n_{k} n_{l} \right) \partial_{j} \left(n_{l} n_{k} \right) \right] = \partial_{x} \left[\left(\partial_{x} \cos^{2} k_{x} x \right)^{2} + \left(\partial_{x} \cos k_{x} x \sin k_{x} x \right)^{2} + \left(\partial_{x} \cos k_{x} x \sin k_{x} x \right)^{2} + \left(\partial_{x} \sin^{2} k_{x} x \right)^{2} \right]$$

$$= \partial_{x} \left[k_{x}^{2} \sin^{2} \left(2k_{x} x \right) + 2 \left(\partial_{x} \frac{1}{2} \sin 2k_{x} x \right)^{2} + k_{x}^{2} \sin^{2} \left(2k_{x} x \right) \right]$$

$$= \partial_{x} \left[2k_{x}^{2} \sin^{2} \left(2k_{x} x \right) + 2k_{x}^{2} \cos^{2} \left(2k_{x} x \right) \right]$$

$$= 0$$

$$(49)$$

Well this is not actually helpful to understanding why the elastic piece is so small – here it is actually zero. However, we can check the rest of the configuration with this scheme. In this case, we get:

$$f_i(x,y) = -\frac{\mu_2}{\mu_1} \frac{3S}{4} \left[8k_x^3 L + \left(A + SB + \frac{3S^2}{2} C \right) k_x \right] \sin(2k_x x)$$
 (50)

Clearly we have that for all $k_y \neq 0$, we have $\hat{f}_{i,k_xk_y} = 0$ (since there is no y-dependence). Additionally, the only nonzero Fourier term is for $k_x = 4\pi/L_x$, and is completely imaginary since only sine is involved. This comes out to be:

$$f_{x,4\pi/L_x,0} = -i\frac{\mu_2}{\mu_1} \frac{3S}{4} \left[8k_x^3 L + \left(A + SB + \frac{3S^2}{2}C \right) k_x \right]$$
 (51)

Note that we only have nonzero \hat{f} for i = x – we see this in previous calculations.