In this document, I derive (in a rather lengthy, but hopefully expository, way) the governing equations for an isothermal active viscous nematic fluid in the absence of external fields. I will consider only temperatures above the critical temperature for the isotropic-nematic transition. In this situation the director does not necessarily persist throughout space. We use the tensorial nematic order parameter,

$$Q_{\alpha\beta} = S(n_\alpha n_\beta - \frac{1}{3}\,\delta_{\alpha\beta}), \tag{0.1}$$

defined here for a uniaxial nematic liquid crystal. Note that I have used indicial notation, which I will throughout, in which like Greek indices (representing directions x, y, and z) are summed over. Latin indices are not summed over unless done so explicitly. See the appendix for useful relations for tensors and corresponding syntax for other notation.

Throughout the document, I make scant reference to any books and articles. Useful references, from which I pulled information are

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I begin with the derivation of a more familiar system, an isotropic viscous fluid in which chemical species may diffuse and undergo chemical reactions. This illustrates the method:

1) Write down the conservation laws for mass, linear momentum, and angular momentum.
2) Write down an expression for the entropy production rate.
3) Simplify the expression for the entropy production rate to enable identification of conjugate thermodynamic fluxes and forces.
4) Expand the thermodynamic fluxes to linear order in the forces, honoring the symmetries of the system and the Onsager reciprocal relations, to obtain the constitutive equations.

1 Illustrative example: diffusion in a viscous fluid

We consider here a multicomponent isotropic viscous fluid.

1.1 Mass conservation

Conservation of total mass is

$$\partial_t \, \rho = -\partial_\alpha \, \rho \, v_\alpha, \tag{1.1}$$

where $\rho = \sum_i \rho_i$, where ρ_i is the density of species i. Using the chain rule on the right hand side, this may alternatively be written as

$$(\partial_t + v_\alpha \partial_\alpha)\rho = -\rho \partial_\alpha v_\alpha, \tag{1.2}$$

where the left hand side is interpreted as the time derivative of the density of a fluid element in a co-moving frame. It is convenient to define the time derivative of the fluid element in the co-moving frame, the so-called *material derivative*,

$$\frac{\mathrm{d}}{\mathrm{d}t} \equiv \partial_t + v_\alpha \partial_\alpha. \tag{1.3}$$

We can also write down the mass conservation relation for species i as

$$\rho \frac{\mathrm{d}}{\mathrm{d}t} \frac{\rho_i}{\rho} = -\partial_\alpha j_{i,\alpha} + m_i \sum_k \nu_{ki} r_k \;\; \forall \, i \tag{1.4}$$

where $j_{i,\alpha}$ is the mass flux of species i with respect to the barycentric motion ($j_{i,\alpha} = \rho_i(v_{i,\alpha} - v_\alpha)$), m_i is its molar mass, and ν_{ki} is the stoichiometric coefficient of species i in chemical reaction k, which proceeds at rate r_k. Using (1.1), this can equivalently be written in terms of the mole fractions, n_i, of the components.

$$\partial_t \, n_i + \partial_\alpha n_i v_\alpha = \frac{\mathrm{d}n_i}{\mathrm{d}t} + n_i \partial_\alpha v_\alpha = -\partial_\alpha \, \frac{j_{i,\alpha}}{m_i} + \sum_k \nu_{ki} r_k \;\; \forall \, i. \tag{1.5}$$

The mass flux of the individual components satisfy

$$\sum_i j_{i,\alpha} = 0. \tag{1.6}$$

1.2 Linear momentum conservation

The statement of linear momentum conservation is

$$\partial_t(\rho v_\alpha) = -\partial_\beta \left[\sigma_{\alpha\beta} + \rho v_\alpha v_\beta\right], \tag{1.7}$$

where $\sigma_{\alpha\beta}$ is the total stress tensor and the bracketed term is the total momentum flux tensor. The left hand side is the rate of change of momentum and the right hand side is the sum forces acting on the fluid (the total momentum flux due to flow). In the co-moving frame, this is

$$\rho \frac{\mathrm{d}v_\alpha}{\mathrm{d}t} = \partial_\beta \sigma_{\alpha\beta}, \tag{1.8}$$

which is perhaps more transparent. It says that the rate of change of momentum in the co-moving frame is given by the forces acting on the fluid.

1.3 Angular momentum conservation

Henceforth, it is convenient to define a small fluid element occupying volume V. The shape of the fluid element may be distorted in time, but the total mass contained therein cannot[1]. The angular momentum of the fluid element is[2]

$$\int_V d^3\mathbf{x}\, \rho\epsilon_{\alpha\beta\gamma} x_\beta v_\gamma, \tag{1.9}$$

where $\epsilon_{\alpha\beta\gamma}$ is the Levi-Civita symbol. The time rate of change of angular momentum is given by the torque acting on the fluid element.

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V d^3\mathbf{x}\, \rho\epsilon_{\alpha\beta\gamma} x_\beta v_\gamma = \int dS_\delta\, \epsilon_{\alpha\beta\gamma}\, x_\beta\, \sigma_{\gamma\delta}, \tag{1.10}$$

where dS_α is a differential surface element with an outward pointing normal, and we have written the expression in the co-moving frame.

1.3.1 Left hand side of angular momentum balance (1.10)

We consider first the left hand side of (1.10). We cannot trivially differentiate under the integral sign, as V changes with time. We can, however, convert the integration over the volume with an integration over the total mass $m = \rho V$, which does not change with time, provided we are in the co-moving frame. Therefore, we can take the material derivative $(\partial_t + v_\alpha \partial_\alpha)$ under the integral sign, giving

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int_V d^3\mathbf{x}\, \rho\epsilon_{\alpha\beta\gamma} x_\beta v_\gamma &= \frac{\mathrm{d}}{\mathrm{d}t}\int dm\, \epsilon_{\alpha\beta\gamma} x_\beta v_\gamma = \int dm\, \epsilon_{\alpha\beta\gamma}\, \frac{\mathrm{d}}{\mathrm{d}t}\, x_\beta v_\gamma \\ &= \int_V d^3\mathbf{x}\, \rho\epsilon_{\alpha\beta\gamma}\, \frac{\mathrm{d}}{\mathrm{d}t}\, x_\beta v_\gamma = \int_V d^3\mathbf{x}\, \epsilon_{\alpha\beta\gamma} x_\beta \rho\, \frac{\mathrm{d}v_\gamma}{\mathrm{d}t} + \int_V d^3\mathbf{x}\, \rho\epsilon_{\alpha\beta\gamma} v_\gamma\, \frac{\mathrm{d}x_\beta}{\mathrm{d}t}.\end{aligned} \tag{1.11}$$

Using linear momentum conservation (1.8), the first integral becomes

$$\int_V d^3\mathbf{x}\, \epsilon_{\alpha\beta\gamma} x_\beta \rho\, \frac{\mathrm{d}v_\gamma}{\mathrm{d}t} = \int_V d^3\mathbf{x}\, \epsilon_{\alpha\beta\gamma} x_\beta \partial_\delta \sigma_{\gamma\delta}. \tag{1.12}$$

Using the fact that $\partial_t x_\beta = v_\beta$ and $\partial_\delta x_\beta = \delta_{\delta\beta}$, the second integral becomes

$$\int_V d^3\mathbf{x}\, \rho\epsilon_{\alpha\beta\gamma} v_\gamma \left(\partial_t + v_\delta \partial_\delta\right) x_\beta = \int_V d^3\mathbf{x}\, \rho\epsilon_{\alpha\beta\gamma} v_\gamma \left(v_\beta + v_\delta \delta_{\delta\beta}\right) = 2\int_V d^3\mathbf{x}\, \rho\epsilon_{\alpha\beta\gamma} v_\beta v_\gamma. \tag{1.13}$$

Now, the tensor $v_\beta v_\gamma$ is symmetric, so $\epsilon_{\alpha\beta\gamma} v_\beta v_\gamma = 0$, and thus the integral vanishes. Therefore, the angular momentum balance is

$$\int_V d^3\mathbf{x}\, \epsilon_{\alpha\beta\gamma} x_\beta \partial_\delta \sigma_{\gamma\delta} = \int dS_\delta\, \epsilon_{\alpha\beta\gamma}\, x_\beta\, \sigma_{\gamma\delta}. \tag{1.14}$$

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[1] I just stated the results of conservation of mass and linear momentum, which are often derived using the concept of a small volume element. They are more familiar, so I just stated them without going into detail on their derivation.

[2] In perhaps more familiar notation, this is $\int_V d^3\mathbf{x}\, \mathbf{x} \times \rho\mathbf{v}$.

1.3.2 Right hand side of angular momentum balance (1.10)

Considering now the right hand side, we can use the divergence theorem to convert the surface integral to a volume integral.

$$\int dS_\delta\, \epsilon_{\alpha\beta\gamma}\, x_\beta\, \sigma_{\gamma\delta} = \int_V d^3\mathbf{x}\, \epsilon_{\alpha\beta\gamma}\, \partial_\delta x_\beta \sigma_{\gamma\delta}. \tag{1.15}$$

Again using the fact that $\partial_\delta x_\beta = \delta_{\delta\beta}$, we can write the integrand as

$$\epsilon_{\alpha\beta\gamma}\, \partial_\delta x_\beta \sigma_{\gamma\delta} = \epsilon_{\alpha\beta\gamma}(\sigma_{\gamma\delta}\delta_{\delta\beta} + x_\beta \partial_\delta \sigma_{\gamma\delta}) = \epsilon_{\alpha\beta\gamma}(\sigma_{\gamma\beta} + x_\beta \partial_\delta \sigma_{\gamma\delta}). \tag{1.16}$$

1.3.3 Result of angular momentum conservation: symmetry of the stress tensor

Equating our new left and right hand sides of (1.10),

$$\int_V d^3\mathbf{x}\, \epsilon_{\alpha\beta\gamma} x_\beta \partial_\delta \sigma_{\gamma\delta} = \int_V d^3\mathbf{x}\, \epsilon_{\alpha\beta\gamma}(\sigma_{\gamma\beta} + x_\beta \partial_\delta \sigma_{\gamma\delta}) \;\Rightarrow \int_V d^3\mathbf{x}\, \epsilon_{\alpha\beta\gamma}\sigma_{\gamma\beta} = 0. \tag{1.17}$$

This must be true for any arbitrary volume element V, so

$$\epsilon_{\alpha\beta\gamma}\sigma_{\gamma\beta} = 0. \tag{1.18}$$

Using properties of the Levi-Civita symbol,

$$\epsilon_{\alpha\beta\gamma} = -\epsilon_{\alpha\gamma\beta} = -\epsilon_{\gamma\beta\alpha}, \tag{1.19}$$

so

$$-\epsilon_{\gamma\beta\alpha}\sigma_{\gamma\beta} = 0. \tag{1.20}$$

Applying $\epsilon_{\delta\mu\alpha}/2$ to both sides gives

$$-\frac{1}{2}\,\epsilon_{\delta\mu\alpha}\epsilon_{\gamma\beta\alpha}\sigma_{\gamma\beta} = -\sigma^a_{\delta\mu} = 0, \tag{1.21}$$

which means that $\sigma_{\alpha\beta}$ is symmetric. This result is true for an isotropic liquid (where we have neglected rotations of its constitutive particles), but is not in general true, e.g., for fluids with nematic or polar order.

1.4 Energy conservation

1.4.1 Total energy balance

Let e be the energy density per unit mass of the fluid, such that the total energy in a fluid element of volume V is $\int_V d^3\mathbf{x}\, \rho e$. The time rate of change of energy in the fluid element is given by the sum of the advective flux of energy out of the volume and the power imparted by body and surface forces. We assume the fluid element is adiabatic (there are no temperature gradients in the fluid), so there is no heat flux. Further, we do not consider here body forces, since we assume there are no fields acting on the fluid. Therefore, the time rate of change of total energy in the fluid element in the co-moving frame is[3]

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V d^3\mathbf{x}\, \rho e = \int_V d^3\mathbf{x}\, \rho \frac{\mathrm{d}e}{\mathrm{d}t} = \int dS_\beta\, \sigma_{\alpha\beta} v_\alpha, \tag{1.22}$$

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[3] In the stationary frame, the expression is $\partial_t \int_V d^3\mathbf{x}\, \rho e = -\int dS_\alpha\, \rho v_\alpha e + \int dS_\beta\, (\sigma_{\alpha\beta} - \rho v_\alpha v_\beta) v_\alpha$.

where we have applied the technique of section 1.3.1 for taking the material derivative under the integral sign. The right hand side is the power imparted by surface forces (force times velocity)[4]. Application of the divergence theorem gives

$$\int_V d^3\mathbf{x}\,\rho\,\frac{\mathrm{d}e}{\mathrm{d}t} = \int_V d\mathbf{x}^3\,\partial_\beta\sigma_{\alpha\beta}v_\alpha. \tag{1.23}$$

This must be true for arbitrary volume V, so

$$\rho\,\frac{\mathrm{d}e}{\mathrm{d}t} = \partial_\beta\sigma_{\alpha\beta}v_\alpha \tag{1.24}$$

1.4.2 Expression for internal energy

The per-mass energy density is given by the sum of the per-mass internal and kinetic energy densities, or

$$e = u + v_\alpha v_\alpha/2. \tag{1.25}$$

Substituting this expression into the expression for total energy conservation (1.24) gives

$$\rho\,\frac{\mathrm{d}}{\mathrm{d}t}(u + v_\alpha v_\alpha/2) = \rho\,\frac{\mathrm{d}u}{\mathrm{d}t} + \rho v_\alpha\,\frac{\mathrm{d}v_\alpha}{\mathrm{d}t} = \rho\,\frac{\mathrm{d}u}{\mathrm{d}t} + v_\alpha\partial_\beta\sigma_{\alpha\beta} = \partial_\beta\sigma_{\alpha\beta}v_\alpha = v_\alpha\partial_\beta\sigma_{\alpha\beta} + \sigma_{\alpha\beta}\partial_\beta v_\alpha \tag{1.26}$$

where we have use the chain rule and the equation for conservation of linear momentum (1.8). This simplifies to

$$\rho\,\frac{\mathrm{d}u}{\mathrm{d}t} = \sigma_{\alpha\beta}\partial_\beta v_\alpha. \tag{1.27}$$

1.5 Entropy production rate

In order to identify the thermodynamic fluxes and forces, we need to write down the entropy production rate of our fluid element. The entropy production rate is due to irreversible ("dissipative") processes within the fluid element. The total entropy in the fluid element can also change due to reversible processes. We shall call the rate of entropy production in the fluid per unit volume per unit time σ, not to be confused with the stress tensor, $\sigma_{\alpha\beta}$. Writing an entropy balance for a fluid element,

$$\rho\,\frac{\mathrm{d}s}{\mathrm{d}t} = -\partial_\alpha\,j_{S,\alpha} + \sigma, \tag{1.28}$$

where s is the per-mass entropy and $j_{S,\alpha}$ is the entropy flux to the surroundings. It is clear then, that the change in entropy by irreversible processes is given by σ. Our goal is to write an expression for $\rho\mathrm{d}s/\mathrm{d}t$ in the form of the above equation in order to identify σ.

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[4] A subtle point: In this analysis, we have neglected the so-called kinetic energy of diffusion. Foreseeing that we will neglect inertial terms in biophysical applications this is justified. For discussions, see section II.4 for de Groot and Mazur, *Non-equilibrium Thermodynamics.*

1.5.1 The Gibbs relation

Using the combined first and second laws of thermodynamics, we can write the differential for the per-volume (i.e., $dV = 0$) internal energy,

$$d(\rho u) = Td(\rho s) + \sum_i \mu_i dn_i, \tag{1.29}$$

where the chemical potential is defined as $\mu_i = \partial(\rho u)/\partial n_i$. We can therefore write the time rate of change of the entropy in the co-moving frame as

$$T\,\frac{\mathrm{d}(\rho s)}{\mathrm{d}t} = \frac{\mathrm{d}\rho u}{\mathrm{d}t} - \sum_i \mu_i \,\frac{\mathrm{d}n_i}{\mathrm{d}t}. \tag{1.30}$$

This is the so-called Gibbs relation.

1.5.2 Identifying σ and $j_{S,\alpha}$

Applying the chain rule to the left and right sides yields

$$\rho T\,\frac{\mathrm{d}s}{\mathrm{d}t} + Ts\,\frac{\mathrm{d}\rho}{\mathrm{d}t} = \rho\,\frac{\mathrm{d}u}{\mathrm{d}t} + u\,\frac{\mathrm{d}\rho}{\mathrm{d}t} - \sum_i \mu_i\,\frac{\mathrm{d}n_i}{\mathrm{d}t}. \tag{1.31}$$

Substituting the continuity equation (1.2), the species mass balance (1.5), and the expression for the time rate of change of internal energy (1.27) gives

$$T\rho\,\frac{\mathrm{d}s}{\mathrm{d}t} - T\rho s\partial_\alpha v_\alpha = \sigma_{\alpha\beta}\partial_\beta v_\alpha - \rho u\partial_\alpha v_\alpha + \sum_i \mu_i \left(n_i\partial_\alpha v_\alpha + \partial_\alpha\,\frac{j_{i,\alpha}}{m_i} - \sum_k \nu_{ki} r_k \right). \tag{1.32}$$

Rearranging,

$$T\rho\,\frac{\mathrm{d}s}{\mathrm{d}t} = \left[\sigma_{\alpha\beta} + (-\rho u + T\rho s + \sum_i \mu_i n_i)\delta_{\alpha\beta} \right] \partial_\beta v_\alpha + \sum_i \mu_i \left(\partial_\alpha\,\frac{j_{i,\alpha}}{m_i} - \sum_k \nu_{ki} r_k \right). \tag{1.33}$$

We apply the chain rule to get

$$\mu_i\partial_\alpha\,\frac{j_{i,\alpha}}{m_i} = \partial_\alpha\mu_i\,\frac{j_{i,\alpha}}{m_i} - \frac{j_{i,\alpha}}{m_i}\,\partial_\alpha\mu_i. \tag{1.34}$$

Using this in our expression for the time rate of change of per-mass entropy density, we get

$$\begin{aligned} T\rho\,\frac{\mathrm{d}s}{\mathrm{d}t} = -\partial_\alpha \left(-\sum_i \mu_i\,\frac{j_{i,\alpha}}{m_i} \right) + \left[\sigma_{\alpha\beta} + (-\rho u + T\rho s + \sum_i \mu_i n_i)\delta_{\alpha\beta} \right] \partial_\beta v_\alpha \\ - \sum_i \left(\frac{j_{i,\alpha}}{m_i}\,\partial_\alpha\mu_i + \mu_i \sum_k \nu_{ki} r_k \right). \end{aligned} \tag{1.35}$$

Comparing to (1.28), we have identified the entropy flux as

$$j_{S,\alpha} = -\frac{\mu_i}{T}\sum_i \frac{j_{i,\alpha}}{m_i}, \tag{1.36}$$

and the entropy production rate as

$$\sigma = \frac{1}{T}\left[\left(\sigma_{\alpha\beta} + (-\rho u + T\rho s + \sum_i \mu_i n_i)\delta_{\alpha\beta} \right) \partial_\beta v_\alpha - \sum_i \left(\frac{j_{i,\alpha}}{m_i}\,\partial_\alpha\mu_i + \mu_i \sum_k \nu_{ki} r_k \right) \right]. \tag{1.37}$$

1.5.3 Consolidating the material flux terms

The fluxes $j_{i,\alpha}$ of the constituent species are not independent, being related by (1.6), which says that the sum of the species fluxes is zero. If we arbitrarily define species 0 to be that which is most abundant (though this abundance specification is not necessary), we can specify the fluxes of the other species using (1.6).

$$\sum_i \frac{j_{i,\alpha}}{m_i}\,\partial_\alpha \mu_i = \frac{j_{0,\alpha}}{m_0}\,\partial_\alpha \mu_0 + \sum_{i\neq 0} \frac{j_{i,\alpha}}{m_i}\,\partial_\alpha \mu_0 = -\frac{\sum_{i\neq 0} j_{i,\alpha}}{m_0}\,\partial_\alpha \mu_i + \sum_{i\neq 0} \frac{j_{i,\alpha}}{m_i}\,\partial_\alpha \mu_i$$

$$= \sum_{i\neq 0} j_{i,\alpha} \partial_\alpha \left(\frac{\mu_i}{m_1} - \frac{\mu_0}{m_0} \right). \tag{1.38}$$

Defining $\bar{\mu}_i \equiv \mu_i/m_i - \mu_0/m_0$, we get

$$\sigma = \frac{1}{T}\left[\left(\sigma_{\alpha\beta} + (-\rho u + T\rho s + \sum_i \mu_i n_i)\delta_{\alpha\beta} \right) \partial_\beta v_\alpha - \sum_{i\neq 0} j_{i,\alpha}\,\partial_\alpha \bar{\mu}_i - \sum_{i,k} r_k \nu_{ki} \mu_i \right]. \tag{1.39}$$

The quantity $A_k \equiv \sum_i \nu_{ki}\mu_i$ is often called the *affinity* of species i in chemical reaction k.

1.5.4 The Ericksen stress

For reversible processes, $\sigma = 0$. We can separate the entropy production rate into terms that are reversible (do not contribute to σ, even in the presence of chemical reactions or chemical potential and velocity gradients) and irreversible (dissipative) terms that contribute positively to σ. Inspecting (1.39), we see that chemical reactions change the entropy production rate. Similarly, if a chemical potential gradient exists, the flux $j_{i,\alpha}$ will be zero for reversible processes. However, if the velocity gradient tensor $\partial_\beta v_\alpha$ is nonzero, we may have zero entropy production if

$$\sigma_{\alpha\beta} = (\rho u - T\rho s - \sum_i \mu_i n_i)\delta_{\alpha\beta}. \tag{1.40}$$

This is the reversible portion of the stress tensor (it does not contribute to dissipation), and we call it the *Ericksen stress.*

$$\sigma^{\mathrm{e}}_{\alpha\beta} = (\rho u - T\rho s - \sum_i \mu_i n_i)\delta_{\alpha\beta} = -p\delta_{\alpha\beta}, \tag{1.41}$$

which in the simple case of an isotropic viscous fluid is just given by the thermodynamic pressure p.

1.5.5 The deviatoric stress

We define the portion of the stress that is responsible for entropy production the *deviatoric stress*, and is given by

$$\sigma^{\mathrm{d}}_{\alpha\beta} \equiv \sigma_{\alpha\beta} - \sigma^{\mathrm{e}}_{\alpha\beta}. \tag{1.42}$$

This is the stress that contributes to dissipation. Using this definition in (1.39), we get

$$\sigma = \frac{1}{T}\left(\sigma^{\mathrm{d}}_{\alpha\beta}\partial_\beta v_\alpha - \sum_{i\neq 0} j_{i,\alpha}\,\partial_\alpha \bar{\mu}_i - \sum_k r_k A_k \right). \tag{1.43}$$

1.5.6 Splitting the stress tensor

It is convenient to split the stress tensor into a diagonal part, a symmetric, traceless part, and an antisymmetric part.

$$\sigma^{\mathrm{d}}_{\alpha\beta} = \delta_{\alpha\beta}\sigma^{\mathrm{d}}_{\gamma\gamma}/3 + \mathring{\sigma}^{\mathrm{d},s}_{\alpha\beta} + \sigma^{a}_{\alpha\beta}, \tag{1.44}$$

where for this case of an isotropic fluid, $\sigma^{a}_{\alpha\beta} = 0$, as we learned from analysis of angular momentum conservation in section 1.3.3. We do the same with the velocity gradient tensor.

$$\begin{aligned}\partial_\beta v_\alpha &= \delta_{\alpha\beta}\partial_\gamma v_\gamma/3 + \left[\frac{1}{2}(\partial_\beta v_\alpha + \partial_\alpha v_\beta/3) - \delta_{\alpha\beta}\partial_\gamma v_\gamma\right] + \frac{1}{2}(\partial_\beta v_\alpha - \partial_\alpha v_\beta) \\ &= \delta_{\alpha\beta}\partial_\gamma v_\gamma/3 + \mathring{u}_{\beta\alpha} + \omega_{\beta\alpha}, \end{aligned} \tag{1.45}$$

where we have defined

$$u_{\alpha\beta} \equiv \frac{1}{2}(\partial_\alpha v_\beta + \partial_\beta v_\alpha) \text{ and } \omega_{\alpha\beta} \equiv \frac{1}{2}(\partial_\alpha v_\beta - \partial_\beta v_\alpha) \tag{1.46}$$

as the symmetric and antisymmetric parts, respectively, of the velocity gradient tensor, using some of the relations listed in the appendix of this document. The latter is related to the vorticity by

$$(\text{vorticity})_\alpha \equiv (\text{curl } \mathbf{v})_\alpha = \epsilon_{\alpha\beta\gamma}\partial_\beta v_\gamma = \epsilon_{\alpha\beta\gamma}\omega_{\beta\gamma}. \tag{1.47}$$

Using tensorial identities and the fact that $\sigma^{a}_{\alpha\beta} = 0$, we get

$$\sigma^{\mathrm{d}}_{\alpha\beta}\partial_\beta v_\alpha = \frac{1}{3}\,\sigma^{\mathrm{d}}_{\alpha\alpha}\partial_\beta v_\beta + \mathring{\sigma}^{\mathrm{d},s}_{\alpha\beta}\mathring{u}_{\beta\alpha}. \tag{1.48}$$

1.5.7 Final expression for the entropy production rate

Using the split stress and velocity gradient tensors, we arrive at the final expression for the entropy production rate.

$$\sigma = \frac{1}{T}\left(\frac{1}{3}\,\sigma^{\mathrm{d}}_{\alpha\alpha}\partial_\beta v_\beta + \mathring{\sigma}^{\mathrm{d},s}_{\alpha\beta}\mathring{u}_{\beta\alpha} - \sum_{i\neq 0} j_{i,\alpha}\,\partial_\alpha\bar{\mu}_i - \sum_k r_k A_k\right). \tag{1.49}$$

1.6 Constitutive relations

1.6.1 Thermodynamic fluxes and forces

Investigating (1.49) reveals that the entropy production rate is given by the sum of conjugate *thermodynamic fluxes and forces*. Let $\mathbf{J}^j$ be a thermodynamic flux and $\mathbf{F}^j$ be its conjugate force. Generically, the entropy production rate is

$$\sigma = \sum_j \mathbf{J}^j\mathbf{F}^j, \tag{1.50}$$

where $\mathbf{J}^j$ and $\mathbf{F}^j$ have the same tensorial character. At equilibrium the fluxes and forces vanish. Close to equilibrium we may expand the fluxes to linear order in the forces.

$$\mathbf{J}^j = \sum_k \mathbf{L}^{jk}\mathbf{F}^j, \tag{1.51}$$

where the tensorial character of $\mathbf{L}^{jk}$ is properly chosen. The coefficients $\mathbf{L}^{jk}$ must respect the symmetries of the system. This is called the *Curie principle.* Similarly, $\mathbf{L}^{jk}$ must be positive definite, since the quadratic form

$$\sigma = \sum_j \mathbf{J}^j \mathbf{F}^j = \sum_{j,k} \mathbf{L}^{jk} \mathbf{F}^k \mathbf{F}^j \tag{1.52}$$

must be positive by the second law of thermodynamics. These are related to the *Onsager reciprocal relations.* Note also the the expansion coefficients can in general be a function of any of the intensive properties of the system.

1.6.2 Identification of fluxes and forces

From (1.49), we can identify the fluxes and forces (modulo a constant factor of $1/T$) and their tensorial character.

flux	force	character
$\sigma^d_{\gamma\gamma}/3$	$\partial_\gamma v_\gamma$	scalar
r_k	$-A_k$	scalar ($\forall k$)
$j_{i,\alpha}$	$-\partial_\alpha \bar{\mu}_i$	polar vector ($\forall i \neq 0$)
$\mathring{\sigma}^{d,s}_{\alpha\beta}$	$\mathring{u}_{\alpha\beta}$	symmetric, traceless tensor

1.6.3 Expansion of fluxes

We carry out the expansions of the fluxes to linear order in the forces. The most general expansion is

$$\sigma^{\mathrm{d}}_{\gamma\gamma}/3 = L^{vv}\partial_\gamma v_\gamma - \sum_k L^{vr_k} A_k - \sum_{i\neq 0} L^{vf_i}_{\alpha} \partial_\alpha \bar{\mu}_i + L^{vs}_{\alpha\beta}\mathring{u}_{\alpha\beta} \tag{1.53}$$

$$r_k = L^{r_k v}\partial_\gamma v_\gamma - \sum_j L^{r_k r_j} A_j - \sum_{i\neq 0} L^{r_k f_i}_{\alpha} \partial_\alpha \bar{\mu}_i + L^{r_k s}_{\alpha\beta}\mathring{u}_{\alpha\beta} \quad \forall k \tag{1.54}$$

$$j_{i,\alpha} = L^{f_i v}_{\alpha}\partial_\gamma v_\gamma - \sum_k L^{f_i r_k}_{\alpha} A_k - \sum_{j\neq 0} L^{f_i f_j}_{\alpha\beta} \partial_\beta \bar{\mu}_j + L^{f_i s}_{\alpha\beta\gamma}\mathring{u}_{\beta\gamma} \quad \forall i \neq 0 \tag{1.55}$$

$$\mathring{\sigma}^{\mathrm{d},s}_{\alpha\beta} = L^{sv}_{\alpha\beta}\partial_\gamma v_\gamma - \sum_k L^{sr_k}_{\alpha\beta} A_k - \sum_{i\neq 0} L^{sf_i}_{\alpha\beta\gamma} \partial_\gamma \bar{\mu}_i + L^{ss}_{\alpha\beta\gamma\delta}\mathring{u}_{\gamma\delta}. \tag{1.56}$$

I have called the expansion coefficients L and labeled the expansion coefficients with a superscript to designate what thermodynamic forces they couple. The code is given below.

superscript	thermodynamic force	description of thermodynamic flux
v	$\partial_\gamma v_\gamma$	compressive stress
r_k	$-A_k$	rate of chemical reaction k
f_i	$-\partial_\alpha \bar{\mu}_i$	diffusive flux of species i
s	$\mathring{u}_{\alpha\beta}$	shear stress

The subscripts of the expansion coefficients L indicate their tensorial order.

1.6.4 The Curie principle

The Curie principle states that the the phenomenological expansion coefficients must honor the spatial symmetry of the system. In particular, if a symmetry in the system exists, application of an orthogonal transformation representing that symmetry must leave the expansion coefficients unchanged.

To codify this notion, we note that application of an orthogonal transformation $R_{\alpha\beta}$ (with $|R_{\alpha\beta}| = \pm 1$) to a tensor $T_{\alpha\beta\gamma\cdots}$ results in a transformed tensor $T'_{\mu\nu\rho\cdots}$

$$T'_{\mu\nu\rho\cdots} = |R|^{\varepsilon}(R_{\mu\alpha}R_{\nu\beta}R_{\rho\gamma}\cdots)T_{\alpha\beta\gamma\cdots}, \tag{1.57}$$

with $\varepsilon = 0$ for polar tensors and $\varepsilon = 1$ for axial tensors. We will denote this transformation as

$$T'_{\alpha\beta\gamma\cdots} = \mathsf{R}T_{\alpha\beta\gamma\cdots}. \tag{1.58}$$

If a tensor is invariant under a transformation $R_{\alpha\beta}$, $T'_{\alpha\beta\gamma\cdots} = \mathsf{R}T_{\alpha\beta\gamma\cdots} = T_{\alpha\beta\gamma\cdots}$.

1.6.5 Application of the Curie principle: invariance under parity inversion

In the case of a simple isotropic fluid, the dynamics must be invariant to parity inversion, $R_{\alpha\beta} = -\delta_{\alpha\beta}$. Therefore, for a tensor L of rank n,

$$L'_{\alpha\beta\gamma\cdots} = \mathsf{R}L_{\alpha\beta\gamma\cdots} = (-1)^{\varepsilon+n}L_{\alpha\beta\gamma\cdots} = L_{\alpha\beta\gamma\cdots}. \tag{1.59}$$

For the isotropic fluid, all $\varepsilon = 0$. Therefore, all tensors with odd order must be zero.

$$L_{\alpha}^{vr_k} = L_{\alpha}^{r_k f_i} = L_{\alpha}^{f_i r_k} = L_{\alpha}^{f_i v} = L_{\alpha\beta\gamma}^{s f_i} = L_{\alpha\beta\gamma}^{f_i s} = 0. \tag{1.60}$$

1.6.6 Application of the Curie principle: invariance under arbitrary rotation

An isotropic fluid is also invariant under an arbitrary rotation. Let $R_{\alpha\beta}$ be a rotation tensor ($|R| = 1$). For scalars,

$$\mathsf{R}L = L \tag{1.61}$$

is satisfied trivially, so all scalar coupling constants are, up to this point, unrestricted.

Polar tensors of order 1. Although we already showed them all to be zero, we consider first order polar tensors, e.g., $L_{\alpha}^{vf_i}$, under arbitrary rotation. They should be invariant to this, so

$$\mathsf{R}L_{\alpha} = L_{\alpha}. \tag{1.62}$$

This holds only if $L_{\alpha} = 0$, which is true of all polar tensors of first order, reiterating that

$$L_{\alpha}^{vf_i} = L_{\alpha}^{r_k f_i} = L_{\alpha}^{r_k f_i} = L_{\alpha}^{f_i r_k} = 0. \tag{1.63}$$

Tensors of order 2. For second order tensors, we have

$$\mathsf{R}L_{\alpha\beta} = R_{\mu\alpha}R_{\nu\beta}L_{\mu\nu} = L_{\alpha\beta}. \tag{1.64}$$

We multiply each side of the equation by a tensor constructed from two arbitrary vectors a_{α} and b_{β} to get the equality of two scalars.

$$R_{\mu\alpha}R_{\nu\beta}L_{\mu\nu}a_{\alpha}b_{\beta} = L_{\alpha\beta}a_{\alpha}b_{\beta}, \tag{1.65}$$

or

$$L_{\mu\nu}R_{\mu\alpha}a_\alpha R_{\nu\beta}b_\beta = L_{\mu\nu}a'_\mu b'_\nu = L_{\alpha\beta}a'_\alpha b'_\beta = L_{\alpha\beta}a_\alpha b_\beta, \tag{1.66}$$

where we have now affected a rotation on a_α and b_β to get the rotated tensors a'_α and b'_β. The above expression indicates that $L_{\alpha\beta}a_\alpha b_\beta$ is the sum of the bilinear invariants of a_α and b_β under rotation. The only bilinear invariant of vectors is the dot product, $a_\alpha b_\alpha$. This implies that $L_{\alpha\beta} = L\delta_{\alpha\beta}$. Explicitly, with respect to the rotations,

$$L\delta_{\mu\nu}R_{\mu\alpha}a_\alpha R_{\nu\beta}b_\beta = LR_{\mu\alpha}R_{\mu\beta}a_\alpha b_\beta = L\delta_{\alpha\beta}a_\alpha b_\beta = La_\alpha b_\alpha, \tag{1.67}$$

where we have used the property of an orthogonal transformation,

$$R_{\gamma\alpha}R_{\gamma\beta} = \delta_{\alpha\beta}. \tag{1.68}$$

Given this is the case for all second order tensors,

$$L^{vs}_{\alpha\beta}\mathring{u}_{\alpha\beta} = L^{vs}\delta_{\alpha\beta}\mathring{u}_{\alpha\beta} = 0, \tag{1.69}$$

$$\text{and } L^{r_k s}_{\alpha\beta}\mathring{u}_{\alpha\beta} = L^{r_k s}\delta_{\alpha\beta}\mathring{u}_{\alpha\beta} = 0, \tag{1.70}$$

since $\mathring{u}_{\alpha\beta}$ is traceless and symmetric. Furthermore, since $\mathring{\sigma}_{\alpha\beta}$ is also symmetric and traceless,

$$L^{sv}_{\alpha\beta}\partial_\gamma v_\gamma = L^{sv}\delta_{\alpha\beta}\partial_\gamma v_\gamma \text{ and } L^{sr_k}_{\alpha\beta}\partial_\gamma v_\gamma = L^{sr_k}\delta_{\alpha\beta}\partial_\gamma v_\gamma \tag{1.71}$$

imply that $L^{sv} = L^{sr_k} = 0$. The remaining second order tensors are

$$L^{f_i f_j}_{\alpha\beta} = L^{f_i f_j}\delta_{\alpha\beta}. \tag{1.72}$$

Note also that because $L_{\alpha\beta} = L\delta_{\alpha\beta}$, $L_{\alpha\beta}$ contracted with any traceless tensor is zero.

Tensors of order 3. Although we already showed them both to be zero as a result of invariance under parity inversion, for instructive purposes, we consider third order tensors under arbitrary rotation. We take a similar strategy as for second order tensors.

$$\mathsf{R}L_{\alpha\beta\gamma} = R_{\mu\alpha}R_{\nu\beta}R_{\rho\gamma}L_{\mu_\nu\rho} = L_{\alpha\beta\gamma} \tag{1.73}$$

We multiply both sides by arbitrary vector a_α and arbitrary tensor $B_{\beta\gamma}$.

$$R_{\mu\alpha}R_{\nu\beta}R_{\rho\gamma}L_{\mu\nu\rho}a_\alpha B_{\beta\gamma} = L_{\alpha\beta\gamma}a_\alpha B_{\beta\gamma} \;\Rightarrow\; L_{\alpha\beta\gamma}a'_\alpha B'_{\beta\gamma} = L_{\alpha\beta\gamma}a_\alpha B_{\beta\gamma}, \tag{1.74}$$

which must be equal to the sum of the third degree invariants under rotation of a_α and $B_{\beta\gamma}$. The only invariant is again a dot product of two vectors, or $a_\alpha\epsilon_{\alpha\beta\gamma}T_{\beta\gamma}$. Therefore,

$$L_{\alpha\beta\gamma} = L\epsilon_{\alpha\beta\gamma}. \tag{1.75}$$

Given this fact,

$$L^{f_i s}_{\alpha\beta\gamma}\mathring{u}_{\beta\gamma} = L^{f_i s}\epsilon_{\alpha\beta\gamma}\mathring{u}_{\beta\gamma} = 0, \tag{1.76}$$

since $\mathring{u}_{\beta\gamma}$ is symmetric. Finally,

$$L^{sf_i}_{\alpha\beta\gamma}\partial_\gamma\bar{\mu}_i = L^{sf_i}\epsilon_{\alpha\beta\gamma}\partial_\gamma\bar{\mu}_i, \tag{1.77}$$

which is an antisymmetric tensor. It must (when summed with other traceless symmetric tensors) be a traceless symmetric tensor, $\mathring{\sigma}^{\mathrm{d},s}$. Therefore, $L_{sf_i} = 0$, which we already knew from invariance under parity inversion.

Tensors of order 4. We use the same strategy for a fourth order tensor, our only one being $L^{ss}_{\alpha\beta\gamma\delta}$.

$$\mathsf{R}L_{\alpha\beta\gamma\delta} = R_{\mu\alpha}R_{\nu\beta}R_{\rho\gamma}R_{\pi\delta}L_{\mu\nu\rho\pi} = L_{\alpha\beta\gamma\delta}. \tag{1.78}$$

Multiplying by arbitrary tensors $A_{\alpha\beta}$ and $B_{\gamma\delta}$,

$$R_{\mu\alpha}R_{\nu\beta}R_{\rho\gamma}R_{\pi\delta}L_{\mu\nu\rho\pi}A_{\alpha\beta}B_{\gamma\delta} = L_{\alpha\beta\gamma\delta}A'_{\alpha\beta}B'_{\gamma\delta} = L_{\alpha\beta\gamma\delta}A_{\alpha\beta}B_{\gamma\delta}. \tag{1.79}$$

Again, this expression must be equal to the sum of the fourth degree invariants under rotation.

$$L_{\alpha\beta\gamma\delta}A_{\alpha\beta}B_{\gamma\delta} = L^a\mathring{A}^s_{\alpha\beta}\mathring{B}^s_{\alpha\beta} + L^bA^a_{\alpha\beta}B^a_{\alpha\beta} + L^cA_{\alpha\alpha}B_{\beta\beta}. \tag{1.80}$$

Therefore, we have

$$L_{\alpha\beta\gamma\delta} = L^a\left(\frac{1}{2}(\delta_{\alpha\delta}\delta_{\beta\gamma} + \delta_{\alpha\gamma}\delta_{\beta\delta}) - \frac{1}{3}\,\delta_{\alpha\beta}\delta_{\gamma\delta}\right) + \frac{L^b}{2}(\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\gamma}\delta_{\beta\delta}) + L^c\delta_{\alpha\beta}\delta_{\gamma\delta}. \tag{1.81}$$

Now, we consider the product of the expansion coefficient with a traceless, symmetric tensor, $\mathring{A}_{\alpha\beta}$.

$$\begin{aligned}L^{ss}_{\alpha\beta\gamma\delta}\mathring{A}_{\alpha\beta} = {}& L^a\left(\frac{1}{2}(\delta_{\alpha\delta}\delta_{\beta\gamma} + \delta_{\alpha\gamma}\delta_{\beta\delta}) - \frac{1}{3}\,\delta_{\alpha\beta}\delta_{\gamma\delta}\right)\mathring{A}_{\alpha\beta} + \frac{L^b}{2}(\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\gamma}\delta_{\beta\delta})\mathring{A}_{\alpha\beta}\\ &+ L^c\delta_{\alpha\beta}\delta_{\gamma\delta}\mathring{A}_{\alpha\beta}.\end{aligned} \tag{1.82}$$

Consider the last term,

$$L^c\delta_{\alpha\beta}\delta_{\gamma\delta}\mathring{A}_{\alpha\beta} = L^c\delta_{\alpha\beta}\mathring{A}_{\gamma\gamma} = 0, \tag{1.83}$$

since $\mathring{A}_{\alpha\beta}$ is traceless. The second term is

$$\frac{L^b}{2}(\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\gamma}\delta_{\beta\delta})\mathring{A}_{\alpha\beta} = \frac{L^b}{2}(\mathring{A}_{\beta\alpha} - \mathring{A}_{\alpha\beta}) = 0, \tag{1.84}$$

since $\mathring{A}_{\alpha\beta}$ is symmetric. Thus, we have

$$\begin{aligned}L^{ss}_{\alpha\beta\gamma\delta}\mathring{A}_{\alpha\beta} &= L^a\left(\frac{1}{2}(\delta_{\alpha\delta}\delta_{\beta\gamma} + \delta_{\alpha\gamma}\delta_{\beta\delta}) - \frac{1}{3}\,\delta_{\alpha\beta}\delta_{\gamma\delta}\right)\mathring{A}_{\alpha\beta} = L^a\left(\frac{1}{2}(\mathring{A}_{\delta\gamma} + \mathring{A}_{\gamma\delta}) - \frac{1}{3}\,\delta_{\gamma\delta}\mathring{A}_{\alpha\alpha}\right)\\ &= L^a\mathring{A}_{\gamma\delta}.\end{aligned} \tag{1.85}$$

Finally, although it does not appear for an isotropic fluid, we consider the product of the expansion coefficient with an antisymmetric tensor, $A^a_{\gamma\delta}$.

$$\begin{aligned}L_{\alpha\beta\gamma\delta}A^a_{\gamma\delta} = {}& L^a\left(\frac{1}{2}(\delta_{\alpha\delta}\delta_{\beta\gamma} + \delta_{\alpha\gamma}\delta_{\beta\delta}) - \frac{1}{3}\,\delta_{\alpha\beta}\delta_{\gamma\delta}\right)A^a_{\gamma\delta} + \frac{L^b}{2}(\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\gamma}\delta_{\beta\delta})A^a_{\gamma\delta}\\ &+ L^c\delta_{\alpha\beta}\delta_{\gamma\delta}A^a_{\gamma\delta}.\end{aligned} \tag{1.86}$$

Consider the last term,

$$L^c \delta_{\alpha\beta}\delta_{\gamma\delta} A^a_{\gamma\delta} = L^c \delta_{\alpha\beta} A^a_{\gamma\gamma} = 0, \tag{1.87}$$

since $A^a_{\alpha\beta}$ is traceless. The first term is

$$L^a \left(\frac{1}{2}(\delta_{\alpha\delta}\delta_{\beta\gamma} + \delta_{\alpha\gamma}\delta_{\beta\delta}) - \frac{1}{3}\,\delta_{\alpha\beta}\delta_{\gamma\delta}\right) A^a_{\gamma\delta} = L^a \left(\frac{1}{2}(A^a_{\beta\alpha} + A^a_{\alpha\beta}) - \frac{1}{3}\,\delta_{\alpha\beta} A^a_{\gamma\gamma}\right) = 0, \tag{1.88}$$

again because $A^a_{\alpha\beta}$ is antisymmetric. Finally, the middle term is

$$\frac{L^b}{2}(\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\gamma}\delta_{\beta\delta}) A^a_{\gamma\delta} = \frac{L^b}{2}(A^a_{\beta\alpha} - A^a_{\alpha\beta}) = -L^b A^a_{\alpha\beta}. \tag{1.89}$$

Therefore, for an antisymmetric tensor $A^a_{\alpha\beta}$ in a system that exhibits rotational invariance,

$$L_{\alpha\beta\gamma\delta} A^a_{\gamma\delta} = L A^a_{\alpha\beta}. \tag{1.90}$$

The result is a traceless, antisymmetric tensor. If this must be equal to a symmetric tensor, $L = 0$.

1.6.7 Updated expansion of fluxes after application of Curie principle

Renaming $L^a = L^{ss}$, we arrive at our updated force/flux relations.

$$\sigma^{\mathrm{d}}_{\gamma\gamma}/3 = L^{vv}\partial_\gamma v_\gamma - \sum_k L^{vr_k} A_k \tag{1.91}$$

$$r_k = L^{r_k v}\partial_\gamma v_\gamma - \sum_j L^{r_k r_j} A_j \;\; \forall k \tag{1.92}$$

$$j_{i,\alpha} = -\sum_{j\neq 0} L^{f_i f_j}\partial_\alpha \bar{\mu}_j \;\; \forall \neq i \tag{1.93}$$

$$\mathring{\sigma}^{\mathrm{d},s}_{\alpha\beta} = L^{ss}\mathring{u}_{\alpha\beta}. \tag{1.94}$$

1.6.8 The Onsager reciprocal relations

The *Onsager reciprocal relations* restrict the values of the coefficients. I will not go into detail here, but see de Groot and Mazur for discussion. They follow from the fact that the positive definiteness of the entropy production rate and properties of the system with respect to time reversal. In particular, we note that the positive definiteness of σ requires that each term in its sum (i.e., each tensorial order) be positive.

The shear viscosity. The easiest relation to see is $L^{ss} > 0$. We define

$$L^{ss} = 2\eta, \tag{1.95}$$

where $\eta (> 0)$ is known as the viscosity.

The bulk viscosity. In the absence of chemical reaction, the entropy must remain positive definite, so $L^{vv} > 0$. We define

$$L^{vv} \equiv \eta_v, \tag{1.96}$$

known as the bulk viscosity.

The chemical reaction rates. The Onsager relations stipulate that when two forces that have opposite signatures under time reversal couple, their expansion coefficients are of the same magnitude and of opposite sign. The $\partial_\gamma v_\gamma$ term changes sign under time reversal, but the chemical affinities A_k do not. Therefore, $L^{r_k v} = -L^{v r_k}$. There is no stipulation on the sign of $L^{r_k v}$.

While there is no stipulation on the sign of L^{rv}, positive definiteness of the entropy production rate σ requires $L^{r_k r_j} < 0$ and further than $L^{r_k r_j} = L^{r_j r_k}$. We will absorb a negative sign into these coefficients and redefine them, $-L^{r_k r_j} \to L^{r_k r_j}$.

Diffusion. We now wish to write the last constitutive relation, $j_{i,\alpha} = -\alpha \partial_\alpha \bar{\mu}_i$, in a more useful form, i.e., as a function of the mole fractions n_i as opposed to $\bar{\mu}_i$. I will not go through the details, since it involves some complicated manipulations, but it is possible to make the transformation between $L^{f_i f_j}$ and D_{ij} such that

$$j_{i,\alpha} = -\sum_{j\neq 0} L^{f_i f_j} \partial_\alpha \bar{\mu}_j = \sum_{j \neq 0} D_{ij} \partial_\alpha n_j. \tag{1.97}$$

(See de Groot and Mazur, chapter XI.) The diffusion coefficients D_{ij} are in general functions of all the intensive parameters of the system. Positive definiteness of the entropy production rate requires D_{ij} be positive definite, with $D_{ii} > 0$ and $D_{ij} = D_{ji}$.

1.6.9 Final constitutive relations

Using the results of the previous sections, we arrive at our final constitutive relations.

$$\sigma^{\mathrm{d}}_{\gamma\gamma}/3 = \eta_v \partial_\gamma v_\gamma - \sum_k \zeta_k A_k \tag{1.98}$$

$$r_k = -L^{v r_k} \partial_\gamma v_\gamma + \sum_j L^{r_k r_j} A_j \;\; \forall k \tag{1.99}$$

$$\mathring{\sigma}^{\mathrm{d}}_{\alpha\beta} = 2\eta \mathring{u}_{\alpha\beta} \tag{1.100}$$

$$j_{i,\alpha} = -m_i \sum_{j\neq 0} D_{ij} \partial_\alpha n_j, \tag{1.101}$$

with the stipulations that

$$\eta_v, \eta, L^{rr}_{kk}, D_{ii} > 0 \;\; \forall k, i, \tag{1.102}$$

and $D_{ij} = D_{ji}$ and $L^{r_k r_j} = L^{r_j r_k}$.

1.7 Dynamical equations

To arrive at the dynamical equations, we first consider conservation of mass. Substitution of the constitutive relation for the flux (1.101) into the conservation law for each species (1.5) yields

$$\frac{\mathrm{d}n_i}{\mathrm{d}t} = -n_i \partial_\alpha v_\alpha + \partial_\alpha \sum_{j\neq 0} D_{ij}\, \partial_\alpha n_j + \sum_k \nu_{ki} r_k. \tag{1.103}$$

To write the remaining dynamical equations, we simply need to write the stress tensor.

$$\sigma_{\alpha\beta} = \sigma^{\mathrm{d}}_{\alpha\beta} + \sigma^{\mathrm{e}}_{\alpha\beta} = \mathring{\sigma}^{\mathrm{d},s}_{\alpha\beta} + \delta_{\alpha\beta}\sigma_{\gamma\gamma}/3 - p\delta_{\alpha\beta} = 2\eta\mathring{u}_{\alpha\beta} + \left(\eta_v\partial_\gamma v_\gamma - p - \sum_k L^{vr_k}A_k\right)\delta_{\alpha\beta} \tag{1.104}$$

$$= \eta(\partial_\alpha v_\beta + \partial_\beta v_\alpha) + \left(\left(\eta_v - \frac{2}{3}\,\eta\right)\partial_\gamma v_\gamma - p - \sum_k L^{vr_k}A_k\right)\delta_{\alpha\beta}, \tag{1.105}$$

where momentum and energy conservation, respectively, are

$$\rho\,\frac{\mathrm{d}v_\alpha}{\mathrm{d}t} = \partial_\beta\sigma_{\alpha\beta} \tag{1.106}$$

$$\rho\,\frac{\mathrm{d}e}{\mathrm{d}t} = \partial_\beta\sigma_{\alpha\beta}v_\alpha. \tag{1.107}$$

If we make the assumption that D_{ij} is diagonal with $D_{ii} \equiv D_i$, that D_i and η are constants, and that the fluid is incompressible ($\partial_\alpha v_\alpha = 0$), we arrive at familiar expressions, the advection-reaction-diffusion equation and the active Navier-Stokes equations (noting that L^{vr_k} is typically zero, i.e., chemical reactions do not exert an active stress).

$$\frac{\mathrm{d}n_i}{\mathrm{d}t} = D_i\,\partial_\alpha n_i - n_i\partial_\alpha v_\alpha + \sum_k \nu_{ki}r_k \tag{1.108}$$

$$\rho\,\frac{\mathrm{d}v_\alpha}{\mathrm{d}t} = -\partial_\alpha\left(p + \sum_k L^{vr_k}A_k\right) + \partial_\beta\partial_\beta v_\alpha. \tag{1.109}$$

2 Nematic liquid crystal above T_c using $Q_{\alpha\beta}$

We now derive the dynamical equations for a nematic liquid crystal above the critical temperature. We neglect temperature gradients and we neglect body forces and external fields. For notational convenience, in this section we will denote

$$\dot{a} \equiv \frac{\mathrm{d}a}{\mathrm{d}t} \tag{2.1}$$

2.1 Nematic order parameters

2.1.1 The director

A nematic liquid crystal has associated with it a *director*, n_α, a unit vector ($n_\alpha n_\alpha = 1$) that points along the direction of the local orientation of the molecules in the liquid crystal. The unit vector is special in that any properties depending on it must be invariant under parity inversion. This is in contrast to a polar fluid, in which the vector specifying the local orientation, p_α, flips sign under parity inversion.

2.1.2 The tensorial order parameter

Below the critical temperature, a nematic liquid crystal is uniaxially ordered over long length scales. Above the critical temperature, the nematic order varies more rapidly through space. We therefore define a *tensorial order parameter* by

$$Q_{\alpha\beta} = S\left(n_\alpha n_\beta - \frac{1}{3}\,\delta_{\alpha\beta}\right), \tag{2.2}$$

where S indicates the magnitude of the order parameter. The tensor order parameter if traceless and symmetric. We will derive the dynamics in terms of $Q_{\alpha\beta}$ and its derivatives, though we could choose to do so in terms of $n_\alpha n_\beta$ and $n_\alpha \mathrm{d}n_\beta/\mathrm{d}t$, which can be a bit easier (see, e.g., Vertogen and de Jeu, *Thermotropic Liquid Crystals, Fundamentals*, chapter 8).

2.2 Mass conservation

All the results derived in section 1.1 hold.

2.3 Linear momentum conservation

All the results derived in section 1.2 hold.

2.4 Angular momentum conservation

The expression given by (1.10) must now be modified to take into account the anisotropy in the fluid.

2.4.1 Total angular momentum density: analogous left hand side of (1.10)

The total angular momentum of the fluid element now has a component due to the rotation of the anisotropic molecules. Let Ω_α be the angular velocity of the rotation and I be the moment of inertia. Then the rate of change of total angular momentum is

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V d^3\mathbf{x}\,[\rho\epsilon_{\alpha\beta\gamma}x_\beta v_\gamma + I\Omega_\alpha]\,, \tag{2.3}$$

and the rate of change of total angular momentum is the material derivative of this expression.

2.4.2 Neglect of the $I\Omega_\alpha$ terms

We compare the size of the two terms on the left hand side of the integral angular momentum balance (2.8). If a is the molecular size of an anisotropic molecules, the moment of inertia of a single molecules $\sim m_1 a^2$, where m_1 is the mass of a single molecule. Then, if there are N molecules per unit volume, the per volume moment of inertia satisfies

$$I \sim \frac{N m_1 a^2}{a^3} \sim \rho a^2, \tag{2.4}$$

since $\rho \sim N m_1/a^3$. Therefore, the second term on the left hand side of (2.8) is

$$I|\Omega| \sim \rho a^2 |\Omega|. \tag{2.5}$$

Now, the first term is $\rho\epsilon_{\alpha\beta\gamma}x_\beta v_\gamma$. If U is the characteristic velocity of the fluid flow and L is the characteristic length scale of the system ($L \gg a$, since this is a hydrodynamic theory), the time scale associated with fluid motion is $\tau = L/U$. Therefore, the first term scale like

$$\rho x v \sim \rho L U \sim \rho L^2/\tau. \tag{2.6}$$

Since $L \gg a$, the second term associated with internal rotations is negligible provided the frequency of the rotations $|\Omega|$ is not orders of magnitude greater than the characteristic flow frequency, τ^{-1}. We will ultimately neglect the contributions of $I\Omega_\alpha$, but we keep them for most of the derivation of the dynamical equations for reference.

2.4.3 Nematic torque and the molecular field: analogous right hand side of (1.10)

In addition to the surface stress taken into account in the right hand side of (1.10), we also must include torques related to alignment of the nematic order. Imagine that the nematic order is different from its equilibrium value. The free energy density of the fluid then changes by ρf_d, the so-called *distortion free energy density.* We define the *molecular field* to be the functional derivative of f_d,

$$H_{\alpha\beta} \equiv -\frac{\delta f_d}{\delta Q_{\alpha\beta}}. \tag{2.7}$$

With this definition, the per-volume torque is $-\epsilon_{\alpha\gamma\delta}H_{\gamma\beta}Q_{\delta\beta} - \epsilon_{\alpha\beta\delta}H_{\gamma\beta}Q_{\gamma\delta}$ (this is a second order tensorial analogue of a cross product). We must include this on the right hand side of the angular momentum balance, giving

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V d^3\mathbf{x}\,[\rho\epsilon_{\alpha\beta\gamma}x_\beta v_\gamma + I\Omega_\alpha] = \int dS_\delta\epsilon_{\alpha\beta\gamma}\,x_\beta\,\sigma_{\gamma\delta} - \int_V d^3\mathbf{x}\,H_{\gamma\beta}\left(\epsilon_{\alpha\gamma\delta}Q_{\delta\beta} + \epsilon_{\alpha\beta\delta}Q_{\gamma\delta}\right). \tag{2.8}$$

2.4.4 Differential expression of angular momentum conservation

We know from section 1.3 that

$$\int dS_\delta\epsilon_{\alpha\beta\gamma}x_\beta\,\sigma_{\gamma\delta} - \frac{\mathrm{d}}{\mathrm{d}t}\int_V d^3\mathbf{x}\,\rho\epsilon_{\alpha\beta\gamma}x_\beta v_\gamma = \int_V d^3\mathbf{x}\,\epsilon_{\alpha\beta\gamma}\sigma_{\gamma\beta}. \tag{2.9}$$

Therefore, the integral expression for conservation of angular momentum (2.8) becomes

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V d^3\mathbf{x}\,I\Omega_\alpha = \int_V d^3\mathbf{x}\left[\epsilon_{\alpha\beta\gamma}\sigma_{\gamma\beta} - H_{\gamma\beta}\left(\epsilon_{\alpha\gamma\delta}Q_{\delta\beta} + \epsilon_{\alpha\beta\delta}Q_{\gamma\delta}\right)\right]. \tag{2.10}$$

Now, we can use the same method as in section 1.3.1 to bring the material derivative under the integral sign, since the moment of inertia is the weighted sum of masses of particles.

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V d^3\mathbf{x}\,I\Omega_\alpha = \int_V d^3\mathbf{x}\,I\dot{\Omega}_\alpha. \tag{2.11}$$

Using this relation, and the fact that angular momentum must be conserved for any arbitrary volume V, we get the differential expression for angular momentum conservation.

$$I\dot{\Omega}_\alpha = \epsilon_{\alpha\beta\gamma}\sigma_{\gamma\beta} - H_{\gamma\beta}\left(\epsilon_{\alpha\gamma\delta}Q_{\delta\beta} + \epsilon_{\alpha\beta\delta}Q_{\gamma\delta}\right) \tag{2.12}$$

2.4.5 The antisymmetric part of the stress tensor

The antisymmetric part of the stress tensor can be computed from (2.12).

$$\begin{aligned}\sigma^a_{\rho\nu} &= \frac{1}{2}\,\epsilon_{\rho\nu\alpha}\epsilon_{\gamma\beta\alpha}\sigma_{\gamma\beta} = -\frac{1}{2}\,\epsilon_{\rho\nu\alpha}\epsilon_{\alpha\beta\gamma}\sigma_{\gamma\beta} \\ &= -\frac{I}{2}\,\epsilon_{\rho\nu\alpha}\,\dot{\Omega}_\alpha - \frac{1}{2}\left(\epsilon_{\rho\nu\alpha}\epsilon_{\alpha\gamma\delta}Q_{\delta\beta} + \epsilon_{\rho\nu\alpha}\epsilon_{\alpha\beta\delta}Q_{\gamma\delta}\right)H_{\gamma\beta}.\end{aligned} \tag{2.13}$$

This can be simplified using identities of the Levi-Civita symbol.

$$\sigma^a_{\rho\nu} = -\frac{I}{2}\,\epsilon_{\rho\nu\alpha}\,\dot{\Omega}_\alpha - \frac{1}{2}\left(H_{\rho\beta}Q_{\nu\beta} - H_{\nu\beta}Q_{\rho\beta} + H_{\gamma\rho}Q_{\gamma\nu} - H_{\gamma\nu}Q_{\gamma\rho}\right) \tag{2.14}$$

Renaming indices gives

$$\sigma^a_{\alpha\beta} = -\frac{I}{2}\,\epsilon_{\alpha\beta\gamma}\,\dot{\Omega}_\gamma - \frac{1}{2}\left(H_{\alpha\gamma}Q_{\beta\gamma} - H_{\beta\gamma}Q_{\alpha\gamma} + H_{\gamma\alpha}Q_{\gamma\beta} - H_{\gamma\beta}Q_{\gamma\alpha}\right) \tag{2.15}$$

Since both $H_{\alpha\beta}$ and $Q_{\alpha\beta}$ are symmetric, this simplifies to

$$\sigma^a_{\alpha\beta} = -\frac{I}{2}\,\epsilon_{\alpha\beta\gamma}\,\dot{\Omega}_\gamma - H_{\alpha\gamma}Q_{\beta\gamma} + H_{\beta\gamma}Q_{\alpha\gamma}. \tag{2.16}$$

2.5 Energy conservation in nematic fluids

2.5.1 Total energy balance

The total energy density e from section 1.4.1 now additionally includes the total internal rotational energy density.

$$\rho e = \rho\,\frac{v_\alpha v_\alpha}{2} + I\,\frac{\Omega_\alpha\Omega_\alpha}{2} + \rho u. \tag{2.17}$$

Therefore the total integral energy balance is

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V d^3\mathbf{x}\left[\rho\left(\frac{v_\alpha v_\alpha}{2} + u\right) + I\,\frac{\Omega_\alpha\Omega_\alpha}{2}\right] = \int dS_\gamma\,\sigma_{\alpha\gamma}v_\alpha = \int_V d^3\mathbf{x}\partial_\gamma\sigma_{\alpha\gamma}v_\alpha, \tag{2.18}$$

where we have used the divergence theorem. This must be true for all arbitrary volumes V, so we arrive at the expression for conservation of energy.

$$\rho\,\frac{\mathrm{d}u}{\mathrm{d}t} + \frac{\rho}{2}\frac{\mathrm{d}v_\alpha v_\alpha}{\mathrm{d}t} + \frac{I}{2}\frac{\mathrm{d}\Omega_\alpha\Omega_\alpha}{\mathrm{d}t} = \partial_\beta\sigma_{\alpha\beta}v_\alpha, \tag{2.19}$$

where we have again taken the material derivative under the integral sign.

2.5.2 Expression for internal energy

We know from section 1.4.2 that

$$\frac{\rho}{2}\frac{\mathrm{d}v_\alpha v_\alpha}{\mathrm{d}t} = v_\alpha\partial_\beta\sigma_{\alpha\beta}. \tag{2.20}$$

Therefore,

$$\rho \frac{\mathrm{d}u}{\mathrm{d}t} = -I\Omega_\alpha \dot{\Omega}_\alpha + \sigma_{\alpha\beta}\partial_\beta v_\alpha, \tag{2.21}$$

where we have used $\sigma_{\alpha\beta}\partial_\beta v_\alpha = \partial_\beta \sigma_{\alpha\beta} v_\alpha - v_\alpha \partial_\beta \sigma_{\alpha\beta}$. Now, multiplication of the conservation of angular momentum equation (2.12) by Ω_α gives

$$I\Omega_\alpha \dot{\Omega}_\alpha = \epsilon_{\alpha\beta\gamma}\Omega_\alpha \sigma_{\gamma\beta} - \Omega_\alpha \left(\epsilon_{\alpha\gamma\delta} Q_{\delta\beta} + \epsilon_{\alpha\beta\delta} Q_{\gamma\delta}\right) H_{\gamma\beta}. \tag{2.22}$$

Therefore, we have

$$\rho \frac{\mathrm{d}u}{\mathrm{d}t} = \sigma_{\alpha\beta}\partial_\beta v_\alpha - \epsilon_{\alpha\beta\gamma}\Omega_\alpha \sigma_{\gamma\beta} + \Omega_\alpha \left(\epsilon_{\alpha\gamma\delta} Q_{\delta\beta} + \epsilon_{\alpha\beta\delta} Q_{\gamma\delta}\right) H_{\gamma\beta}. \tag{2.23}$$

2.6 Nematic entropy production rate

We again proceed to write the entropy balance in the form of (1.28) in order to identify the entropy production rate σ.

2.6.1 Nematic distortion internal energy

The total free energy density, ρf, is given by performing a Legendre transform on the T and ρs conjugate variables. For a nematic fluid, in contrast to an isotropic fluid, there are contributions to the free energy coming from energetics associated with the director. We will call this free energy the *distortion free energy density*, ρf_d. The corresponding distortion internal energy is ρu_d. By writing the total differentials of the free energy and internal energy.

$$d(\rho f) = -\rho s dT + \sum_i \mu_i dn_i + d\rho f_d \tag{2.24}$$

$$d(\rho u) = d(\rho s) + \sum_i \mu_i dn_i + d\rho u_d \tag{2.25}$$

Since ρf and ρu are related by Legendre transform of the T and ρs conjugate pair, $d\rho u_d = d\rho f_d$, from which it follows that $du_d = df_d$.

We write the distortion free energy as a function $Q_{\alpha\beta}$ and $\partial_\gamma Q_{\alpha\beta}$ and expand to first order in $Q_{\alpha\beta}$ and its gradient.

$$df_d = du_d = \phi_{\alpha\beta}\, dQ_{\alpha\beta} + \pi_{\alpha\beta\gamma}\, d\partial_\gamma Q_{\alpha\beta}, \tag{2.26}$$

where have have defined

$$\phi_{\alpha\beta} \equiv \frac{\partial f_d}{\partial Q_{\alpha\beta}} \text{ and } \pi_{\alpha\beta\gamma} \equiv \frac{\partial f_d}{\partial(\partial_\gamma Q_{\alpha\beta})}. \tag{2.27}$$

Given the prescribed functional dependence of f_d on $Q_{\alpha\beta}$ and $\partial_\gamma Q_{\alpha\beta}$, we may write the molecular field as the functional derivative of f_d with respect to $Q_{\alpha\beta}$.

$$H_{\alpha\beta} \equiv -\frac{\delta f_d}{\delta Q_{\alpha\beta}} = -\phi_{\alpha\beta} + \partial_\gamma \pi_{\alpha\beta\gamma}. \tag{2.28}$$

2.6.2 Nematic Gibbs relation

The Gibbs relation follows from (2.25)

$$T\,\frac{\mathrm{d}\rho s}{\mathrm{d}t}=\frac{\mathrm{d}\rho u}{\mathrm{d}t}-\frac{\mathrm{d}u_d}{\mathrm{d}t}-\sum_i\mu_i\,\frac{\mathrm{d}n_i}{\mathrm{d}t}. \tag{2.29}$$

Using (2.26), this is

$$T\,\frac{\mathrm{d}\rho s}{\mathrm{d}t}=\frac{\mathrm{d}\rho u}{\mathrm{d}t}-\phi_{\alpha\beta}\,\frac{\mathrm{d}Q_{\alpha\beta}}{\mathrm{d}t}-\pi_{\alpha\beta\gamma}\,\frac{\mathrm{d}}{\mathrm{d}t}\left(\partial_\gamma Q_{\alpha\beta}\right)-\sum_i\mu_i\,\frac{\mathrm{d}n_i}{\mathrm{d}t}. \tag{2.30}$$

To put this in a more convenient form, we note that

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\left(\partial_\gamma Q_{\alpha\beta}\right)&=(\partial_t+v_\delta\partial_\delta)\partial_\gamma Q_{\alpha\beta}=\partial_\gamma\partial_t Q_{\alpha\beta}+v_\delta\partial_\gamma(\partial_\delta Q_{\alpha\beta})\\&=\partial_\gamma\partial_t Q_{\alpha\beta}+\partial_\gamma v_\delta\partial_\delta Q_{\alpha\beta}-(\partial_\delta Q_{\alpha\beta})\partial_\gamma v_\delta=\partial_\gamma\,\frac{\mathrm{d}Q_{\alpha\beta}}{\mathrm{d}t}-(\partial_\delta Q_{\alpha\beta})\partial_\gamma v_\delta.\end{aligned} \tag{2.31}$$

Thus,

$$T\,\frac{\mathrm{d}\rho s}{\mathrm{d}t}=\frac{\mathrm{d}\rho u}{\mathrm{d}t}-\phi_{\alpha\beta}\,\dot{Q}_{\alpha\beta}-\pi_{\alpha\beta\gamma}\left(\partial_\gamma\,\dot{Q}_{\alpha\beta}-(\partial_\delta Q_{\alpha\beta})\partial_\gamma v_\delta\right)-\sum_i\mu_i\,\dot{n}_i. \tag{2.32}$$

2.6.3 Identifying σ and $j_{S,\alpha}$ for a nematic fluid

Substitution of the expression for the time rate of change of the internal energy (2.23) into the nematic Gibbs relation (2.32) and application of simplifications of section 1.5.2 yield

$$\begin{aligned}T\rho\,\frac{\mathrm{d}s}{\mathrm{d}t}=&\left\{-\partial_\alpha\left(-\sum_i\mu_i\,\frac{j_{i,\alpha}}{m_i}\right)+\left[\sigma_{\alpha\beta}+\left(-\rho u+T\rho s+\sum_i\mu_i n_i\right)\delta_{\alpha\beta}\right]\partial_\beta v_\alpha\right\}\\&-\epsilon_{\alpha\beta\gamma}\Omega_\alpha\sigma_{\gamma\beta}+\Omega_\alpha\left(\epsilon_{\alpha\gamma\delta}Q_{\delta\beta}+\epsilon_{\alpha\beta\delta}Q_{\gamma\delta}\right)H_{\gamma\beta}-\phi_{\alpha\beta}\dot{Q}_{\alpha\beta}-\pi_{\alpha\beta\gamma}\left(\partial_\gamma\dot{Q}_{\alpha\beta}-(\partial_\delta Q_{\alpha\beta})\partial_\gamma v_\delta\right)\\&-\left\{\sum_i\left(\frac{j_{i,\alpha}}{m_i}\,\partial_\alpha\mu_i+\mu_i\sum_k\nu_{ki}r_k\right)\right\},\end{aligned} \tag{2.33}$$

where the terms in braces appear for an isotropic fluid. We now apply the chain rule to rewrite

$$\pi_{\alpha\beta\gamma}\partial_\gamma\dot{Q}_{\alpha\beta}=\partial_\gamma\pi_{\alpha\beta\gamma}\dot{Q}_{\alpha\beta}-\dot{Q}_{\alpha\beta}\partial_\gamma\pi_{\alpha\beta\gamma}. \tag{2.34}$$

Using this relation and relabeling some indices, we get

$$\begin{aligned}T\rho\,\frac{\mathrm{d}s}{\mathrm{d}t}=&-\partial_\gamma\left(-\sum_i\mu_i\,\frac{j_{i,\gamma}}{m_i}+\pi_{\alpha\beta\gamma}\dot{Q}_{\alpha\beta}\right)+\left(\sigma_{\alpha\beta}+p\delta_{\alpha\beta}+\pi_{\gamma\delta\beta}\partial_\alpha Q_{\gamma\delta}\right)\partial_\beta v_\alpha\\&-\epsilon_{\alpha\beta\gamma}\Omega_\alpha\sigma_{\gamma\beta}+\Omega_\alpha\left(\epsilon_{\alpha\gamma\delta}Q_{\delta\beta}+\epsilon_{\alpha\beta\delta}Q_{\gamma\delta}\right)H_{\gamma\beta}+[\partial_\gamma\pi_{\alpha\beta\gamma}-\phi_{\alpha\beta}]\dot{Q}_{\alpha\beta}\\&-\sum_i\left(\frac{j_{i,\alpha}}{m_i}\,\partial_\alpha\mu_i+\mu_i\sum_k\nu_{ki}r_k\right),\end{aligned} \tag{2.35}$$

where the bracketed expression is the molecular field $H_{\alpha\beta}$ and we have again identified

$$p = -\rho u + T\rho s + \sum_i \mu_i n_i. \tag{2.36}$$

We can now identify

$$T j_{s,\alpha} = -\sum_i \mu_i \frac{j_{i,\gamma}}{m_i} + \pi_{\alpha\beta\gamma}\dot{Q}_{\alpha\beta} \tag{2.37}$$

and

$$\begin{aligned} T\sigma = &\left(\sigma_{\alpha\beta} + p\delta_{\alpha\beta} + \pi_{\gamma\delta\beta}\partial_\alpha Q_{\gamma\delta}\right)\partial_\beta v_\alpha - \epsilon_{\alpha\beta\gamma}\Omega_\alpha \sigma_{\gamma\beta} + \Omega_\alpha\left(\epsilon_{\alpha\gamma\delta}Q_{\delta\beta} + \epsilon_{\alpha\beta\delta}Q_{\gamma\delta}\right)H_{\gamma\beta} \\ &+ H_{\alpha\beta}\dot{Q}_{\alpha\beta} - \sum_i \left(\frac{j_{i,\alpha}}{m_i}\partial_\alpha \mu_i + \mu_i \sum_k \nu_{ki} r_k\right). \end{aligned} \tag{2.38}$$

2.6.4 Consolidating the material flux terms

We again consolidate the material flux terms as in section 1.5.3. We additionally simplify the terms involving Ω_α.

$$\begin{aligned} T\sigma = &\left(\sigma_{\alpha\beta} + p\delta_{\alpha\beta} + \pi_{\gamma\delta\beta}\partial_\alpha Q_{\gamma\delta}\right)\partial_\beta v_\alpha - \Omega_\alpha\left(\epsilon_{\alpha\beta\gamma}\sigma_{\gamma\beta} - \left(\epsilon_{\alpha\gamma\delta}Q_{\delta\beta} + \epsilon_{\alpha\beta\delta}Q_{\gamma\delta}\right)H_{\gamma\beta}\right) \\ &+ H_{\alpha\beta}\dot{Q}_{\alpha\beta} - \sum_{i\neq 0} j_{i,\alpha}\,\partial_\alpha \bar{\mu}_i - \sum_k r_k A_k, \end{aligned} \tag{2.39}$$

where we have again defined the affinity A_k.

2.6.5 Reversible terms and the nematic Ericksen stress

We identify the portions of the stress and nematic ordering interactions that are reversible, i.e., those that do not contribute to the production of entropy, as those for which $\sigma = 0$, even when $\partial_\beta v_\alpha$, Ω_α, and $\dot{Q}_{\alpha\beta}$ are all nonzero. The first identifies the Ericksen stress for a nematic liquid crystal.

$$\sigma^{\mathrm{e}}_{\alpha\beta} = -p\delta_{\alpha\beta} - \pi_{\gamma\delta\beta}\partial_\alpha Q_{\gamma\delta}, \tag{2.40}$$

with the deviatoric stress again being $\sigma^{\mathrm{d}}_{\alpha\beta} = \sigma_{\alpha\beta} - \sigma^{\mathrm{e}}_{\alpha\beta}$. Note that both terms in the Ericksen stress are symmetric, and we can write it as

$$\sigma^{\mathrm{e}}_{\alpha\beta} = -p\delta_{\alpha\beta} - \pi_{\gamma\delta\alpha}\partial_\beta Q_{\gamma\delta}, \tag{2.41}$$

The second relation defining a reversible process comes from the Ω_α term.

$$\epsilon_{\alpha\beta\gamma}\sigma^{(r)}_{\gamma\beta} = \left(\epsilon_{\alpha\gamma\delta}Q_{\delta\beta} + \epsilon_{\alpha\beta\delta}Q_{\gamma\delta}\right)H_{\gamma\beta}, \tag{2.42}$$

which describes the antisymmetric part of the reversible stress. This can be re-written by multiplying both sides by $\epsilon_{\alpha\beta\gamma}$ and contracting, using identities of the Levi-Citiva symbol.

$$\sigma^{(r)}_{\alpha\beta} = \frac{1}{3}\left(H_{\gamma\beta}Q_{\gamma\alpha} - H_{\alpha\gamma}Q_{\beta\gamma}\right). \tag{2.43}$$

2.6.6 Splitting the stress tensor

We split the tensors $\sigma^{\mathrm{d}}_{\alpha\beta}$ and $\partial_\beta v_\alpha$ into their trace, antisymmetric, and traceless and symmetric parts. Note that $\dot{Q}_{\alpha\beta}$ is traceless and symmetric and $H_{\alpha\beta}$ is symmetric. Doing this gives the entropy production rate

$$\begin{aligned} T\sigma =& \mathring{\sigma}^{\mathrm{d},s}_{\alpha\beta}\mathring{u}_{\alpha\beta} - \sigma^{\mathrm{d},a}_{\alpha\beta}\omega_{\alpha\beta} + \sigma^{\mathrm{d}}_{\alpha\alpha}\partial_\gamma v_\gamma/3 - \Omega_\alpha\left(\epsilon_{\alpha\beta\gamma}\sigma_{\gamma\beta} - \left(\epsilon_{\alpha\gamma\delta}Q_{\delta\beta} + \epsilon_{\alpha\beta\delta}Q_{\gamma\delta}\right)H_{\gamma\beta}\right) \\ &+ \mathring{H}_{\alpha\beta}\dot{Q}_{\alpha\beta} - \sum_{i\neq 0} j_{i,\alpha}\,\partial_\alpha\bar{\mu}_i - \sum_k r_k A_k. \end{aligned} \tag{2.44}$$

2.6.7 Incorporating the antisymmetric part of the stress tensor

Because the Ericksen stress is symmetric, the antisymmetric part of the stress tensor appears exclusively in the deviatoric stress, i.e.,

$$\sigma^{\mathrm{d},a}_{\alpha\beta} = -\frac{I}{2}\,\epsilon_{\alpha\beta\gamma}\,\dot{\Omega}_\gamma - H_{\alpha\gamma}Q_{\beta\gamma} + H_{\beta\gamma}Q_{\alpha\gamma}. \tag{2.45}$$

Therefore,

$$\begin{aligned} -\sigma^{\mathrm{d},a}_{\alpha\beta}\omega_{\alpha\beta} &= \frac{I}{2}\,\epsilon_{\alpha\beta\gamma}\,\dot{\Omega}_\gamma\omega_{\alpha\beta} + (H_{\alpha\gamma}Q_{\beta\gamma} - H_{\beta\gamma}Q_{\alpha\gamma})\omega_{\alpha\beta} \\ &= \frac{I}{2}\,\epsilon_{\alpha\beta\gamma}\,\dot{\Omega}_\gamma\omega_{\alpha\beta} + H_{\alpha\beta}(Q_{\gamma\beta}\omega_{\alpha\gamma} + Q_{\gamma\alpha}\omega_{\beta\gamma}), \end{aligned} \tag{2.46}$$

where we have relabeled indices and taken advantage of the symmetry of $H_{\alpha\beta}$ and the antisymmetry of $\omega_{\alpha\beta}$. Defining the co-moving, co-rotational derivative of $Q_{\alpha\beta}$ as

$$\frac{DQ_{\alpha\beta}}{Dt} \equiv \frac{\mathrm{d}Q_{\alpha\beta}}{\mathrm{d}t} + Q_{\gamma\beta}\omega_{\alpha\gamma} + Q_{\gamma\alpha}\omega_{\beta\gamma}, \tag{2.47}$$

we can write the entropy production rate as

$$\begin{aligned} T\sigma =& \mathring{\sigma}^{\mathrm{d},s}_{\alpha\beta}\mathring{u}_{\alpha\beta} + \sigma^{\mathrm{d}}_{\alpha\alpha}\partial_\gamma v_\gamma/3 + \frac{I}{2}\,\epsilon_{\alpha\beta\gamma}\,\dot{\Omega}_\gamma\omega_{\alpha\beta} - \Omega_\alpha\left(\epsilon_{\alpha\beta\gamma}\sigma_{\gamma\beta} - \left(\epsilon_{\alpha\gamma\delta}Q_{\delta\beta} + \epsilon_{\alpha\beta\delta}Q_{\gamma\delta}\right)H_{\gamma\beta}\right) \\ &+ \mathring{H}_{\alpha\beta}\frac{DQ_{\alpha\beta}}{Dt} - \sum_{i\neq 0} j_{i,\alpha}\,\partial_\alpha\bar{\mu}_i - \sum_k r_k A_k. \end{aligned} \tag{2.48}$$

Note that $DQ_{\alpha\beta}/Dt$ is traceless and symmetric.

2.6.8 The axial vector Ω_α as a second order antisymmetric tensor

An axial vector may be written as an antisymmetric second order tensor. We therefore define

$$\Omega_{\alpha\beta} = \epsilon_{\alpha\beta\gamma}\Omega_\gamma. \tag{2.49}$$

Using this fact and symmetry properties of second order tensors, the entropy production rate is, after relabeling indices,

$$T\sigma = \mathring{\sigma}^{\mathrm{d},s}_{\alpha\beta}\mathring{u}_{\alpha\beta} + \sigma^{\mathrm{d}}_{\alpha\alpha}\partial_\gamma v_\gamma/3 + \frac{I}{2}\,\dot{\Omega}_{\alpha\beta}\omega_{\alpha\beta} + \left[\Omega_{\alpha\beta}(\sigma_{\alpha\beta} - H_{\gamma\beta}Q_{\gamma\alpha} + H_{\alpha\gamma}Q_{\beta\gamma})\right]$$

$$+\,\mathring{H}_{\alpha\beta}\frac{DQ_{\alpha\beta}}{Dt}-\sum_{i\neq 0}j_{i,\alpha}\,\partial_\alpha\bar{\mu}_i-\sum_k r_k A_k. \tag{2.50}$$

Since $\Omega_{\alpha\beta}$ is antisymmetric, as is the sum $H_{\alpha\gamma}Q_{\beta\gamma}-H_{\gamma\beta}Q_{\gamma\alpha}$ only the antisymmetric part of the stress tensor may contribute to the entropy production rate in the bracketed term. Using the expression for the antisymmetric part of the stress tensor (2.16), we get, for the bracketed term

$$\Omega_{\alpha\beta}(\sigma_{\alpha\beta}-H_{\gamma\beta}Q_{\gamma\alpha}+H_{\alpha\gamma}Q_{\beta\gamma})=-I\Omega_{\alpha\beta}\dot{\Omega}_{\alpha\beta}/2 \tag{2.51}$$

Therefore, the entropy production rate is

$$T\sigma=\mathring{\sigma}^{\mathrm{d},s}_{\alpha\beta}\mathring{u}_{\alpha\beta}+\sigma^{\mathrm{d}}_{\alpha\alpha}\partial_\gamma v_\gamma/3+\frac{I}{2}\dot{\Omega}_{\alpha\beta}(\omega_{\alpha\beta}-\Omega_{\alpha\beta})+\mathring{H}_{\alpha\beta}\frac{DQ_{\alpha\beta}}{Dt}-\sum_{i\neq 0}j_{i,\alpha}\,\partial_\alpha\bar{\mu}_i-\sum_k r_k A_k. \tag{2.52}$$

2.7 Constitutive relations

2.7.1 Identification of fluxes and forces

Using our expression for the entropy production rate, we identify the thermodynamic fluxes and forces, identifying the molecular field as a *force.*

flux	force	character
$\sigma^{d}_{\gamma\gamma}/3$	$\partial_\gamma v_\gamma$	scalar
r_k	$-A_k$	scalar ($\forall k$)
$j_{i,\alpha}$	$-\partial_\alpha\bar{\mu}_i$	polar vector ($\forall i\neq 0$)
$\mathring{\sigma}^{d,s}_{\alpha\beta}$	$\mathring{u}_{\alpha\beta}$	symmetric, traceless tensor
$DQ_{\alpha\beta}/Dt$	$\mathring{H}_{\alpha\beta}$	symmetric, traceless tensor
$I\dot{\Omega}_{\alpha\beta}/2$	$\omega_{\alpha\beta}-\Omega_{\alpha\beta}$	antisymmetric tensor

2.7.2 Expansion of fluxes

We carry out the expansions of the fluxes to linear order in the forces. With nematic order, the tensors are still invariant to parity inversion. This means, again, that all tensors of odd order are zero. Using this fact, the most general expansion is

$$\sigma^{\mathrm{d}}_{\gamma\gamma}/3=L^{vv}\partial_\gamma v_\gamma-\sum_k L^{vr_k}A_k+L^{vs}_{\alpha\beta}\mathring{u}_{\alpha\beta}+L^{vq}_{\alpha\beta}\mathring{H}_{\alpha\beta}+L^{va}_{\alpha\beta}(\omega_{\alpha\beta}-\Omega_{\alpha\beta}). \tag{2.53}$$

$$r_k=L^{r_k v}\partial_\gamma v_\gamma-\sum_j L^{r_k r_j}A_j+L^{r_k s}_{\alpha\beta}\mathring{u}_{\alpha\beta}+L^{r_k q}_{\alpha\beta}\mathring{H}_{\alpha\beta}+L^{r_k a}_{\alpha\beta}(\omega_{\alpha\beta}-\Omega_{\alpha\beta}).\ \ \forall k \tag{2.54}$$

$$j_{i,\alpha}=-\sum_{j\neq 0}L^{f_i f_j}_{\alpha\beta}\partial_\beta\bar{\mu}_j\ \ \forall i\neq 0 \tag{2.55}$$

$$\mathring{\sigma}^{\mathrm{d},s}_{\alpha\beta}=L^{sv}_{\alpha\beta}\partial_\gamma v_\gamma-\sum_k L^{sr_k}_{\alpha\beta}A_k+L^{ss}_{\alpha\beta\gamma\delta}\mathring{u}_{\gamma\delta}+L^{sq}_{\alpha\beta\gamma\delta}\mathring{H}_{\gamma\delta}+L^{sa}_{\alpha\beta\gamma\delta}(\omega_{\gamma\delta}-\Omega_{\gamma\delta}). \tag{2.56}$$

$$\frac{DQ_{\alpha\beta}}{Dt} = L^{qv}_{\alpha\beta}\partial_\gamma v_\gamma - \sum_k L^{qr_k}_{\alpha\beta} A_k + L^{qs}_{\alpha\beta\gamma\delta}\mathring{u}_{\gamma\delta} + L^{qq}_{\alpha\beta\gamma\delta}\mathring{H}_{\gamma\delta} + L^{qa}_{\alpha\beta\gamma\delta}(\omega_{\gamma\delta} - \Omega_{\gamma\delta}). \tag{2.57}$$

$$I\dot{\Omega}_{\alpha\beta}/2 = L^{av}_{\alpha\beta}\partial_\gamma v_\gamma - \sum_k L^{ar_k}_{\alpha\beta} A_k + L^{as}_{\alpha\beta\gamma\delta}\mathring{u}_{\gamma\delta} + L^{aq}_{\alpha\beta\gamma\delta}\mathring{H}_{\gamma\delta} + L^{aa}_{\alpha\beta\gamma\delta}(\omega_{\gamma\delta} - \Omega_{\gamma\delta}). \tag{2.58}$$

I have called the expansion coefficients L and labeled the expansion coefficients with a superscript to designate what thermodynamic forces they couple. The code is given below.

superscript	thermodynamic force	description of thermodynamic flux
v	$\partial_\gamma v_\gamma$	compressive stress
r_k	$-A_k$	rate of chemical reaction k
f_i	$-\partial_\alpha \bar{\mu}_i$	diffusive flux of species i
s	$\mathring{u}_{\alpha\beta}$	shear stress
q	$\mathring{H}_{\alpha\beta}$	order parameter alignment
a	$\omega_{\alpha\beta} - \Omega_{\alpha\beta}$	rotational stress

The subscripts of the expansion coefficients L indicate their tensorial order.

2.7.3 Rotational invariance: application of the Curie principle

The system must have the same symmetry properties as the order parameter. In general the expansion coefficients (the Ls), are functions of the intensive thermodynamic variables, including the order parameter $Q_{\alpha\beta}$. Therefore, the zeroth order L tensors may be written as expansions of $Q_{\alpha\beta}$,

$$L = L_0 + L_2 Q_{\alpha\beta} Q_{\alpha\beta} + \ldots, \tag{2.59}$$

where the first order term vanishes because $Q_{\alpha\alpha} = 0$. Similarly, the second order tensors may be expanded as

$$L_{\alpha\beta} = L_0 \delta_{\alpha\beta} + L_1 Q_{\alpha\beta} + L_2 Q_{\alpha\gamma} Q_{\gamma\beta} + \ldots, \tag{2.60}$$

where we have taken the zeroth order term to be that appearing in the absense of nematic order. Likewise for fourth order tensors,

$$\begin{aligned} L_{\alpha\beta\gamma\delta} =& L^a_0 \left(\frac{1}{2}(\delta_{\alpha\delta}\delta_{\beta\gamma} + \delta_{\alpha\gamma}\delta_{\beta\delta}) - \frac{1}{3}\delta_{\alpha\beta}\delta_{\gamma\delta}\right) + \frac{L^b_0}{2}(\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\gamma}\delta_{\beta\delta}) + L^c_0 \delta_{\alpha\beta}\delta_{\gamma\delta} \\ &+ L^a_1 Q_{\beta\delta}\delta_{\alpha\gamma} + L^b_1 Q_{\beta\gamma}\delta_{\alpha\delta} + L^c_1 Q_{\alpha\gamma}\delta_{\beta\delta} + L^d_1 Q_{\alpha\delta}\delta_{\beta\gamma} + L^e_1 Q_{\gamma\delta}\delta_{\alpha\beta} + L^f_1 Q_{\alpha\beta}\delta_{\gamma\delta} \\ &+ L_2 Q_{\alpha\beta} Q_{\gamma\delta} + \ldots. \end{aligned} \tag{2.61}$$

There are six terms that are first order in $Q_{\alpha\beta}$, since $Q_{\alpha\beta}$ and $\delta_{\alpha\beta}$ are symmetric. If they were not, there would be 24 terms, e.g., $Q_{\alpha\beta}\delta_{\gamma\delta} = Q_{\alpha\beta}\delta_{\delta\gamma} = Q_{\beta\alpha}\delta_{\gamma\delta} = Q_{\beta\alpha}\delta_{\delta\gamma}$.

Going forward, we will only consider terms up to first order in $Q_{\alpha\beta}$ and use the above relations for the expansion coefficients, (the Ls).

Compressive stress. We now consider the constitutive relation for the compressive stress, $\sigma^{\mathrm{d}}_{\gamma\gamma}$. Using the above relations,

$$L^{vs}_{\alpha\beta} = L^{vs}_0 \delta_{\alpha\beta} + L^{vs} Q_{\alpha\beta}, \quad L^{vq}_{\alpha\beta} = L^{vq}_0 \delta_{\alpha\beta} + L^{vq} Q_{\alpha\beta}, \text{ and } L^{va}_{\alpha\beta} = L^{va}_0 \delta_{\alpha\beta} + L^{va}_1 Q_{\alpha\beta}. \tag{2.62}$$

Therefore, we have

$$L^{va}_{\alpha\beta}(\omega_{\alpha\beta} - \Omega_{\alpha\beta}) = 0, \tag{2.63}$$

due to the symmetry (to first order in the order parameter) of $L^{va}_{\alpha\beta}$ and the antisymmetry of $\omega_{\alpha\beta}$ and $\Omega_{\alpha\beta}$. Due to the tracelessness of $\mathring{u}_{\alpha\beta}$ and $\mathring{H}_{\alpha\beta}$,

$$L^{vs}_{\alpha\beta}\mathring{u}_{\alpha\beta} = L^{vs}Q_{\alpha\beta}\mathring{u}_{\alpha\beta}, \tag{2.64}$$

$$L^{vs}_{\alpha\beta}\mathring{H}_{\alpha\beta} = L^{vq}Q_{\alpha\beta}\mathring{H}_{\alpha\beta}. \tag{2.65}$$

Thus, we have

$$\sigma^{\mathrm{d}}_{\gamma\gamma}/3 = L^{vv}\partial_\gamma v_\gamma - \sum_k L^{vr_k}A_k + L^{vs}Q_{\alpha\beta}\mathring{u}_{\alpha\beta} + L^{vq}Q_{\alpha\beta}\mathring{H}_{\alpha\beta}. \tag{2.66}$$

Chemical reaction rates. We now consider the constitutive relations for the chemical reaction rates. As scalar quantities, their constitutive relations are similar to the compressive stress.

$$r_k = L^{r_k v}\partial_\gamma v_\gamma - \sum_j L^{r_k r_j}A_j + L^{r_k s}Q_{\alpha\beta}\mathring{u}_{\alpha\beta} + L^{r_k q}Q_{\alpha\beta}\mathring{H}_{\alpha\beta} \;\forall k. \tag{2.67}$$

Chemical fluxes. The chemical fluxes, to first order in $Q_{\alpha\beta}$ are

$$j_{i,\alpha} = -\sum_{j\neq 0}\left(L^{f_i f_j}_0 \partial_\alpha \bar{\mu}_j + L^{f_i f_j}_1 Q_{\alpha\beta}\partial_\beta\bar{\mu}_j\right) \;\; \forall i. \tag{2.68}$$

Shear stress. We now consider the shear stress to first order in $Q_{\alpha\beta}$. Recall

$$\mathring{\sigma}^{\mathrm{d},s}_{\alpha\beta} = L^{sv}_{\alpha\beta}\partial_\gamma v_\gamma - \sum_k L^{sr_k}_{\alpha\beta}A_k + L^{ss}_{\alpha\beta\gamma\delta}\mathring{u}_{\gamma\delta} + L^{sq}_{\alpha\beta\gamma\delta}\mathring{H}_{\gamma\delta} + L^{sa}_{\alpha\beta\gamma\delta}(\omega_{\gamma\delta} - \Omega_{\gamma\delta}). \tag{2.69}$$

We first consider

$$L^{sv}_{\alpha\beta}\partial_\gamma v_\gamma = \left(L^{sv}_0\delta_{\alpha\beta} + L^{sv}_1 Q_{\alpha\beta}\right)\partial_\gamma v_\gamma. \tag{2.70}$$

Because $\mathring{\sigma}^{\mathrm{d},s}_{\alpha\beta}$ is traceless, $L^{sv}_0 = 0$. Similar arguments hold for $L^{sr_k}_{\alpha\beta}A_k$. Next, consider

$$\begin{aligned} L^{ss}_{\alpha\beta\gamma\delta}\mathring{u}_{\gamma\delta} = {} & \left(L^{ss,a}_0\left(\frac{1}{2}(\delta_{\alpha\delta}\delta_{\beta\gamma} + \delta_{\alpha\gamma}\delta_{\beta\delta}) - \frac{1}{3}\,\delta_{\alpha\beta}\delta_{\gamma\delta}\right) + \frac{L^{ss,b}_0}{2}(\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\gamma}\delta_{\beta\delta}) + L^{ss,c}_0\delta_{\alpha\beta}\delta_{\gamma\delta}\right)\mathring{u}_{\gamma\delta} \\ & + \left(L^{ss,a}_1 Q_{\beta\delta}\delta_{\alpha\gamma} + L^{ss,b}_1 Q_{\beta\gamma}\delta_{\alpha\delta} + L^{ss,c}_1 Q_{\alpha\gamma}\delta_{\beta\delta} + L^{ss,d}_1 Q_{\alpha\delta}\delta_{\beta\gamma} + L^{ss,e}_1 Q_{\gamma\delta}\delta_{\alpha\beta} + L^{ss,f}_1 Q_{\alpha\beta}\delta_{\gamma\delta}\right)\mathring{u}_{\gamma\delta}. \end{aligned} \tag{2.71}$$

By the same arguments as in section 1.6.6, the first term is $L^{ss,a}_0\mathring{u}_{\alpha\beta}$. We now consider the remaining terms.

$$L^{ss,a}_1 Q_{\beta\delta}\delta_{\alpha\gamma}\mathring{u}_{\gamma\delta} = L^{ss,a}_1 Q_{\beta\delta}\mathring{u}_{\alpha\delta} = L^{ss,a}_1 Q_{\beta\gamma}\mathring{u}_{\gamma\alpha} \tag{2.72}$$

$$L^{ss,b}_1 Q_{\beta\gamma}\delta_{\alpha\delta}\mathring{u}_{\gamma\delta} = L^{ss,b}_1 Q_{\beta\gamma}\mathring{u}_{\gamma\alpha} \tag{2.73}$$

$$L^{ss,c}_1 Q_{\alpha\gamma}\delta_{\beta\delta}\mathring{u}_{\gamma\alpha} = L^{ss,c}_1 Q_{\alpha\gamma}\mathring{u}_{\gamma\beta} \tag{2.74}$$

$$L_1^{ss,d} Q_{\alpha\delta}\delta_{\beta\gamma}\mathring{u}_{\gamma\delta} = L_1^{ss,d} Q_{\alpha\delta}\mathring{u}_{\beta\delta} = L_1^{ss,d} Q_{\alpha\gamma}\mathring{u}_{\gamma\beta} \tag{2.75}$$

$$L_1^{ss,e} Q_{\gamma\delta}\delta_{\alpha\beta}\mathring{u}_{\gamma\delta} = L_1^{ss,e}(Q_{\gamma\delta}\mathring{u}_{\gamma\delta})\delta_{\alpha\beta} \tag{2.76}$$

$$L_1^{ss,f} Q_{\alpha\beta}\delta_{\gamma\delta}\mathring{u}_{\gamma\delta} = L_1^{ss,f} Q_{\alpha\beta}\mathring{u}_{\delta\delta} = 0. \tag{2.77}$$

Therefore, we have

$$L^{ss}_{\alpha\beta\gamma\delta}\mathring{u}_{\gamma\delta} = L_0^{ss,a}\mathring{u}_{\alpha\beta} + \left(L_1^{ss,a} + L_1^{ss,b}\right) Q_{\beta\gamma}\mathring{u}_{\gamma\alpha} + \left(L_1^{ss,c} + L_1^{ss,d}\right) Q_{\alpha\gamma}\mathring{u}_{\gamma\beta} + L_1^{ss,e}(Q_{\gamma\delta}\mathring{u}_{\gamma\delta})\delta_{\alpha\beta}. \tag{2.78}$$

In order for $\mathring{\sigma}^{\mathrm{d},s}_{\alpha\beta}$ to be traceless and symmetric, $L_1^{ss,a} = L_1^{ss,b} = L_1^{ss,c} = L_1^{ss,d} \equiv L_1^{ss}/4$, and $L_1^{ss,e} = -L_1^{ss}/3$. Therefore,

$$L^{ss}_{\alpha\beta\gamma\delta}\mathring{u}_{\gamma\delta} = L_0^{ss}\mathring{u}_{\alpha\beta} + L_1^{ss}\left(\frac{1}{2}(Q_{\beta\gamma}\mathring{u}_{\gamma\alpha} + Q_{\alpha\gamma}\mathring{u}_{\gamma\beta}) - \frac{1}{3}(Q_{\gamma\delta}\mathring{u}_{\delta\gamma})\delta_{\alpha\beta}\right). \tag{2.79}$$

Similar arguments apply for the $L^{sq}_{\alpha\beta\gamma\delta}\mathring{H}_{\gamma\delta}$ term.

$$L^{sq}_{\alpha\beta\gamma\delta}\mathring{u}_{\gamma\delta} = L_0^{sq}\mathring{H}_{\alpha\beta} + L_1^{sq}\left(\frac{1}{2}(Q_{\beta\gamma}\mathring{H}_{\gamma\alpha} + Q_{\alpha\gamma}\mathring{H}_{\gamma\beta}) - \frac{1}{3}(Q_{\gamma\delta}\mathring{H}_{\delta\gamma})\delta_{\alpha\beta}\right). \tag{2.80}$$

For the $L^{sa}_{\alpha\beta\gamma\delta}(\omega_{\alpha\beta} - \Omega_{\alpha\beta})$ term, the first term vanishes, again by the same arguments as in section 1.6.6. Defining $A^a_{\alpha\beta} = \omega_{\alpha\beta} - \Omega_{\alpha\beta}$ for notational convenience, he latter terms linear in the order parameter are

$$L_1^{sa,a} Q_{\beta\delta}\delta_{\alpha\gamma}A^a_{\gamma\delta} = L_1^{sa,a} Q_{\beta\delta}A^a_{\alpha\delta} = L_1^{sa,a} Q_{\beta\gamma}A^a_{\gamma\alpha} \tag{2.81}$$

$$L_1^{sa,b} Q_{\beta\gamma}\delta_{\alpha\delta}A^a_{\gamma\delta} = L_1^{sa,b} Q_{\beta\gamma}A^a_{\gamma\alpha} \tag{2.82}$$

$$L_1^{sa,c} Q_{\alpha\gamma}\delta_{\beta\delta}A^a_{\gamma\alpha} = L_1^{sa,c} Q_{\alpha\gamma}A^a_{\gamma\beta} \tag{2.83}$$

$$L_1^{sa,d} Q_{\alpha\delta}\delta_{\beta\gamma}A^a_{\gamma\delta} = L_1^{sa,d} Q_{\alpha\delta}A^a_{\beta\delta} = L_1^{sa,d} Q_{\alpha\gamma}A^a_{\gamma\beta} \tag{2.84}$$

$$L_1^{sa,e} Q_{\gamma\delta}\delta_{\alpha\beta}A^a_{\gamma\delta} = L_1^{sa,e}(Q_{\gamma\delta}A^a_{\gamma\delta})\delta_{\alpha\beta} = 0 \tag{2.85}$$

$$L_1^{sa,f} Q_{\alpha\beta}\delta_{\gamma\delta}A^a_{\gamma\delta} = L_1^{sa,f} Q_{\alpha\beta}A^a_{\delta\delta} = 0. \tag{2.86}$$

Thus, we have

$$L^{sa}_{\alpha\beta\gamma\delta}A^a_{\gamma\delta} = \left(L_1^{sa,a} + L_1^{sa,b}\right) Q_{\beta\gamma}A^a_{\gamma\alpha} + \left(L_1^{sa,c} + L_1^{sa,d}\right) Q_{\alpha\gamma}A^a_{\gamma\beta}. \tag{2.87}$$

In order for $\mathring{\sigma}_{\alpha\beta}$ to be symmetric (tracelessness is automatically satisfied), $L_1^{sa,a} = L_1^{sa,b} = -L_1^{sa,c} = -L_1^{sa,d} \equiv L^{sa}/4$. Therefore, we have, to first order in $Q_{\alpha\beta}$,

$$\begin{aligned}\mathring{\sigma}^{\mathrm{d},s}_{\alpha\beta} =& L^{sv}Q_{\alpha\beta}\partial_\gamma v_\gamma - \sum_k L^{sr_k}Q_{\alpha\beta}A_k + L_0^{ss}\mathring{u}_{\alpha\beta} + L_1^{ss}\left(\frac{1}{2}(Q_{\beta\gamma}\mathring{u}_{\gamma\alpha} + Q_{\alpha\gamma}\mathring{u}_{\gamma\beta}) - \frac{1}{3}(Q_{\gamma\delta}\mathring{u}_{\delta\gamma})\delta_{\alpha\beta}\right)\\ &+ L_0^{sq}\mathring{H}_{\alpha\beta} + L_1^{sq}\left(\frac{1}{2}(Q_{\beta\gamma}\mathring{H}_{\gamma\alpha} + Q_{\alpha\gamma}\mathring{H}_{\gamma\beta}) - \frac{1}{3}(Q_{\gamma\delta}\mathring{H}_{\delta\gamma})\delta_{\alpha\beta}\right)\\ &+ L^{sa}\left(Q_{\alpha\gamma}(\omega_{\gamma\beta} - \Omega_{\gamma\beta}) - Q_{\beta\gamma}(\omega_{\gamma\alpha} - \Omega_{\gamma\alpha})\right).\end{aligned} \tag{2.88}$$

Order parameter alignment. The analysis for order parameter alignment proceeds exactly as for the shear stress.

$$\begin{aligned}\frac{DQ_{\alpha\beta}}{Dt} &= L^{qv}Q_{\alpha\beta}\partial_\gamma v_\gamma - \sum_k L^{qr_k}Q_{\alpha\beta}A_k + L_0^{qs}\mathring{u}_{\alpha\beta} + L_1^{qs}\left(\frac{1}{2}(Q_{\beta\gamma}\mathring{u}_{\gamma\alpha} + Q_{\alpha\gamma}\mathring{u}_{\gamma\beta}) - \frac{1}{3}(Q_{\gamma\delta}\mathring{u}_{\delta\gamma})\delta_{\alpha\beta}\right) \\ &\quad + L_0^{qq}\mathring{H}_{\alpha\beta} + L_1^{qq}\left(\frac{1}{2}(Q_{\beta\gamma}\mathring{H}_{\gamma\alpha} + Q_{\alpha\gamma}\mathring{H}_{\gamma\beta}) - \frac{1}{3}(Q_{\gamma\delta}\mathring{H}_{\delta\gamma})\delta_{\alpha\beta}\right) \\ &\quad + L^{qa}\left(Q_{\alpha\gamma}(\omega_{\gamma\beta} - \Omega_{\gamma\beta}) - Q_{\beta\gamma}(\omega_{\gamma\alpha} - \Omega_{\gamma\alpha})\right). \end{aligned} \tag{2.89}$$

Rotational stress. The rate of change rotational stress is an antisymmetric tensor. Recall,

$$I\dot{\Omega}_{\alpha\beta}/2 = L^{av}_{\alpha\beta}\partial_\gamma v_\gamma - \sum_k L^{ar_k}_{\alpha\beta}A_k + L^{as}_{\alpha\beta\gamma\delta}\mathring{u}_{\gamma\delta} + L^{aq}_{\alpha\beta\gamma\delta}\mathring{H}_{\gamma\delta} + L^{aa}_{\alpha\beta\gamma\delta}(\omega_{\gamma\delta} - \Omega_{\gamma\delta}). \tag{2.90}$$

Since $L^{av}_{\alpha\beta} = L_0^{av}\delta_{\alpha\beta} + L_1^{av}Q_{\alpha\beta}$ is a symmetric tensor, $L^{av}_{\alpha\beta}\partial_\gamma v_\gamma = 0$. A similar argument holds for $L^{ar_k}_{\alpha\beta}$. We now consider

$$\begin{aligned} L^{as}_{\alpha\beta\gamma\delta}\mathring{u}_{\gamma\delta} &= \left(L_0^{as,a}\left(\frac{1}{2}(\delta_{\alpha\delta}\delta_{\beta\gamma} + \delta_{\alpha\gamma}\delta_{\beta\delta}) - \frac{1}{3}\delta_{\alpha\beta}\delta_{\gamma\delta}\right) + \frac{L_0^{as,b}}{2}(\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\gamma}\delta_{\beta\delta}) + L_0^{as,c}\delta_{\alpha\beta}\delta_{\gamma\delta}\right)\mathring{u}_{\gamma\delta} \\ &\quad + \left(L_1^{as,a}Q_{\beta\delta}\delta_{\alpha\gamma} + L_1^{as,b}Q_{\beta\gamma}\delta_{\alpha\delta} + L_1^{as,c}Q_{\alpha\gamma}\delta_{\beta\delta} + L_1^{as,d}Q_{\alpha\delta}\delta_{\beta\gamma} + L_1^{as,e}Q_{\gamma\delta}\delta_{\alpha\beta} + L_1^{as,f}Q_{\alpha\beta}\delta_{\gamma\delta}\right)\mathring{u}_{\gamma\delta}. \end{aligned} \tag{2.91}$$

By the same arguments of section 1.6.6, the term that is zero order in $Q_{\alpha\beta}$ vanishes. Using the results from our analysis of the shear stress, we have

$$L^{as}_{\alpha\beta\gamma\delta}\mathring{u}_{\gamma\delta} = \left(L_1^{as,a} + L_1^{as,b}\right)Q_{\beta\gamma}\mathring{u}_{\gamma\alpha} + \left(L_1^{as,c} + L_1^{as,d}\right)Q_{\alpha\gamma}\mathring{u}_{\gamma\beta} + L_1^{as,e}(Q_{\gamma\delta}\mathring{u}_{\gamma\delta})\delta_{\alpha\beta}. \tag{2.92}$$

In order for this to equal an antisymmetric tensor, $L_1^{as,a} = L_1^{as,b} = -L_1^{as,c} = -L_1^{as,d} \equiv -L_1^{as}/4$, and $L_1^{as,e} = 0$. Thus, we have

$$L^{as}_{\alpha\beta\gamma\delta}\mathring{u}_{\gamma\delta} = \frac{L_1^{as}}{2}(Q_{\beta\gamma}\mathring{u}_{\gamma\alpha} - Q_{\alpha\gamma}\mathring{u}_{\gamma\beta}). \tag{2.93}$$

Similarly,

$$L^{as}_{\alpha\beta\gamma\delta}\mathring{H}_{\gamma\delta} = \frac{L_1^{aq}}{2}(Q_{\beta\gamma}\mathring{H}_{\gamma\alpha} - Q_{\alpha\gamma}\mathring{H}_{\gamma\beta}). \tag{2.94}$$

Finally,

$$L^{aa}_{\alpha\beta\gamma\delta}A^a_{\gamma\delta} = \left(L_1^{aa,a} + L_1^{aa,b}\right)Q_{\beta\gamma}A^a_{\gamma\alpha} + \left(L_1^{aa,c} + L_1^{aa,d}\right)Q_{\alpha\gamma}A^a_{\gamma\beta} + L_1^{aa,e}(Q_{\gamma\delta}A^a_{\gamma\delta})\delta_{\alpha\beta}. \tag{2.95}$$

For this to equal an antisymmetric tensor, $L_1^{aa,a} = L_1^{aa,b} = L_1^{aa,c} = L_1^{aa,d} \equiv L_1^{aa}/4$. Note that $Q_{\gamma\delta}A^a_{\gamma\delta} = 0$. Therefore, we have

$$\begin{aligned} I\dot{\Omega}_{\alpha\beta}/2 &= \frac{L_1^{as}}{2}(Q_{\beta\gamma}\mathring{u}_{\gamma\alpha} - Q_{\alpha\gamma}\mathring{u}_{\gamma\beta}) + \frac{L_1^{aq}}{2}(Q_{\beta\gamma}\mathring{H}_{\gamma\alpha} - Q_{\alpha\gamma}\mathring{H}_{\gamma\beta}) \\ &\quad + \frac{L_1^{aa}}{2}\left(Q_{\beta\gamma}(\omega_{\gamma\alpha} - \Omega_{\gamma\alpha}) + Q_{\alpha\gamma}(\omega_{\gamma\beta} - \Omega_{\gamma\beta})\right). \end{aligned} \tag{2.96}$$

Updated consitutive relations. The updated constitutive relations are

$$\sigma^{\mathrm{d}}_{\gamma\gamma}/3 = L^{vv}\partial_\gamma v_\gamma - \sum_k L^{vr_k} A_k + L^{vs} Q_{\alpha\beta}\mathring{u}_{\alpha\beta} + L^{vq} Q_{\alpha\beta}\mathring{H}_{\alpha\beta} \tag{2.97}$$

$$r_k = L^{r_k v}\partial_\gamma v_\gamma - \sum_j L^{r_k r_j} A_j + L^{r_k s} Q_{\alpha\beta}\mathring{u}_{\alpha\beta} + L^{r_k q} Q_{\alpha\beta}\mathring{H}_{\alpha\beta} \;\forall k \tag{2.98}$$

$$j_{i,\alpha} = -\sum_{j\neq 0}\left(L_0^{f_i f_j}\partial_\alpha \bar{\mu}_j + L_1^{f_i f_j} Q_{\alpha\beta}\partial_\beta \bar{\mu}_j\right) \quad \forall i \tag{2.99}$$

$$\begin{aligned}
\mathring{\sigma}^{\mathrm{d},s}_{\alpha\beta} = {} & L^{sv} Q_{\alpha\beta}\partial_\gamma v_\gamma - \sum_k L^{sr_k} Q_{\alpha\beta} A_k + L_0^{ss}\mathring{u}_{\alpha\beta} + L_1^{ss}\left(\frac{1}{2}(Q_{\beta\gamma}\mathring{u}_{\gamma\alpha} + Q_{\alpha\gamma}\mathring{u}_{\gamma\beta}) - \frac{1}{3}(Q_{\gamma\delta}\mathring{u}_{\delta\gamma})\delta_{\alpha\beta}\right) \\
& + L_0^{sq}\mathring{H}_{\alpha\beta} + L_1^{sq}\left(\frac{1}{2}(Q_{\beta\gamma}\mathring{H}_{\gamma\alpha} + Q_{\alpha\gamma}\mathring{H}_{\gamma\beta}) - \frac{1}{3}(Q_{\gamma\delta}\mathring{H}_{\delta\gamma})\delta_{\alpha\beta}\right) \\
& + L^{sa}\left(Q_{\alpha\gamma}(\omega_{\gamma\beta} - \Omega_{\gamma\beta}) - Q_{\beta\gamma}(\omega_{\gamma\alpha} - \Omega_{\gamma\alpha})\right)
\end{aligned} \tag{2.100}$$

$$\begin{aligned}
\frac{DQ_{\alpha\beta}}{Dt} = {} & L^{qv} Q_{\alpha\beta}\partial_\gamma v_\gamma - \sum_k L^{qr_k} Q_{\alpha\beta} A_k + L_0^{qs}\mathring{u}_{\alpha\beta} + L_1^{qs}\left(\frac{1}{2}(Q_{\beta\gamma}\mathring{u}_{\gamma\alpha} + Q_{\alpha\gamma}\mathring{u}_{\gamma\beta}) - \frac{1}{3}(Q_{\gamma\delta}\mathring{u}_{\delta\gamma})\delta_{\alpha\beta}\right) \\
& + L_0^{qq}\mathring{H}_{\alpha\beta} + L_1^{qq}\left(\frac{1}{2}(Q_{\beta\gamma}\mathring{H}_{\gamma\alpha} + Q_{\alpha\gamma}\mathring{H}_{\gamma\beta}) - \frac{1}{3}(Q_{\gamma\delta}\mathring{H}_{\delta\gamma})\delta_{\alpha\beta}\right) \\
& + L^{qa}\left(Q_{\alpha\gamma}(\omega_{\gamma\beta} - \Omega_{\gamma\beta}) - Q_{\beta\gamma}(\omega_{\gamma\alpha} - \Omega_{\gamma\alpha})\right)
\end{aligned} \tag{2.101}$$

$$\begin{aligned}
I\dot{\Omega}_{\alpha\beta}/2 = {} & \frac{L_1^{as}}{2}(Q_{\beta\gamma}\mathring{u}_{\gamma\alpha} - Q_{\alpha\gamma}\mathring{u}_{\gamma\beta}) + \frac{L_1^{aq}}{2}(Q_{\beta\gamma}\mathring{H}_{\gamma\alpha} - Q_{\alpha\gamma}\mathring{H}_{\gamma\beta}) \\
& + \frac{L_1^{aa}}{2}\left(Q_{\beta\gamma}(\omega_{\gamma\alpha} - \Omega_{\gamma\alpha}) + Q_{\alpha\gamma}(\omega_{\gamma\beta} - \Omega_{\gamma\beta})\right).
\end{aligned} \tag{2.102}$$

2.7.4 Onsager relations

The Onsager relations stipulate

$$L^{vr_k} = -L^{r_k v} \;\forall k \tag{2.103}$$

$$L^{vs} = L^{sv} \tag{2.104}$$

$$L^{vq} = -L^{qv} \tag{2.105}$$

$$L^{r_k s} = -L^{sr_k} \;\forall k \tag{2.106}$$

$$L^{r_k q} = L^{qr_k} \;\forall k \tag{2.107}$$

$$L_0^{f_i f_j} = L_0^{f_j f_i} \;\forall i, j \tag{2.108}$$

$$L_0^{sq} = -L_0^{qs} \tag{2.109}$$

$$L_1^{sq} = -L_1^{qs} \tag{2.110}$$

$$L^{sa} = L^{as}. \tag{2.111}$$

Furthermore,

$$L^{jj} > 0 \, \forall j \in \{v, r_k, f_i, s, q, a\}. \tag{2.112}$$

2.7.5 Simplification of constitutive relations: neglect of internal inertia and $Q_{\alpha\beta}$-dependence of viscosity

We now make a few simplifying assumptions. First, we neglect the internal rotation, as described in section 2.4.2. This means that all terms involving $\omega_{\alpha\beta} - \Omega_{\alpha\beta}$ are ignored. Secondly, we assume that the viscosities are independent of the order parameter (as suggested by Olmsted and Goldbart, *PRA*, 1990). This means that all fourth order tensors are expanded only to zeroth order in $Q_{\alpha\beta}$. Finally, we now make the following definitions.

$$\eta_v \equiv L^{vv}, \ \eta \equiv L_0^{ss}/2, \beta_1 \equiv -L_0^{sq}, \ \beta_2 \equiv 1/L_0^{qq}. \tag{2.113}$$

We then get the following constitutive relations, also applying the Onsager relations.

$$\sigma^{\mathrm{d}}_{\gamma\gamma}/3 = \eta_v \partial_\gamma v_\gamma + \sum_k L^{r_k v} A_k \tag{2.114}$$

$$r_k = L^{r_k v} \partial_\gamma v_\gamma - \sum_j L^{r_k r_j} A_j + L^{r_k s} Q_{\alpha\beta} \mathring{u}_{\alpha\beta} + L^{r_k q} Q_{\alpha\beta} \mathring{H}_{\alpha\beta} \ \ \forall k \tag{2.115}$$

$$j_{i,\alpha} = -\sum_{j\neq 0} \left(L_0^{f_i f_j} \partial_\alpha \bar{\mu}_j + L_1^{f_i f_j} Q_{\alpha\beta} \partial_\beta \bar{\mu}_j \right) \ \ \forall i \tag{2.116}$$

$$\mathring{\sigma}^{\mathrm{d},s}_{\alpha\beta} = \sum_k L^{r_k s} Q_{\alpha\beta} A_k + 2\eta \mathring{u}_{\alpha\beta} - \beta_1 \mathring{H}_{\alpha\beta} \tag{2.117}$$

$$\frac{DQ_{\alpha\beta}}{Dt} = L^{r_k q} Q_{\alpha\beta} A_k + \beta_1 \mathring{u}_{\alpha\beta} + \beta_2^{-1} \mathring{H}_{\alpha\beta}. \tag{2.118}$$

2.7.6 Further simplification of constitutive relations: neglect of anisotropic diffusion

We should treat the diffusion as anisotropic, with non-vanishing $L_1^{f_i f_j}$. We defer this until later, and for now assume diffusion is isotropic. We can again define a diffusivity tensor and write

$$j_{i,\alpha} = -m_i \sum_{j\neq 0} D_{ij} \partial_\alpha n_j. \tag{2.119}$$

2.8 Nematic dynamical equations

The dynamical equations are given by

$$\frac{\mathrm{d}n_i}{\mathrm{d}t} = -n_i \partial_\alpha v_\alpha + \partial_\alpha \sum_{j\neq 0} D_{ij} \, \partial_\alpha n_j + \sum_k \nu_{ki} r_k \tag{2.120}$$

$$\rho \frac{\mathrm{d}v_\alpha}{\mathrm{d}t} = \partial_\beta \sigma_{\alpha\beta} \tag{2.121}$$

$$\frac{DQ_{\alpha\beta}}{Dt} = L^{r_k q} Q_{\alpha\beta} A_k + \beta_1 \mathring{u}_{\alpha\beta} + \beta_2^{-1} \mathring{H}_{\alpha\beta}, \tag{2.122}$$

where the latter is simply a constitutive relation.

2.8.1 The total stress tensor

The total stress tensor is

$$\sigma_{\alpha\beta} = \sigma^{\mathrm{d}}_{\alpha\beta} + \sigma^{\mathrm{e}}_{\alpha\beta} = \mathring{\sigma}^{\mathrm{d},s}_{\alpha\beta} + \frac{1}{3}\sigma^{\mathrm{d}}_{\gamma\gamma}\delta_{\alpha\beta} + \sigma^{\mathrm{d},a}_{\alpha\beta} + \sigma^{\mathrm{e}}_{\alpha\beta}. \tag{2.123}$$

We use the above constitutive relations for $\mathring{\sigma}^{\mathrm{d},s}_{\alpha\beta}$ and $\sigma^{\mathrm{d}}_{\gamma\gamma}$, (2.16) for $\sigma^{\mathrm{d},a}_{\alpha\beta}$, and (2.41) for the $\sigma^{\mathrm{e}}_{\alpha\beta}$. Therefore, the total stress tensor is

$$\begin{aligned} \sigma_{\alpha\beta} = {} & 2\eta\mathring{u}_{\alpha\beta} + \eta_v \partial_\gamma v_\gamma \delta_{\alpha\beta} \\ & - \beta_1 \mathring{H}_{\alpha\beta} \\ & + \sum_k L^{r_k s} Q_{\alpha\beta} A_k + \sum_k L^{r_k v} A_k \delta_{\alpha\beta} \\ & - H_{\alpha\gamma} Q_{\beta\gamma} + H_{\beta\gamma} Q_{\alpha\gamma} \\ & - p\delta_{\alpha\beta} - \pi_{\gamma\delta\alpha} \partial_\beta Q_{\gamma\delta}. \end{aligned} \tag{2.124}$$

The first line is the isotropic deviatoric stress, the second is the stress due to alignment with the molecular field, the third is the active stress (due to chemical reactions), the fourth is the antisymmetric part of the deviatoric stress, and the last line is the reversible (Ericksen) stress.

2.8.2 Simplification of the total stress: neglect of second order terms in $H_{\alpha\beta}$ and $Q_{\alpha\beta}$

The total stress tensor is further simplified if we neglect terms that are above first order in the molecular field and order parameter. In this case, the stress tensor is symmetric.

$$\sigma_{\alpha\beta} = 2\eta\mathring{u}_{\alpha\beta} + \eta_v \partial_\gamma v_\gamma \delta_{\alpha\beta} - \beta_1 \mathring{H}_{\alpha\beta} + \sum_k L^{r_k s} Q_{\alpha\beta} A_k + \sum_k L^{r_k v} A_k \delta_{\alpha\beta} - p\delta_{\alpha\beta}. \tag{2.125}$$

2.8.3 Further simplification of the total stress: equality of viscosities

We make a further approximation that $\eta_v = \eta$. Then, we have

$$\sigma_{\alpha\beta} = 2\eta u_{\alpha\beta} - \beta_1 \mathring{H}_{\alpha\beta} + \sum_k L^{r_k s} Q_{\alpha\beta} A_k + \sum_k L^{r_k v} A_k \delta_{\alpha\beta} - p\delta_{\alpha\beta}, \tag{2.126}$$

where $u_{\alpha\beta} \equiv (\partial_\alpha v_\beta + \partial_\beta v_\alpha)/2$ is the symmetric part of the velocity gradient tensor.

2.8.4 Special case: fast ATP consumption, mass action kinetics, incompressible fluid, diagonal diffusivity tensor

We now consider the special case where ATP is in abundance and diffuses infinitely quickly. In this case, the affinity for the hydrolysis of ATP,

$$\mathrm{ATP} \rightarrow \mathrm{ADP} + \mathrm{Pi}, \tag{2.127}$$

which we will call reaction 0, is

$$A_0 = \mu_{\mathrm{ADP}} + \mu_{\mathrm{Pi}} - \mu_{\mathrm{ATP}} \equiv \Delta\mu, \tag{2.128}$$

which is constant. We define $L^{r_0 s} = \zeta$, $L^{r_0 v} = \bar{\zeta}$, and $L^{r_0 q} = \lambda$. We assume that no other chemical reactions contribute to the stress of alignment of the order parameter, or $L^{r_k s} = L^{r_k q} = 0 \quad \forall k \neq 0$. Thus, the stress tensor is

$$\sigma_{\alpha\beta} = 2\eta u_{\alpha\beta} - \beta_1 \mathring{H}_{\alpha\beta} + \zeta \Delta\mu Q_{\alpha\beta} + (\bar{\zeta}\Delta\mu - p)\delta_{\alpha\beta}. \tag{2.129}$$

The order parameter is governed by

$$\frac{DQ_{\alpha\beta}}{Dt} = \beta_1 \mathring{u}_{\alpha\beta} + \beta_2^{-1}\mathring{H}_{\alpha\beta} + \lambda\Delta\mu Q_{\alpha\beta}. \tag{2.130}$$

If we further assume that the chemical reaction rates (with the exception of ATP hydrolysis), are governed by mass action kinetics, i.e.,

$$r_k \approx \prod_{i \text{ for which } \nu_{ki}<0} k_{ki} n_i^{-\nu_{ki}}. \tag{2.131}$$

This means that the terms containing to the chemical affinities in the constitutive relation for r_k dominate the other terms in the sum. Further, is we assume the diffusivity tensor is diagonal, we have

$$\frac{\mathrm{d}n_i}{\mathrm{d}t} = -n_i \partial_\alpha v_\alpha + D_i \partial_\alpha \partial_\alpha n_i + \sum_k \nu_{ki} \prod_{i \text{ for which } \nu_{ki}<0} k_{ki} n_i^{-\nu_{ki}}. \tag{2.132}$$

If we further assume that the fluid is incompressible ($\partial_\gamma v_\gamma = 0$ and $u_{\alpha\beta} = \mathring{u}_{\alpha\beta}$), we get

$$\sigma_{\alpha\beta} = 2\eta u_{\alpha\beta} - \beta_1 \mathring{H}_{\alpha\beta} - \zeta\Delta\mu Q_{\alpha\beta} - p\delta_{\alpha\beta} \tag{2.133}$$

$$\frac{DQ_{\alpha\beta}}{Dt} = \beta_1 u_{\alpha\beta} + \beta_2^{-1}\mathring{H}_{\alpha\beta} + \lambda\Delta\mu Q_{\alpha\beta}. \tag{2.134}$$

The $\bar{\zeta}\Delta\mu$ term vanished because if appears as an expansion of the diagonal portion of the deviatoric stress, which is zero for an incompressible fluid. We can write the stress in terms of $DQ_{\alpha\beta}/Dt$ by eliminating the molecular field.

$$\sigma_{\alpha\beta} = \left(2\eta + \beta_1^2\beta_2\right) u_{\alpha\beta} - p\delta_{\alpha\beta} + \zeta'\Delta\mu Q_{\alpha\beta} - \beta_1\beta_2 \frac{DQ_{\alpha\beta}}{Dt}, \tag{2.135}$$

where $\zeta' \equiv \zeta + \beta_1\beta_2\lambda$.

2.8.5 The Landau-de Gennes expansion

We can write the distortion energy as a *Landau-de Gennes expansion*. Formally, we may write the distortion energy as a function of the order parameter, $Q_{\alpha\beta}$. The coefficients of the expansion are in general tensorial, so most generally,

$$f_d = A_{\alpha\beta\gamma\delta} Q_{\alpha\beta} Q_{\gamma\delta} + B_{\alpha\beta\gamma\delta\mu\nu} Q_{\alpha\beta} Q_{\gamma\delta} Q_{\gamma\delta} Q_{\mu\nu} + \dots, \tag{2.136}$$

where we have not included the dependence of the distortion free energy on the derivatives of the order parameter. Considering symmetry properties of a uniaxial nematic (which I will not go into here), the Landau-de Gennes expansion to second order in the order parameter and its derivative is

$$f_d = \frac{\chi}{2} Q_{\alpha\beta} Q_{\alpha\beta} + \frac{L_1}{2} (\partial_\gamma Q_{\alpha\beta})(\partial_\gamma Q_{\alpha\beta}) + \frac{L_2}{2} (\partial_\alpha Q_{\alpha\gamma})(\partial_\beta Q_{\gamma\beta}). \tag{2.137}$$

The first order terms are all zero, because of the scalar nature of f_d. It can be shown that to second order in S (see Vertogen and de Jeu, page 232), that L_1 and L_2 are related to the Frank elastic constants, K_1, K_2, and K_3, by

$$K_1 = K_3 = 2\left(L_1 + L_2/2\right) S^2 \tag{2.138}$$

$$K_2 = 2 L_1 S^2, \tag{2.139}$$

where truncation of the Landau-de Gennes expansion necessitates that $K_1 = K_3$ (inclusion of further terms would result in $K_1 \neq K_3$). If we make the *one constant approximation* that $K_1 = K_2 = K_3$, then $L_2 = 0$, and we define $L \equiv L_1$. Therefore, we have a distortion energy of

$$f_d = \frac{\chi}{2} Q_{\alpha\beta} Q_{\alpha\beta} + \frac{L}{2} (\partial_\gamma Q_{\alpha\beta})(\partial_\gamma Q_{\alpha\beta}). \tag{2.140}$$

2.8.6 The molecular field as determined by the Landau-de Gennes expansion

We can use the distortion energy to compute the molecular field.

$$H_{\alpha\beta} = -\frac{\delta f_d}{\delta Q_{\alpha\beta}} = -\chi Q_{\alpha\beta} + L \partial_\gamma \partial_\gamma Q_{\alpha\beta}. \tag{2.141}$$

With this in place, we can get an expression for $DQ_{\alpha\beta}/Dt$.

$$\frac{DQ_{\alpha\beta}}{Dt} = \beta_1 u_{\alpha\beta} - \beta_2^{-1} \left(\chi' Q_{\alpha\beta} - L \partial_\gamma \partial_\gamma Q_{\alpha\beta}\right), \tag{2.142}$$

where $\chi' \equiv \chi - \beta_2 \lambda \Delta\mu$. Keep in mind that with this definition, terms containing χ' result from both active and passive processes.

Substitution of (2.142) into (2.135) yields

$$\sigma_{\alpha\beta} = 2\eta u_{\alpha\beta} - p\delta_{\alpha\beta} + \left(\zeta' \Delta\mu + \beta_1 \chi' - \beta_1 L \partial_\gamma \partial_\gamma\right) Q_{\alpha\beta}. \tag{2.143}$$

2.9 A thin sheet of active nematic liquid crystal

We now consider a thin sheet of active nematic liquid crystal. We stipulate the the filaments are aligned in the xy-plane, meaning $Q_{xz} = Q_{yz} = 0$ and $Q_{zz} = -1/3$. We define the equilibrium state of the liquid crystal to be disordered in the plane, naturally absent of flow and active processes. The equilibrium order parameter is then given by

$$Q^0_{xx} = Q^0_{yy} = \frac{1}{6}, \;\; Q^0_{zz} = -\frac{1}{3}, \tag{2.144}$$

with the other entries being zero. We define $Q'_{\alpha\beta}$ as the deviation from the equilibrium configuration,

$$Q_{\alpha\beta} = Q^0_{\alpha\beta} + Q'_{\alpha\beta}. \tag{2.145}$$

$Q'_{\alpha\beta}$ is uniquely defined by $Q'_{xx} = -Q'_{yy} \equiv \tilde{Q}$ and $Q'_{xy} = Q'_{yx} \equiv q$, with all other entries being zero.

In addition the thinness of the sheet affects the scale of the fluid velocities in the respective directions. The sheet is thin in the z direction, say with thickness h, compared to the x and y directions, say with extent ℓ. If characteristic velocity in the x and y directions is U, then the continuity equation, $\partial_\gamma v_\gamma = 0$, specifies that the characteristic velocity in the z-direction, U_z is

$$U_z \sim \frac{h}{\ell} U. \tag{2.146}$$

I.e., $U_z \ll U$ since $h \ll \ell$.

2.9.1 The Landau-de Gennes expansion under the thin sheet constraint

Given the thin sheet constraint and that the equilibrium value of the order parameter is $Q^0_{\alpha\beta}$, the Landau-de Gennes expansion of the distortion free energy is

$$f_d = \frac{\chi}{2} Q'_{\alpha\beta} Q'_{\alpha\beta} + \frac{L}{2} (\partial_\gamma Q'_{\alpha\beta})(\partial_\gamma Q'_{\alpha\beta}). \tag{2.147}$$

The resulting molecular field is

$$H_{\alpha\beta} = -\frac{\delta f_d}{\delta Q'_{\alpha\beta}} = -\chi Q'_{\alpha\beta} + L \partial_\gamma \partial_\gamma Q'_{\alpha\beta}. \tag{2.148}$$

2.9.2 Expression for $DQ_{\alpha\beta}/Dt$ under thin sheet constraint

Using the expression for the molecular field in the thin sheet,

$$\begin{aligned} \frac{DQ_{xx}}{Dt} = \frac{DQ'_{xx}}{Dt} &= \beta_1 u_{xx} - \beta_2^{-1} \left(\chi Q'_{xx} - L \partial_\gamma \partial_\gamma Q'_{xx} \right) + \lambda \Delta\mu (Q^0_{xx} + Q'_{xx}) \\ &= \beta_1 u_{xx} - \beta_2^{-1} \left(\chi' - L \partial_\gamma \partial_\gamma \right) Q'_{xx} + \lambda \Delta\mu Q^0_{xx}, \end{aligned} \tag{2.149}$$

and similarly,

$$\begin{aligned} \frac{DQ_{yy}}{Dt} = -\frac{DQ'_{xx}}{Dt} &= \beta_1 u_{yy} - \beta_2^{-1} \left(\chi Q'_{yy} - L \partial_\gamma \partial_\gamma Q'_{yy} \right) + \lambda \Delta\mu (Q^0_{yy} + Q'_{yy}) \\ &= \beta_1 u_{yy} + \beta_2^{-1} \left(\chi' - L \partial_\gamma \partial_\gamma \right) Q'_{xx} - \lambda \Delta\mu Q^0_{xx}, \end{aligned} \tag{2.150}$$

where we have used the fact that $Q'_{xx} = -Q'_{yy}$. Subtracting the two equations gives

$$\frac{DQ'_{xx}}{Dt} - \frac{DQ'_{yy}}{Dt} = 2\frac{D\tilde{Q}}{Dt} = \beta_1 (u_{xx} - u_{yy}) - 2\beta_2^{-1} \left(\chi' - L \partial_\gamma \partial_\gamma \right) \tilde{Q}. \tag{2.151}$$

Thus, we have

$$\frac{D\tilde{Q}}{Dt} = \frac{\beta_1}{2} (u_{xx} - u_{yy}) - \beta_2^{-1} \left(\chi' - L(\partial_x^2 + \partial_y^2) \right) \tilde{Q}. \tag{2.152}$$

Finally, we can trivially compute

$$\frac{DQ'_{xy}}{Dt} = \frac{Dq}{Dt} = \beta_1 u_{xy} - \beta_2^{-1} \left(\chi' - L(\partial_x^2 + \partial_y^2) \right) q. \tag{2.153}$$

Note that

$$\frac{D\tilde{Q}}{Dt} = \partial_t \tilde{Q} + v_\gamma \partial_\gamma \tilde{Q} + q(\partial_x v_y - \partial_y v_x) \tag{2.154}$$

$$\frac{Dq}{Dt} = \partial_t q + v_\gamma \partial_\gamma q - \tilde{Q}(\partial_x v_y - \partial_y v_x). \tag{2.155}$$

2.9.3 The stress tensor for a thin film

The stress tensor for the thin film is

$$\sigma_{\alpha\beta} = 2\eta u_{\alpha\beta} - p\delta_{\alpha\beta} + \zeta' \Delta\mu (Q^0_{\alpha\beta} + Q'_{\alpha\beta}) + \left[\beta_1^2 \beta_2 u_{\alpha\beta} - \beta_1 \beta_2 \frac{DQ_{\alpha\beta}}{Dt}\right]. \tag{2.156}$$

We now compute the bracketed term. Note that

$$\frac{DQ_{xz}}{Dt} = \frac{DQ_{zx}}{Dt} = \frac{DQ_{yz}}{Dt} = \frac{DQ_{zy}}{Dt} = \frac{DQ_{zz}}{Dt} = 0. \tag{2.157}$$

Therefore, for the bracketed term,

$$\beta_1^2 \beta_2 u_{\alpha\beta} - \beta_1 \beta_2 \frac{DQ_{\alpha\beta}}{Dt} = \beta_1^2 \beta_2 u_{\alpha\beta} \text{ if } \alpha \text{ or } \beta = z. \tag{2.158}$$

Considering now the other three independent terms,

$$\beta_1^2 \beta_2 u_{xx} - \beta_1 \beta_2 \frac{DQ_{xx}}{Dt} = \frac{\beta_1^2 \beta_2}{2}(u_{xx} + u_{yy}) + \beta_1 \left(\chi' - L(\partial_x^2 + \partial_y^2)\right) \tilde{Q} \tag{2.159}$$

$$\beta_1^2 \beta_2 u_{yy} - \beta_1 \beta_2 \frac{DQ_{yy}}{Dt} = \frac{\beta_1^2 \beta_2}{2}(u_{xx} + u_{yy}) + \beta_1 \left(\chi' - L(\partial_x^2 + \partial_y^2)\right) \tilde{Q} \tag{2.160}$$

$$\beta_1^2 \beta_2 u_{xy} - \beta_1 \beta_2 \frac{DQ_{xy}}{Dt} = \beta_1 \left(\chi' - L(\partial_x^2 + \partial_y^2)\right) q. \tag{2.161}$$

Therefore, the bracketed term is

$$\beta_1^2 \beta_2 u_{\alpha\beta} - \beta_1 \beta_2 \frac{DQ_{\alpha\beta}}{Dt} = \begin{cases} \beta_1^2 \beta_2 u_{\alpha\beta} & \alpha \text{ or } \beta = z \\ \frac{\beta_1^2 \beta_2}{2}(u_{xx} + u_{yy}) + \beta_1 \left(\chi' - L(\partial_x^2 + \partial_y^2)\right) \tilde{Q} & \alpha = \beta \neq z \\ \beta_1 \left(\chi' - L(\partial_x^2 + \partial_y^2)\right) q & \alpha \neq \beta, \ \alpha, \beta \neq z \end{cases}. \tag{2.162}$$

This can be written in a more compact form,

$$\begin{aligned} \beta_1^2 \beta_2 u_{\alpha\beta} - \beta_1 \beta_2 \frac{DQ_{\alpha\beta}}{Dt} = &\beta_1^2 \beta_2 u_{\alpha\beta} (\delta_{\alpha z} + \delta_{\beta z} - \delta_{\alpha z}\delta_{\beta z}) + \frac{u_{xx} + u_{yy}}{2} (\delta_{\alpha x}\delta_{\beta x} + \delta_{\alpha y}\delta_{\beta y}) \\ &+ \beta_1 \left(\chi' - L(\partial_x^2 + \partial_y^2)\right) Q'_{\alpha\beta}. \end{aligned} \tag{2.163}$$

Defining $w_{\alpha\beta} \equiv \beta_1^2 \beta_2 u_{\alpha\beta}(\delta_{\alpha z} + \delta_{\beta z} - \delta_{\alpha z}\delta_{\beta z}) + (u_{xx} + u_{yy}) (\delta_{\alpha x}\delta_{\beta x} + \delta_{\alpha y}\delta_{\beta y})/2$, the stress tensor is

$$\sigma_{\alpha\beta} = 2\eta u_{\alpha\beta} - p\delta_{\alpha\beta} + \zeta' \Delta\mu Q^0_{\alpha\beta} + \left(\zeta\Delta\mu + \beta_1 \chi - \beta_1 L(\partial_x^2 + \partial_y^2)\right) Q'_{\alpha\beta} + \beta_1^2 \beta_2 w_{\alpha\beta}. \tag{2.164}$$

As pointed out by Salbreux, et al., the $w_{\alpha\beta}$ term represents anisotropy of the viscosity (arising because we constrained the order parameter for alignment in the *xy*-plane), which we already specifically neglected in section 2.7.5, so the $w_{\alpha\beta}$ term, may also be neglected.

For reference, we now write all the components of the stress tensor.

$$\sigma_{xx} = 2\eta\partial_x v_x - p + (\zeta\Delta\mu + \beta_1\beta_2\lambda\Delta\mu)Q^0_{xx} + \left(\zeta\Delta\mu + \beta_1\chi - \beta_1 L(\partial_x^2 + \partial_y^2)\right)\tilde{Q} \tag{2.165}$$

$$\sigma_{xy} = \sigma_{yx} = \eta(\partial_x v_y + \partial_y v_x) + \left(\zeta\Delta\mu + \beta_1\chi - \beta_1 L(\partial_x^2 + \partial_y^2)\right) q \tag{2.166}$$

$$\sigma_{xz} = \sigma_{zx} = \eta(\partial_x v_z + \partial_z v_x) \tag{2.167}$$

$$\sigma_{yy} = 2\eta\partial_y v_y - p + (\zeta\Delta\mu + \beta_1\beta_2\lambda\Delta\mu)Q^0_{yy} - \left(\zeta\Delta\mu + \beta_1\chi - \beta_1 L(\partial_x^2 + \partial_y^2)\right)\tilde{Q} \tag{2.168}$$

$$\sigma_{yz} = \sigma_{zy} = \eta(\partial_y v_z + \partial_z v_y) \tag{2.169}$$

$$\sigma_{zz} = 2\eta\partial_z v_z - p + (\zeta\Delta\mu + \beta_1\beta_2\lambda\Delta\mu)Q^0_{zz}, \tag{2.170}$$

where, as noted before, $Q^0_{xx} = Q^0_{yy} = 1/6$ and $Q^0_{zz} = -1/3$.

2.9.4 Equations of motion

Given the expression for the stress tensor, we can write the equations of motion. We assume that all phenomenological coefficients that are not active are constants. This includes η, β_1, β_2, χ, and L.

$$\begin{aligned}\rho\frac{\mathrm{d}v_x}{\mathrm{d}t} &= \partial_\beta\sigma_{x\beta} = \eta\left(\partial_x^2 + \partial_y^2 + \partial_z^2\right)v_x - \partial_x p + \beta_1\chi\left(\partial_x\tilde{Q} + \partial_y q\right) - \beta_1 L\left((\partial_x^3 + \partial_x\partial_y^2)\tilde{Q} + (\partial_x^2\partial_y + \partial_y^3)q\right)\\ &\quad + Q^0_{xx}\partial_x\zeta\Delta\mu + \partial_x(\zeta\Delta\mu\tilde{Q}) + \partial_y(\zeta\Delta\mu q) + \beta_1\beta_2 Q^0_{xx}\partial_x\lambda\Delta\mu \end{aligned}\tag{2.171}$$

$$\begin{aligned}\rho\frac{\mathrm{d}v_y}{\mathrm{d}t} &= \partial_\beta\sigma_{y\beta} = \eta\left(\partial_x^2 + \partial_y^2 + \partial_z^2\right)v_y - \partial_y p + \beta_1\chi\left(\partial_x q - \partial_y\tilde{Q}\right) - \beta_1 L\left((\partial_x^3 + \partial_x\partial_y^2)q - (\partial_x^2\partial_y + \partial_y^3)\tilde{Q}\right)\\ &\quad + Q^0_{yy}\partial_y\zeta\Delta\mu + \partial_x(\zeta\Delta\mu q) - \partial_y(\zeta\Delta\mu\tilde{Q}) + \beta_1\beta_2 Q^0_{yy}\partial_y\lambda\Delta\mu, \end{aligned}\tag{2.172}$$

where we have used incompressibility, $\partial_\gamma v_\gamma = 0$. The second line of the two equations represent the active terms.

If we do not have rigid plates on either side of the thin sheet, we assume that the stress normal to the sheet vanishes, or $\sigma_{zz} = 0$. If this is the case, the pressure is set by

$$p = -2\eta(\partial_x v_x + \partial_y v_y) + (\zeta\Delta\mu + \beta_1\beta_2\lambda\Delta\mu)Q^0_{zz}, \tag{2.173}$$

The equations of motion then become

$$\begin{aligned}\rho\frac{\mathrm{d}v_x}{\mathrm{d}t} &= \eta\left(\partial_x^2 + \partial_y^2 + \partial_z^2\right)v_x + 2\eta\partial_x(\partial_x v_x + \partial_y v_y)\\ &\quad + \beta_1\chi\left(\partial_x\tilde{Q} + \partial_y q\right) - \beta_1 L\left((\partial_x^3 + \partial_x\partial_y^2)\tilde{Q} + (\partial_x^2\partial_y + \partial_y^3)q\right)\\ &\quad + (Q^0_{xx} - Q^0_{zz})\partial_x\zeta\Delta\mu + \partial_x(\zeta\Delta\mu\tilde{Q}) + \partial_y(\zeta\Delta\mu q) + \beta_1\beta_2(Q^0_{xx} - Q^0_{zz})\partial_x\lambda\Delta\mu \end{aligned}\tag{2.174}$$

$$\begin{aligned}\rho\frac{\mathrm{d}v_y}{\mathrm{d}t} &= \eta\left(\partial_x^2 + \partial_y^2 + \partial_z^2\right)v_y + 2\eta\partial_y(\partial_x v_x + \partial_y v_y)\\ &\quad + \beta_1\chi\left(\partial_x q - \partial_y\tilde{Q}\right) - \beta_1 L\left((\partial_x^3 + \partial_x\partial_y^2)q - (\partial_x^2\partial_y + \partial_y^3)\tilde{Q}\right)\end{aligned}$$

$$+ (Q^0_{yy} - Q^0_{zz})\partial_y \zeta\Delta\mu + \partial_x(\zeta\Delta\mu q) - \partial_y(\zeta\Delta\mu\tilde{Q}) + \beta_1\beta_2(Q^0_{yy} - Q^0_{zz})\partial_y\lambda\Delta\mu. \tag{2.175}$$

As suggested by Guillaume, we can use the definition of the stress tensor and the continuity equation to re-write the first two terms (2.174) and (2.175). We note that

$$\eta\partial_z^2 v_x = \partial_z\sigma_{xz} - \eta\partial_z\partial_x v_z = \partial_z\sigma_{xz} + \eta\partial_x(\partial_x v_x + \partial_y v_y), \tag{2.176}$$

by the expression we derived for the stress tensor and continuity. Similarly,

$$\eta\partial_z^2 v_y = \partial_z\sigma_{xy} - \eta\partial_z\partial_y v_z = \partial_z\sigma_{yz} + \eta\partial_y(\partial_x v_x + \partial_y v_y). \tag{2.177}$$

Substitution of these two equations into (2.174) and (2.175) gives, after rearranging,

$$\begin{aligned}
\rho\frac{\mathrm{d}v_x}{\mathrm{d}t} &= \partial_z\sigma_{xz} + \eta(\partial_x^2 + \partial_y^2)v_x + 3\eta\partial_x(\partial_x v_x + \partial_y v_y) \\
&\quad + \beta_1\chi\left(\partial_x\tilde{Q} + \partial_y q\right) - \beta_1 L\left((\partial_x^3 + \partial_x\partial_y^2)\tilde{Q} + (\partial_x^2\partial_y + \partial_y^3)q\right) \\
&\quad + (Q^0_{xx} - Q^0_{zz})\partial_x\zeta\Delta\mu + \partial_x(\zeta\Delta\mu\tilde{Q}) + \partial_y(\zeta\Delta\mu q) + \beta_1\beta_2(Q^0_{xx} - Q^0_{zz})\partial_x\lambda\Delta\mu
\end{aligned} \tag{2.178}$$

$$\begin{aligned}
\rho\frac{\mathrm{d}v_y}{\mathrm{d}t} &= \partial_z\sigma_{xz} + \eta(\partial_x^2 + \partial_y^2)v_y + 3\eta\partial_y(\partial_x v_x + \partial_y v_y) \\
&\quad + \beta_1\chi\left(\partial_x q - \partial_y\tilde{Q}\right) - \beta_1 L\left((\partial_x^3 + \partial_x\partial_y^2)q - (\partial_x^2\partial_y + \partial_y^3)\tilde{Q}\right) \\
&\quad + (Q^0_{yy} - Q^0_{zz})\partial_y\zeta\Delta\mu + \partial_x(\zeta\Delta\mu q) - \partial_y(\zeta\Delta\mu\tilde{Q}) + \beta_1\beta_2(Q^0_{yy} - Q^0_{zz})\partial_y\lambda\Delta\mu.
\end{aligned} \tag{2.179}$$

2.9.5 Averaging over the z-dimension

To get a two-dimensional description of the active nematic fluid, we must average over the z-dimension. In general, for a quantity a, the average over the thin dimension of the film (z, with thickness h), is

$$\bar{a} \equiv \frac{1}{h}\int_0^h dz\, a. \tag{2.180}$$

Note that

$$\overline{\partial_x a} = \frac{1}{h}\int_0^h dz\,\partial_x a = \frac{1}{h}\partial_x\int_0^h dz\, a - a\partial_x h = \partial_x\left(\frac{1}{h}\int_0^h dz\, a\right) - (\partial_x h)\left(a + \frac{1}{h^2}\int_0^h dz\, a\right). \tag{2.181}$$

If $\partial_x h \approx 0$, then $\overline{\partial_x a} \approx \partial_x\bar{a}$. Similar results hold for $\overline{\partial_y a}$, $\overline{\partial_x^2 a}$, $\overline{\partial_y^2 a}$, and $\overline{\partial_x\partial_y a}$. Note that, in general $\overline{ab} \neq \bar{a}\bar{b}$, unless $\partial_z a = 0$ or $\partial_z b = 0$. In addition to the constant coefficients, we also assume that ρ, n_i, and $Q_{\alpha\beta}$ do not change appreciably over z.

We can now perform the average over the equations of motion, (2.178) and (2.179), using the above relations and assumptions, further assuming that the thickness is approximately constant in space. The only integrals that arise that we have not yet addressed are of the form

$$\frac{1}{h}\int_0^h dz\sigma_{xz} = \frac{\sigma_{xz}|_0^h}{h}. \tag{2.182}$$

Therefore, the integral is proportional to a shear stress at the surface of the fluid. This could be a stress against, e.g., a cell membrane or cytoplasm. The stress can depend only on local parameters, and cannot depend on the order parameter, as can be seen for the expression we derived for σ_{xz}. The stress is not normal, so it cannot depend on the pressure. This leaves only the average velocity. Therefore, we take

$$\frac{1}{h}\int_0^h dz\sigma_{xz} = \frac{\sigma_{xz}|_0^h}{h} = -\gamma\bar{v}_x, \tag{2.183}$$

where γ is a friction coefficient capturing the proportionality between the surface shear stress and the velocity. A similar relation holds in the y direction.

Performing the averaging yields

$$\begin{aligned}
\rho\partial_t\bar{v}_x + \rho\overline{v_\gamma\partial_\gamma v_x} = {} & \eta(\partial_x^2+\partial_y^2)\bar{v}_x + 3\eta\partial_x(\partial_x\bar{v}_x+\partial_y\bar{v}_y) - \gamma\bar{v}_x + \beta_1\chi\left(\partial_x\tilde{Q}+\partial_y q\right) \\
& - \beta_1 L\left((\partial_x^3+\partial_x\partial_y^2)\tilde{Q} + (\partial_x^2\partial_y+\partial_y^3)q\right) + (Q^0_{xx}-Q^0_{zz})\partial_x\bar{\zeta}\Delta\mu \\
& + \partial_x(\bar{\zeta}\Delta\mu\tilde{Q}) + \partial_y(\bar{\zeta}\Delta\mu q) + \beta_1\beta_2(Q^0_{xx}-Q^0_{zz})\partial_x\bar{\lambda}\Delta\mu,
\end{aligned} \tag{2.184}$$

$$\begin{aligned}
\rho\partial_t\bar{v}_y + \rho\overline{v_\gamma\partial_\gamma v_y} = {} & \eta\left(\partial_x^2+\partial_y^2\right)\bar{v}_y + 3\eta\partial_y(\partial_x\bar{v}_x+\partial_y\bar{v}_y) - \gamma\bar{v}_y + \beta_1\chi\left(\partial_x q-\partial_y\tilde{Q}\right) \\
& - \beta_1 L\left((\partial_x^3+\partial_x\partial_y^2)q - (\partial_x^2\partial_y+\partial_y^3)\tilde{Q}\right) + (Q^0_{yy}-Q^0_{zz})\partial_y\bar{\zeta}\Delta\mu \\
& + \partial_x(\bar{\zeta}\Delta\mu q) - \partial_y(\bar{\zeta}\Delta\mu\tilde{Q}) + \beta_1\beta_2(Q^0_{yy}-Q^0_{zz})\partial_y\bar{\lambda}\Delta\mu,
\end{aligned} \tag{2.185}$$

where $\bar{\zeta}$ is not to be confused with the previous use of that symbol representing the Onsager coefficient L^{rov}. The nonlinear term on the left hand side presents a difficulty. Under circumstances where the Reynolds number is low, this term may be ignored. We retain the time derivative term, which may remain, even at small Reynolds number, if the Strouhal number is also small, i.e., if there is another slow process (e.g., slow diffusion of chemical reaction) occurring in addition to fluid motion. Going forward, we neglect the nonlinear term on the left hand side.

Averaging the equation describing the dynamics of the order parameter, again assuming $\partial_z Q_{\alpha\beta}\approx 0$, yields

$$\begin{aligned}
\partial_t\tilde{Q} = {} & -(\bar{v}_x\partial_x+\bar{v}_y\partial_y)\tilde{Q} - q(\partial_x\bar{v}_y-\partial_y\bar{v}_x) + \frac{\beta_1}{2}(\partial_x\bar{v}_x-\partial_y\bar{v}_y) \\
& - \left(\frac{\chi}{\beta_2} - \frac{L}{\beta_2}(\partial_x^2+\partial_y^2)\right)\tilde{Q} + \bar{\lambda}\Delta\mu\tilde{Q}
\end{aligned} \tag{2.186}$$

$$\begin{aligned}
\partial_t q = {} & -(\bar{v}_x\partial_x+\bar{v}_y\partial_y)q + \tilde{Q}(\partial_x\bar{v}_y-\partial_y\bar{v}_x) + \frac{\beta_1}{2}(\partial_x\bar{v}_y+\partial_y\bar{v}_x) \\
& - \left(\frac{\chi}{\beta_2} - \frac{L}{\beta_2}(\partial_x^2+\partial_y^2)\right)q + \bar{\lambda}\Delta\mu q.
\end{aligned} \tag{2.187}$$

We note that in order to maintain a constant thickness, material must be brought into and out of the thin layer. The rate at which material flows in and out may be found by averaging the incompressibility condition, $\partial_\gamma v_\gamma = 0$.

$$v_z|_0^h = -h(\partial_x\bar{v}_x+\partial_y\bar{v}_y). \tag{2.188}$$

The left hand side is interpreted as the fluid velocity of material flowing out of the thin layer in the z direction.

Averaging the reaction-diffusion-advection equation for a chemical species, assuming $\partial_z n_i \approx 0$ and a diagonal diffusivity tensor, yields

$$\partial_t n_i = D_i(\partial_x^2 + \partial_y^2)n_i - \partial_x(n_i \bar{v}_x) - \partial_y(n_i \bar{v}_y) + \left[-\frac{n_i v_z|_0^h}{h}\right] + \sum_k \nu_{ki} r_k. \tag{2.189}$$

The term in brackets represents the flux of species i out of the thin film. The expression for this term is given by (2.188). We may, however, imagine a situation where fluid may be exchanged through the boundaries of the thin film, but not diffusing species i. We introduce a parameter, $\alpha_i \in [0, 1]$ to allow for this situation.[5] If $\alpha_i < 1$, the exit of species i from the boundaries of the thin film is inhibited. Thus, we get

$$\partial_t n_i = D_i(\partial_x^2 + \partial_y^2)n_i - (1 - \alpha_i)n_i(\partial_x \bar{v}_x + \partial_y \bar{v}_y) - \bar{v}_x \partial_x n_i - \bar{v}_y \partial_y n_i + \sum_k \nu_{ki} r_k. \tag{2.190}$$

2.9.6 Summary of governing equations

In summary, the governing dynamical equations for a thin film of active viscous nematic fluid in which species can diffuse, taking all the assumptions thus far mentioned are

$$\begin{aligned}\rho\partial_t v_x = {} & \eta(\partial_x^2 + \partial_y^2)v_x + \eta_v^{2d}\partial_x(\partial_x v_x + \partial_y v_y) + \beta_1\chi\left(\partial_x\tilde{Q} + \partial_y q\right) - \beta_1 L\left((\partial_x^3 + \partial_x\partial_y^2)\tilde{Q} + (\partial_x^2\partial_y + \partial_y^3)q\right) \\ & + (Q_{xx}^0 - Q_{zz}^0)\partial_x\zeta\Delta\mu + \partial_x(\zeta\Delta\mu\tilde{Q}) + \partial_y(\zeta\Delta\mu q) + \beta_1\beta_2(Q_{xx}^0 - Q_{zz}^0)\partial_x\lambda\Delta\mu - \gamma v_x\end{aligned} \tag{2.191}$$

$$\begin{aligned}\rho\partial_t v_y = {} & \eta\left(\partial_x^2 + \partial_y^2\right)v_y + \eta_v^{2d}\partial_y(\partial_x v_x + \partial_y v_y) + \beta_1\chi\left(\partial_x q - \partial_y\tilde{Q}\right) - \beta_1 L\left((\partial_x^3 + \partial_x\partial_y^2)q - (\partial_x^2\partial_y + \partial_y^3)\tilde{Q}\right) \\ & + (Q_{yy}^0 - Q_{zz}^0)\partial_y\zeta\Delta\mu + \partial_x(\zeta\Delta\mu q) - \partial_y(\zeta\Delta\mu\tilde{Q}) + \beta_1\beta_2(Q_{yy}^0 - Q_{zz}^0)\partial_y\lambda\Delta\mu - \gamma v_y\end{aligned} \tag{2.192}$$

$$\begin{aligned}\partial_t\tilde{Q} = {} & -(v_x\partial_x + v_y\partial_y)\tilde{Q} - q(\partial_x v_y - \partial_y v_x) + \frac{\beta_1}{2}(\partial_x v_x - \partial_y v_y) \\ & - \left(\frac{\chi}{\beta_2} - \frac{L}{\beta_2}(\partial_x^2 + \partial_y^2)\right)\tilde{Q} + \lambda\Delta\mu\tilde{Q}\end{aligned} \tag{2.193}$$

$$\begin{aligned}\partial_t q = {} & -(v_x\partial_x + v_y\partial_y)q + \tilde{Q}(\partial_x v_y - \partial_y v_x) + \frac{\beta_1}{2}(\partial_x v_y + \partial_y v_x) \\ & - \left(\frac{\chi}{\beta_2} - \frac{L}{\beta_2}(\partial_x^2 + \partial_y^2)\right)q + \lambda\Delta\mu q\end{aligned} \tag{2.194}$$

$$\partial_t n_i = D_i(\partial_x^2 + \partial_y^2)n_i - (1 - \alpha_i)n_i(\partial_x v_x + \partial_y v_y) - v_x\partial_x n_i - v_y\partial_y n_i + \sum_k \nu_{ki} r_k, \tag{2.195}$$

where we have removed the overbars for notational convenience. We have defined η_v^{2d} to be the two-dimensional bulk viscosity, which we have derived to be $\eta_v^{2d} = 3\eta$. Note that, in general, any of the coefficients may depend on the concentrations n_i. Of particular interest are the active terms, $\zeta\Delta\mu$ and $\lambda\Delta\mu$.

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[5] This is a simplistic way to do it, since the tacit assumption is that the concentration of regulator in the medium in which it can exchange is the same as it is *locally* in x and y in the film. A more reasonable expression can be derived, depending on the nature of the medium that the thin film can exchange material with.

3 Sponanteous flow and nematic alignment

We now consider the possibility that a thin film of an active nematic fluid, initially isotropic and without flow, can spontaneously align and flow. To do so, we consider the following simple case.

1) The Reynolds number is so small that the time derivatives in (2.191) and (2.192) may be neglected ($\tilde{\eta}\tilde{\chi}\mathrm{Re} \approx 0$, cf. section 4).
2) We treat the fluid as a single species.
3) There is a single regulator or active stress and active alignment, i.e., $\zeta\Delta\mu = \zeta\Delta\mu(n)$ and $\lambda\Delta\mu = \lambda\Delta\mu(n)$.
4) There are no other chemical reactions besides those generating active processes.

3.1 The quiescent, isotropic, homogeneous steady state

The isotropic, quiescent, homogeneous steady state has $\tilde{Q} = q = 0$ and $n = n_0$. Then, by (2.191) and (2.192),

$$(\partial_x^2 + \partial_y^2)v_x + \eta_v^{2d}\partial_x(\partial_x v_x + \partial_y v_y) = \tilde{\gamma} v_x \tag{3.1}$$

$$(\partial_x^2 + \partial_y^2)v_y + \eta_v^{2d}\partial_y(\partial_x v_x + \partial_y v_y) = \tilde{\gamma} v_y, \tag{3.2}$$

so $v_x = v_y = 0$. Therefore, we also have $\partial_t\tilde{Q} = \partial_t q = 0$ by (2.193) and (2.194), consistent with our putative isotropic steady state. We consider a perturbation to this steady state,

$$\tilde{Q} = \delta\tilde{Q}\mathrm{e}^{st+ik_x x+ik_y y} \tag{3.3}$$

$$q = \delta q\mathrm{e}^{st+ik_x x+ik_y y} \tag{3.4}$$

$$n = n_0 + \delta n\mathrm{e}^{st+ik_x x+ik_y y}. \tag{3.5}$$

The steady state active stress is $\zeta\Delta\mu(n_0)$, and under the perturbation, the active stress, to first order in the perturbation, is

$$\zeta\Delta\mu(n) = \zeta\Delta\mu(n_0) + \delta n\mathrm{e}^{st+ik_x x+ik_y y}\,\partial_n\zeta\Delta\mu(n_0) = \zeta\Delta\mu(n_0) + n'\,\partial_n\zeta\Delta\mu(n_0), \tag{3.6}$$

where we have defined

$$n' \equiv \delta n\mathrm{e}^{st+ik_x x+ik_y y} \tag{3.7}$$

for notational convenience. Note that the derivatives are easily calculated, e.g.,

$$\partial_x q = ik_x q, \;\; \partial_t q = sq, \text{ etc.} \tag{3.8}$$

3.2 Velocity profiles

We insert the perturbations in $\tilde{Q}$, q, and n into (2.191) and (2.192) (using $Q^0_{xx} - Q^0_{zz} = Q^0_{yy} - Q^0_{zz} = 1/2$) to get, to linear order in the perturbation,

$$i\left((\eta(\partial_x^2 + \partial_y^2) - \gamma)v_x + \eta_v^{2d}\partial_x(\partial_x v_x + \partial_y v_y)\right) = \beta_1\chi(k_x\tilde{Q} + k_y q) + \beta_1 L\left((k_x^3 + k_x k_y^2)\tilde{Q} + (k_x^2 k_y + k_y^3)q\right)$$

$$+ \frac{k_x}{2}\,\zeta_n n' + k_x\zeta_0\tilde{Q} + k_y\zeta_0 q + \frac{k_x}{2}\,\beta_1\beta_2\lambda_n n' \tag{3.9}$$

$$i\left((\eta(\partial_x^2+\partial_y^2)-\gamma)v_y + \eta_v^{2d}\partial_y(\partial_x v_x + \partial_y v_y)\right) = \beta_1\chi(k_x q - k_y\tilde{Q}) + \beta_1 L\left((k_x^3 + k_x k_y^2)q - (k_x^2 k_y + k_y^3)\tilde{Q}\right)$$

$$+ \frac{k_y}{2}\,\zeta_n n' + k_x\zeta_0 q - k_y\zeta_0\tilde{Q} + \frac{k_y}{2}\,\beta_1\beta_2\lambda_n n', \tag{3.10}$$

where we have used the fact that $Q^0_{xx} - Q^0_{zz} = Q^0_{yy} - Q^0_{zz} = 1/2$. We have also defined

$$\zeta_0 \equiv \zeta\Delta\mu(n_0), \;\; \zeta_n \equiv \partial_n\zeta\Delta\mu(n_0) \tag{3.11}$$

$$\lambda_0 \equiv \lambda\Delta\mu(n_0), \;\; \lambda_n \equiv \partial_n\lambda\Delta\mu(n_0) \tag{3.12}$$

for notational convenience. The velocities are easily solved for by Fourier transform to give

$$v_x = \frac{\left(\eta k^2 + \eta_v^{2d}k_y^2 + \gamma\right) g_x - \eta_v^{2d}k_x k_y g_y}{\left((\eta + \eta_v^{2d})k^2 + \gamma\right)\left(\eta k^2 + \gamma\right)} \tag{3.13}$$

$$v_y = \frac{\left(\eta k^2 + \eta_v^{2d}k_x^2 + \gamma\right) g_y - \eta_v^{2d}k_x k_y g_x}{\left((\eta + \eta_v^{2d})k^2 + \gamma\right)\left(\eta k^2 + \gamma\right)}, \tag{3.14}$$

where $k \equiv \sqrt{k_x^2 + k_y^2}$ and

$$g_x \equiv i\left[\beta_1(\chi + Lk^2)(k_x\tilde{Q} + k_y q) + \frac{k_x}{2}\,\zeta_n n' + \zeta_0(k_x\tilde{Q} + k_y q) + \frac{\beta_1\beta_2}{2}\,k_x\lambda_n n'\right], \tag{3.15}$$

$$g_y \equiv i\left[\beta_1(\chi + Lk^2)(k_x q - k_y\tilde{Q}) + \frac{k_y}{2}\,\zeta_n n' + \zeta_0(k_x q - k_y\tilde{Q}) + \frac{\beta_1\beta_2}{2}\,k_y\lambda_n n'\right]. \tag{3.16}$$

For convenience, we compute

$$\begin{aligned}
d(\partial_x v_x - \partial_y v_y) &= id(k_x v_x - k_y v_y)\\
&= -\beta_1\left(\chi + Lk^2\right)\left[\left(k^2\left(\eta k^2 + \gamma\right) + 4\eta_v^{2d}k_x^2k_y^2\right)\tilde{Q} - 2\eta_v^{2d}(k_x^2 - k_y^2)k_x k_y q\right]\\
&\quad - \frac{1}{2}(k_x^2 - k_y^2)(\eta k^2 + \gamma)\zeta_n n' - \left(k^2(\eta k^2 + \gamma) + 4\eta_v^{2d}k_x^2k_y^2\right)\zeta_0\tilde{Q}\\
&\quad + 2\eta_v^{2d}k_x k_y(k_x^2 - k_y^2)\zeta_0 q - \frac{\beta_1\beta_2}{2}(k_x^2 - k_y^2)(\eta k^2 + \gamma)\lambda_n n' \qquad (3.17)\\
d(\partial_x v_y + \partial_y v_x) &= id(k_x v_y + k_y v_x)\\
&= \beta_1\left(\chi + Lk^2\right)\left[2\eta_v^{2d}(k_x^2 - k_y^2)k_x k_y\tilde{Q} - \left(k^2\left(\eta k^2 + \gamma\right) + \eta_v^{2d}(k_x^2 - k_y^2)^2\right)\tilde{q}\right]\\
&\quad - k_x k_y(\eta k^2 + \gamma)\zeta_n n' + 2\eta_v^{2d}k_x k_y(k_x^2 - k_y^2)\zeta_0\tilde{Q}\\
&\quad - \left(k^2(\eta k^2 + \gamma) + \eta_v^{2d}(k_x^2 - k_y^2)^2\right)\zeta_0 q - \beta_1\beta_2 k_x k_y(\eta k^2 + \gamma)\lambda_n n', \qquad (3.18)\\
d(\partial_x v_x + \partial_y v_y) &= id(k_x v_x + k_y v_y)
\end{aligned}$$

$$\begin{aligned} &= -\beta_1\left(\chi + Lk^2\right)\left(\eta k^2 + \gamma\right)\Big((k_x^2 - k_y^2)\tilde{Q} + 2k_xk_yq\Big) - \frac{k^2}{2}(\eta k^2 + \gamma)\zeta_n n' \\ &\quad - (\eta k^2 + \gamma)\zeta_0\Big((k_x^2 - k_y^2)\tilde{Q} + 2k_xk_yq\Big) - \frac{\beta_1\beta_2}{2}\,k^2(\eta k^2 + \gamma)\lambda_n n', \end{aligned} \tag{3.19}$$

where

$$d = \Big((\eta + \eta_v^{2d})k^2 + \gamma\Big)\left(\eta k^2 + \gamma\right), \tag{3.20}$$

the denominator in the expressions for velocities.

3.2.1 Dispersion relation

We next substitute the velocity profiles into (2.193), (2.194) and (2.195). The first two terms of the right hand sides of (2.193) and (2.194) then result in terms of order $\delta\tilde{Q}^2$, δq^2, and $\delta\tilde{Q}\delta q$. These are second order in the perturbation, so we neglect them. Similarly, note that the $v_x\partial_x n$ and $v_y\partial_y n$ terms in (2.195) are second order in the perturbation and therefore neglected. We get, then, to first order in the perturbation,

$$s\tilde{Q} = l_{11}\tilde{Q} + l_{12}q + l_{13}n' \tag{3.21}$$

$$sq = l_{21}\tilde{Q} + l_{22}q + l_{23}n' \tag{3.22}$$

$$sn' = l_{31}\tilde{Q} + l_{32}q + l_{33}n', \tag{3.23}$$

with

$$l_{11} = -\frac{\beta_1}{2d}\Big(k^2(\eta k^2 + \gamma) + 4\eta_v^{2d}k_x^2k_y^2\Big)\left(\beta_1(\chi + Lk^2) + \zeta_0\right) - \frac{1}{\beta_2}\left(\chi + Lk^2\right) + \lambda_0, \tag{3.24}$$

$$l_{12} = \frac{\beta_1}{d}\,\eta_v^{2d}k_xk_y(k_x^2 - k_y^2)\left(\beta_1(\chi + Lk^2) + \zeta_0\right), \tag{3.25}$$

$$l_{13} = -\frac{\beta_1}{4d}(k_x^2 - k_y^2)(\eta k^2 + \gamma)\left(\zeta_n + \beta_1\beta_2\lambda_n\right), \tag{3.26}$$

$$l_{21} = l_{12}, \tag{3.27}$$

$$l_{22} = -\frac{\beta_1}{2d}\Big(k^2(\eta k^2 + \gamma) + \eta_v^{2d}(k_x^2 - k_y^2)^2\Big)\left(\beta_1(\chi + Lk^2) + \zeta_0\right) - \frac{1}{\beta_2}\left(\chi + Lk^2\right) + \lambda_0, \tag{3.28}$$

$$l_{23} = -\frac{\beta_1}{2d}k_xk_y\left(\eta k^2 + \gamma\right)\left(\zeta_n + \beta_1\beta_2\lambda_n\right) \tag{3.29}$$

$$l_{31} = \frac{1}{d}\,(1 - \alpha)n_0(\eta k^2 + \gamma)\left(k_x^2 - k_y^2\right)\left(\beta_1(\chi + Lk^2) + \zeta_0\right) \tag{3.30}$$

$$l_{32} = \frac{2}{d}\,(1 - \alpha)n_0(\eta k^2 + \gamma)k_xk_y\left(\beta_1(\chi + Lk^2) + \zeta_0\right) \tag{3.31}$$

$$l_{33} = -Dk^2 + \frac{k^2(1 - \alpha)n_0}{2d}(\eta k^2 + \gamma)(\zeta_n + \beta_1\beta_2\lambda_n). \tag{3.32}$$

Therefore, s is given by the eigenvalues of the 3×3 matrix with entries l_{ij} described above.

To obtain the dispersion relation, we must compute these eigenvalues. There is an analytical expression, but it is very complicated, consisting of the roots of a cubic polynomial, so it is of little use. We are better off plotting the dispersion relation for given parameter values. Nonetheless, we note that it is possible to have imaginary eigenvalues, so an oscillatory instability is possible.

3.3 Special cases

We will eventually look are dispersion relations for various parameter values. For now, we consider some special cases that can be treated analytically.

3.3.1 Very weak coupling of nematic order

If the coupling to nematic order is very weak, i.e., $\beta_1 = \lambda = \beta_2^{-1} = 0$, we essentially recover the situation described in Bois, Jülicher, and Grill (with an extra factor of 1/2 multiplying the active stress, $\alpha = 0$, and $\eta \to \eta + \eta_v^{2d}$). In this case, the dispersion relation is

$$s = -Dk^2 + \frac{(1-\alpha)n_0 k^2}{2\left((\eta + \eta_v^{2d})k^2 + \gamma\right)}\partial_n \, \zeta\Delta\mu(n_0). \tag{3.33}$$

Note that if the active stress is expansive $\zeta\Delta\mu(n_0) < 0$, and the homogeneous steady state is unstable regardless of the sign of $\partial_n\zeta\Delta\mu(n_0)$ (i.e., regardless of whether we have an active stress up-regulator or down-regulator). However, if we have a contractile active stress, the results are as described in Bois, Jülicher, and Grill.

3.3.2 Constant active terms

If $\zeta\Delta\mu$ and $\lambda\Delta\mu$ are not functions of n, the dispersion relation simplifies to

$$s_1 = -\frac{\beta_1}{(\eta + \eta_v^{2d})k^2 + \gamma}\, k^2 \left(\beta_1(\chi + Lk^2) + \zeta_0\right) - \frac{2}{\beta_2}(\chi + Lk^2) + 2\lambda_0, \tag{3.34}$$

$$s_2 = -\frac{\beta_1}{\eta k^2 + \gamma}\, k^2 \left(\beta_1(\chi + Lk^2) + \zeta_0\right) - \frac{2}{\beta_2}(\chi + Lk^2) + 2\lambda_0. \tag{3.35}$$

Note that we have real eigenvalues, so we do not have an oscillatory instability. If we have a contractile active stress ($\zeta_0 > 0$), the first two terms are negative for all k. They reach a maximum (minimal absolute value) when $k = 0$. Therefore, the onset of instability of the isotropic steady state is

$$\lambda_0 = \frac{\chi}{\beta_2}. \tag{3.36}$$

Therefore, if λ_0 is sufficiently large, we can get an instability.

However, we might expect $\lambda_0 = 0$ in the absense of crosslinking of the nematic filaments. In this case, the only alignment is by flow. In the absense of crosslinking, one can imagine an active stress imparted on the fluid as a result of motors carrying cargo along the filaments, as opposed to sliding filaments relative to each other. Here, one could consider the cargoes as a set of Stokeslets. If a Stokeslet has a force F_α, then the resultant pressure is

$$p = \frac{F_\alpha x_\alpha}{4\pi(x_\alpha x_\alpha)^{\frac{3}{2}}} + p_0, \tag{3.37}$$

where x is the Cartesian distance from the Stokeslet and p_0 is the ambient pressure. Depending on the system geometry, the resulting pressure can have either a positive or negative sign, so it is at least possible in principle that $\zeta_0 < 0$. This is a delicate point that needs more thought, and might benefit from treatment of a polar fluid as well.

3.3.3 Constant $\zeta\Delta\mu < 0$ with $\lambda\Delta\mu = 0$

We now consider the case where $\zeta_0 < 0$ and $\lambda_0 = 0$. Given that one of the eigenvalues is positive, the larger is s_2. Therefore, the pertinent dispersion relation is

$$s(k) = \frac{\beta_1}{\eta k^2 + \gamma} k^2 \left(|\zeta_0| - \beta_1(\chi + Lk^2)\right) - \frac{2}{\beta_2}(\chi + Lk^2), \tag{3.38}$$

where we use the absolute value of ζ_0, remembering that $\zeta_0 < 0$. Note that for $k = 0$, $s = -2\chi/\beta_2 < 0$, so the zero mode is always stable, provided we have friction. The homogeneous steady state is unstable if there is a k for which

$$|\zeta_0| > \left(\beta_1 + \frac{2}{\beta_1\beta_2 k^2}(\eta k^2 + \gamma)\right)(\chi + Lk^2). \tag{3.39}$$

The fastest growning mode occurs when

$$\partial_k s(k) = 0 \text{ and } \partial_k^2 s(k) < 0. \tag{3.40}$$

We have

$$\partial_k s(k) = k\left[\frac{2\beta_1}{(\eta k^2 + \gamma)^2}\left(\gamma|\zeta_0| - \beta_1\left(Lk^2(\eta k^2 + \gamma) + \gamma(\chi + Lk^2)\right)\right) - \frac{4L}{\beta_2}\right]. \tag{3.41}$$

Clearly, $s(k)$ has an extremum at $k = 0$. As shown before, $s(0) < 0$, and this extremum is a minimum if $|\zeta_0|$ is sufficiently large. We can solve $\partial_k s(k) = 0$ for k, use this value to find the value of $|\zeta_0|$ for which $s(k) = 0$ to determine the onset of instability. The resulting expression is enormous and not particularly informative. We are better off generating stability diagrams.

3.3.4 Constant $\zeta\Delta\mu < 0$ with $\lambda\Delta\mu = 0$ with $\gamma = 0$

In the absense of friction ($\gamma = 0$), things are simpler.

$$s(k) = \frac{\beta_1}{\eta}\left[|\zeta_0| - \beta_1(\chi + Lk^2)\right] - \frac{2}{\beta_2}(\chi + Lk^2), \tag{3.42}$$

so s reaches a maximum at $k = 0$. Thus, in the absense of friction, the fastest growing mode of an instability is the zero mode (global flow and alignment), which occurs if

$$|\zeta_0| > \chi\left(\beta_1 + \frac{2\eta}{\beta_1\beta_2}\right). \tag{3.43}$$

In other words, the active stress must be strong enough to overcome the tendency for the filaments to remain randomly aligned, as measured by the inverse susceptability χ from the Landau-de Gennes expansion.

Further, for a given χ, a small viscosity can lead to an instability, while a large viscosity will not. Therefore, if everything else is constant, the bifurcation between an isotropic quiescent state to an ordered, flowing state may be crossed by moving the viscosity down.

3.3.5 Consequences on studies of ooplasmic streaming

This is a proof of principle that regulation of viscosity can result in moving from an isotropic quiescent state (pre-streaming) to an ordered, flowing state (streaming) in filamentous active fluids. Two things are important to note. First, this analysis requires an *expansive* active stress, as opposed to a contractile one. Typically, the active stresses are contractile in nature for crosslinked networks of filaments. However,

It is important to note that this is a *nematic* fluid. In the oocyte, the active stresses are acted along microtubules, which, in the geometry of the oocyte are *polar*, not nematic. An interesting experimental observation is that the absense or presence of dynein can result in kinesin-driven streaming or not, respectively. This cannot be captured with a nematic fluid, since the directionality of the motors is not taken into account. In a polar fluid, the active stress couples to a polar order parameter, so two fighting motors in opposite direction, result in lower active stress coupling to fluid flow. For a nematic fluid, the directionality cannot be distinguished, since the flow couples to a nematic order parameter. Finally, it is interesting to note that we did not have to take into account viscoelasticity in this theory.

4 Dimensionless equations

To make the governing equations (written in section 2.9.6) dimensionless, we need to define characteristic length, time, and velocity scales as ℓ, τ, and U, respectively. It is also useful to know the following dimensions of the parameters.

$$\beta_1 \; [=] \; \text{dimensionless} \tag{4.1}$$

$$\beta_2 \; [=] \; \frac{M}{LT} \; [=] \; \text{viscosity} \tag{4.2}$$

$$\chi \; [=] \; \frac{M}{LT^2} \; [=] \; \text{stress} \tag{4.3}$$

$$L \; [=] \; \frac{ML}{T^2} \; [=] \; \text{force} \tag{4.4}$$

$$\gamma \; [=] \; \frac{M}{L^3 T} \; [=] \; \frac{\text{force density}}{\text{velocity}} \tag{4.5}$$

$$\lambda \Delta\mu \; [=] \; T^{-1} \tag{4.6}$$

$$\zeta \Delta\mu \; [=] \; \frac{M}{LT^2} \; [=] \; \text{stress} \tag{4.7}$$

4.1 Dimensionless parameters

This is a general specification, and the exact values of these depend on the particular geometry and physical constraints of a given system. We define the characteristic length as ℓ and the characteristic time scale as τ. The characteristic active stress is $(\zeta\Delta\mu)_0$ and the characteristic active alignment is $(\lambda\Delta\mu)_0$. We define the characteristic velocity of be U, and this is set by $(\zeta\Delta\mu)_0$, as we will show in a moment. For now, we define dimensionless variables

$$\tilde{x} = x/\ell \tag{4.8}$$

$$\tilde{y} = y/\ell \tag{4.9}$$

$$\tilde{v}_x = v_x/U \tag{4.10}$$

$$\tilde{v}_y = v_y/U \tag{4.11}$$

$$\tilde{t} = t/\tau \tag{4.12}$$

$$\widetilde{\zeta\Delta\mu} = \zeta\Delta\mu/(\zeta\Delta\mu)_0 \tag{4.13}$$

$$\widetilde{\lambda\Delta\mu} = \lambda\Delta\mu/(\lambda\Delta\mu)_0. \tag{4.14}$$

To determine the characteristic velocity, we rewrite the equation of motion in 1D, neglecting the contribution of the order parameter and assuming a zero Reynolds number.

$$\frac{1}{2}\,\partial_x\zeta\Delta\mu = -\eta\partial_x^2 v_x + \gamma v_x \tag{4.15}$$

$$\Rightarrow\quad \frac{(\zeta\Delta\mu)_0}{\ell}\,\partial_{\tilde{x}}\widetilde{\zeta\Delta\mu} = -\frac{\eta U}{\ell^2}\left(\partial_{\tilde{x}}^2\tilde{v}_x + \frac{\gamma}{\eta}\,\tilde{v}_x\right). \tag{4.16}$$

To have both sides of the equations be of the same magnitude, the characteristic velocity is set by $U = (\zeta\Delta\mu)_0\ell/\eta$. If we consider an infinite domain, the only length scale present is $\sqrt{\eta/\gamma}$. This sets the characteristic velocity as $U = (\zeta\Delta\mu)_0/\sqrt{\eta\gamma}$. However, if we have no friction and $\gamma = 0$, there is no characteristc length scale. Indeed, on an infinite domain the equation of motion has no physical solution in the absense of friction. For a finite system the length scale is set by the size of the system itself. For example, if we consider $\widetilde{\zeta\Delta\mu} = \Theta(x)$, where $\Theta(x)$ is the Heaviside step function, and we consider $v_x(-\ell/2) = v_x(\ell/2) = 0$, we get

$$v_x = \frac{(\zeta\Delta\mu)_0\ell}{8\eta}\left(1 - 2\,\frac{|x|}{\ell}\right). \tag{4.17}$$

So, generally speaking, the characteristic velocity is given by

$$U = \frac{(\zeta\Delta\mu)_0\ell}{\eta}. \tag{4.18}$$

For convenience, we define two length scales, the hydrodynamic length scale and the nematic correlation length, defined respectively by

$$\ell_h = \sqrt{\eta/\gamma} \text{ and } \ell_n = \sqrt{L/\chi}. \tag{4.19}$$

Using these definitions, the governing equations become

$$\begin{aligned}\frac{\mathrm{Re}}{\mathrm{Sr}}\,\partial_t v_x = {} & (\partial_x^2 + \partial_y^2)v_x + \tilde{\eta}_v^{2d}\partial_x(\partial_x v_x + \partial_y v_y)\\ & + \beta_1\tilde{\chi}\left(\partial_x\tilde{Q} + \partial_y q\right) - \beta_1\tilde{\chi}\lambda_n^2\left((\partial_x^3 + \partial_x\partial_y^2)\tilde{Q} + (\partial_x^2\partial_y + \partial_y^3)q\right)\\ & + \left((Q_{xx}^0 - Q_{zz}^0)\partial_x\zeta\Delta\mu + \partial_x(\zeta\Delta\mu\tilde{Q}) + \partial_y(\zeta\Delta\mu q)\right)\\ & + \beta_1\mathrm{Sr}^{-1}(Q_{xx}^0 - Q_{zz}^0)\partial_x\lambda\Delta\mu - \lambda_h^{-2}\,v_x,\end{aligned} \tag{4.20}$$

$$
\begin{aligned}
\frac{\mathrm{Re}}{\mathrm{Sr}}\,\partial_t v_y = {} & (\partial_x^2+\partial_y^2)v_y + \tilde{\eta}_v^{2d}\partial_y(\partial_x v_x + \partial_y v_y) \\
& + \frac{\beta_1\tilde{\chi}}{\lambda_h}\left(\partial_x q - \partial_y \tilde{Q}\right) - \frac{\beta_1\tilde{\chi}\lambda_n^2}{\lambda_h}\left((\partial_x^3 + \partial_x\partial_y^2)q - (\partial_x^2\partial_y + \partial_y^3)\tilde{Q}\right) \\
& + \lambda_h^{-1}\left((Q_{yy}^0 - Q_{zz}^0)\partial_y\zeta\Delta\mu + \partial_x(\zeta\Delta\mu q) - \partial_y(\zeta\Delta\mu\tilde{Q})\right) \\
& + \beta_1\tilde{\beta_2}\mathrm{Sr}^{-1}(Q_{yy}^0 - Q_{zz}^0)\partial_y\lambda\Delta\mu - \lambda_h^{-2}\, v_y,
\end{aligned}
\tag{4.21}
$$

$$
\begin{aligned}
\mathrm{Sr}^{-1}\partial_t\tilde{Q} = {} & -(v_x\partial_x + v_y\partial_y)\tilde{Q} - q(\partial_x v_y - \partial_y v_x) + \frac{\beta_1}{2}(\partial_x v_x - \partial_y v_y) - \frac{\tilde{\chi}}{\tilde{\beta_2}\lambda_h}\left(1 - \lambda_n^2(\partial_x^2 + \partial_y^2)\right)\tilde{Q} \\
& + \lambda\Delta\mu\tilde{Q},
\end{aligned}
\tag{4.22}
$$

$$
\begin{aligned}
\mathrm{Sr}^{-1}\partial_t q = {} & -(v_x\partial_x + v_y\partial_y)q + \tilde{Q}(\partial_x v_y - \partial_y v_x) + \frac{\beta_1}{2}(\partial_x v_y + \partial_y v_x) - \frac{\tilde{\chi}}{\tilde{\beta_2}\lambda_h}\left(1 - \lambda_n^2(\partial_x^2 + \partial_y^2)\right)q \\
& + \lambda\Delta\mu q,
\end{aligned}
\tag{4.23}
$$

$$
\partial_t n_i = \tilde{D}_i(\partial_x^2 + \partial_y^2)n_i - \mathrm{Sr}\left[(1-\alpha_i)n_i(\partial_x v_x + \partial_y v_y) + v_x\partial_x n_i + v_y\partial_y n_i\right] + \tau\sum_k \nu_{ki}r_k. \tag{4.24}
$$

Here, we have omitted tildes on variables for notational convenience. The chemical reaction rates are still dimensional as written, and are nondimensionalized in the mass conservation equation by being multiplied by the characteristic time, τ. The dimensionless parameters are defined as

$$
\text{Reynolds number} = \mathrm{Re} = \frac{\rho U \ell}{\eta} = \text{ratio of inertial to viscous forces} \tag{4.25}
$$

$$
\text{Strouhal number} = \mathrm{Sr} = \frac{U\tau}{\ell} = \text{ratio of times scale of interest to time scale of fluid flow} \tag{4.26}
$$

$$
\tilde{\eta}_v^{2d} = \eta_v^{2d}/\eta = \text{ratio of 2d bulk to shear viscosity } (= 3) \tag{4.27}
$$

$$
\beta_1 = \text{coupling constant of stress to molecular field} \tag{4.28}
$$

$$
\tilde{\chi} \equiv \frac{\chi}{(\zeta\Delta\mu)_0} = \frac{\chi}{U\sqrt{\eta\gamma}} = \text{ratio of alignment forces due to molecular field to active stress} \tag{4.29}
$$

$$
\tilde{\beta_2} \equiv \frac{\beta_2}{\eta} = \text{ratio of viscosity of rotational alignment to viscosity} \tag{4.30}
$$

$$
\lambda_h \equiv \ell_h/\ell = \text{ratio of hydrodynamic length scale to characteristic length} \tag{4.31}
$$

$$
\lambda_n \equiv \ell_n/\ell = \text{ratio of nematic correlation length to characteristic length} \tag{4.32}
$$

$$
\tilde{D}_i \equiv \frac{D_i\tau}{\ell^2} = \text{ratio of characteristic time scale to diffusive time scale} \tag{4.33}
$$

4.2 Dimensionless equations for particular choice of ℓ, τ, and U

Following Bois, Jülicher, and Grill, *PRL*, we consider only flows driven against viscous dissipation and frictional losses by active processes. Here, the emphasis is on studying dynamics due to regulation of active stress by diffusing, being advocated, and reacting species. To this end, we take $\ell = \ell_h \equiv \sqrt{\eta/\gamma}$ as the characteristic length. This is the decay length of the velocity profile due to a step in active stress in the absence of nematic order. The resulting velocity has a maximum of order

$$U = \frac{(\zeta\Delta\mu)_0}{\sqrt{\eta\gamma}} = \frac{(\zeta\Delta\mu)_0}{\gamma\ell}, \tag{4.34}$$

which we take to be our characteristic velocity. Finally, we take the time scale of interest to be the diffusive time scale of species 1, $\tau = \tau_D \equiv \ell^2/D_1$. In this case, the Strouhal number is a Péclet number.

$$\mathrm{Sr} = \mathrm{Pe} = \frac{U\ell}{D_1} = \frac{(\zeta\Delta\mu)_0}{\gamma D_1}. \tag{4.35}$$

Then, the governing equations are

$$\begin{aligned}
\frac{\mathrm{Re}}{\mathrm{Pe}}\,\partial_t v_x = {} & (\partial_x^2 + \partial_y^2)v_x + 3\partial_x(\partial_x v_x + \partial_y v_y) \\
& + \beta_1\tilde{\chi}\left(\partial_x\tilde{Q} + \partial_y q\right) - \beta_1\tilde{\chi}\lambda_n^2\left((\partial_x^3 + \partial_x\partial_y^2)\tilde{Q} + (\partial_x^2\partial_y + \partial_y^3)q\right) \\
& + (Q_{xx}^0 - Q_{zz}^0)\partial_x\zeta\Delta\mu + \partial_x(\zeta\Delta\mu\tilde{Q}) + \partial_y(\zeta\Delta\mu q) \\
& + \beta_1\tilde{\beta}_2\mathrm{Pe}^{-1}(Q_{xx}^0 - Q_{zz}^0)\partial_x\lambda\Delta\mu - v_x,
\end{aligned} \tag{4.36}$$

$$\begin{aligned}
\frac{\mathrm{Re}}{\mathrm{Pe}}\,\partial_t v_y = {} & (\partial_x^2 + \partial_y^2)v_y + 3\partial_y(\partial_x v_x + \partial_y v_y) \\
& + \beta_1\tilde{\chi}\left(\partial_x q - \partial_y\tilde{Q}\right) - \beta_1\tilde{\chi}\lambda_n^2\left((\partial_x^3 + \partial_x\partial_y^2)q - (\partial_x^2\partial_y + \partial_y^3)\tilde{Q}\right) \\
& + (Q_{yy}^0 - Q_{zz}^0)\partial_y\zeta\Delta\mu + \partial_x(\zeta\Delta\mu q) - \partial_y(\zeta\Delta\mu\tilde{Q}) \\
& + \beta_1\tilde{\beta}_2\mathrm{Pe}^{-1}(Q_{yy}^0 - Q_{zz}^0)\partial_y\lambda\Delta\mu - v_y,
\end{aligned} \tag{4.37}$$

$$\begin{aligned}
\mathrm{Pe}^{-1}\partial_t\tilde{Q} = {} & -(v_x\partial_x + v_y\partial_y)\tilde{Q} - q(\partial_x v_y - \partial_y v_x) + \frac{\beta_1}{2}(\partial_x v_x - \partial_y v_y) - \frac{\tilde{\chi}}{\tilde{\beta}_2}\left(1 - \lambda_n^2(\partial_x^2 + \partial_y^2)\right)\tilde{Q} \\
& + \lambda\Delta\mu\tilde{Q},
\end{aligned} \tag{4.38}$$

$$\begin{aligned}
\mathrm{Pe}^{-1}\partial_t q = {} & -(v_x\partial_x + v_y\partial_y)q + \tilde{Q}(\partial_x v_y - \partial_y v_x) + \frac{\beta_1}{2}(\partial_x v_y + \partial_y v_x) - \frac{\tilde{\chi}}{\tilde{\beta}_2\lambda_h}\left(1 - \lambda_n^2(\partial_x^2 + \partial_y^2)\right)q \\
& + \lambda\Delta\mu q,
\end{aligned} \tag{4.39}$$

$$\partial_t n_i = (\partial_x^2 + \partial_y^2)n_i - \mathrm{Pe}\left[(1 - \alpha_i)n_i(\partial_x v_x + \partial_y v_y) + v_x\partial_x n_i + v_y\partial_y n_i\right] + \tau_D\sum_k \nu_{ki}r_k. \tag{4.40}$$

5 Numerical solution strategy

To solve equations (2.191), (2.192), (2.193), (2.194), and (2.195), we employ implicit-explicit (IMEX) methods. We split the problem into the linear and nonlinear parts. The linear parts are integrated with implicit time stepping and the nonlinear parts explicitly. We do all of this in Fourier space with $Re/Sr \approx 0$ (i.e., the left hand sides of (2.191) and (2.192) are both zero). We will also take $\alpha_i = 0\ \forall i$. Further, note that $Q^0_{xx} - Q^0_{zz} = Q^0_{yy} - Q^0_{zz} = 1/2$. We solve for the velocity at each time step and integrate $\tilde{Q}$, q, and n_i in time.

For this discussion, we assume we have periodic boundary conditions in both x and y.

5.1 Generic VSIMEX strategy

We adopt a variable step size IMEX scheme. The step sizes are chosen using a PID controller that keeps the relative change in values of the solution within a set tolerance. I know give the basic VSIMEX strategy.

Consider a set of PDEs,

$$\partial_t u = f(u) + g(u), \tag{5.1}$$

where $f(u)$ is a nonlinear function of u and $g(u)$ is linear. Note that both $f(u)$ and $g(u)$ may contain spatial differential operators, but for $g(u)$, these operators must be linear. Let k_n be the step size for numerical integration step n. Let U^n be the numerical solution for step n and let $\omega_{n+i} = k_{n+i}/k_n$. The general s-step VSIMEX scheme is, as given by Wang and Ruuth, *J. Comp. Math.*, **26**, 838–855 (2008),

$$\frac{1}{k_{n+s-1}} \sum_{j=0}^{s} \alpha_{j,n} U^{n+j} = \sum_{j=0}^{s-1} \beta_{j,n} f\left(U^{n+j}\right) + \sum_{j=0}^{s} \gamma_{j,n} g\left(U^{n+j}\right). \tag{5.2}$$

The constants α, β, and γ are given in the Wang and Ruuth paper. We see that the current step appears on both sides, but only in linear terms. Therefore, only the linear terms have implicit time stepping, so we do not have to solve nonlinear equations at each time step. We instead need to solve a linear system, which involves inverting a (potentially large and stiff) matrix. As we will see, doing the time stepping in Fourier space often avoids the necessity to perform this matrix inversion. Instead, for our particular system, we need only to invert a 2×2 matrix.

The special cases we apply are second order semi-implicit backward differencing formula (SBDF2) and second order Crank-Nicholson-Adams-Bashforth (CNAB2). In these cases, we have

$$\text{CNAB2}: \quad \frac{U^{n+2} - U^{n+1}}{k_{n+1}} = \left(1 + \frac{\omega}{2}\right) f(U^{n+1}) - \frac{\omega}{2} f(U^n) + \frac{1}{2}\left(g(U^{n+2}) + g(U^{n+1})\right), \tag{5.3}$$

$$\text{SBDF2}: \quad \frac{1}{k_{n+1}} \left(\frac{1+2\omega}{1+\omega} U^{n+2} - (1+\omega)U^{n+1} + \frac{\omega^2}{1+\omega} U^n\right) = (1+\omega) f(U^{n+1}) - \omega f(U^n) + g(U^{n+2}), \tag{5.4}$$

where we have taken $\omega = \omega_{n+1} = k_{n+1}/k_n$ for simpler notation.

5.2 Our problem in Fourier space

Re-writing (2.191) and (2.192) in Fourier space gives

$$k^2 \hat{v}_x + \tilde{\eta}_v^{2d} \left(k_x^2 \hat{v}_x + k_x k_y \hat{v}_y\right) + \ell_h^{-2} \hat{v}_x = \hat{f}_x \tag{5.5}$$

$$k^2\hat{v}_y + \tilde{\eta}_v^{2d}\left(k_x k_y \hat{v}_x + k_y^2\hat{v}_y\right) + \ell_h^{-2}\hat{v}_y = \hat{f}_y, \tag{5.6}$$

where

$$\hat{f}_x = \frac{i}{\eta}\left[\beta_1\chi(k_x\hat{Q} + k_y\hat{q}) + \beta_1 L k^2(k_x\hat{Q} + k_y\hat{q}) + \frac{k_x}{2}\,\widehat{\zeta\Delta\mu} + k_x\widehat{\zeta\Delta\mu Q} + k_y\widehat{\zeta\Delta\mu q} + \frac{\beta_1\beta_2}{2}\,k_x\widehat{\lambda\Delta\mu}\right] \tag{5.7}$$

$$\hat{f}_y = \frac{i}{\eta}\left[\beta_1\chi(k_x\hat{q} - k_y\hat{Q}) + \beta_1 L k^2(k_x\hat{q} - k_y\hat{Q}) + \frac{k_y}{2}\,\widehat{\zeta\Delta\mu} + k_x\widehat{\zeta\Delta\mu q} - k_y\widehat{\zeta\Delta\mu Q} + \frac{\beta_1\beta_2}{2}\,k_y\widehat{\lambda\Delta\mu}\right]. \tag{5.8}$$

To simplify notation, we have denoted the Fourier transform of $\tilde{Q}$ as $\hat{Q}$. We can solve (5.5) and (5.6) for $\hat{v}_x$ and $\hat{v}_y$.

$$\hat{v}_x = \frac{\left(k^2 + \tilde{\eta}_v^{2d}k_y^2 + \ell_h^{-2}\right)\hat{f}_x - \tilde{\eta}_v^{2d}k_x k_y\hat{f}_y}{\left((1+\tilde{\eta}_v^{2d})k^2 + \ell_h^{-2}\right)\left(k^2 + \ell_h^{-2}\right)} \tag{5.9}$$

$$\hat{v}_y = \frac{\left(k^2 + \tilde{\eta}_v^{2d}k_x^2 + \ell_h^{-2}\right)\hat{f}_y - \tilde{\eta}_v^{2d}k_x k_y\hat{f}_x}{\left((1+\tilde{\eta}_v^{2d})k^2 + \ell_h^{-2}\right)\left(k^2 + \ell_h^{-2}\right)}. \tag{5.10}$$

We can take an inverse Fourier transform to solve for v_x and v_y. An important caveat, however, is that when $\gamma = 0$ (and therefore $\ell_h^{-2} = 0$), the solution of (2.191) and (2.192) is only unique up to an additive constant with periodic boundary conditions. I.e., $v_x = v_x^0 + v_x^1(x,y)$ and $v_y = v_y^0 + v_y^1(x,y)$. Conveniently, this additive constant is given by the zero mode in Fourier space. The reason for this is that $\hat{f}_x$ and $\hat{f}_y$ are both functions of derivatives of periodic functions. This means than when the right hand side of (5.5) and (5.6) is written as a Fourier series, there is no constant term. Therefore, the zero mode of $\hat{v}_x$ and $\hat{v}_y$ must be zero.

With (5.9) and (5.10) in hand, and denoting the Fourier transform as F, we have

$$\begin{aligned}
\eta d F[\partial_x v_x - \partial_y v_y] &= i\eta d(k_x\hat{v}_x - k_y\hat{v}_y)\\
&= -\beta_1\chi\left[\left(k^2\left(k^2 + \ell_h^{-2}\right) + 4\tilde{\eta}_v^{2d}k_x^2k_y^2\right)\hat{Q} - 2\tilde{\eta}_v^{2d}(k_x^2 - k_y^2)k_xk_y\hat{q}\right]\\
&\quad - \beta_1 L k^2\left[\left(k^2\left(k^2 + \lambda_h^{-2}\right) + 4\tilde{\eta}_v^{2d}k_x^2k_y^2\right)\hat{Q} - 2\tilde{\eta}_v^{2d}(k_x^2 - k_y^2)k_xk_y\hat{q}\right]\\
&\quad - \frac{1}{2}(k_x^2 - k_y^2)(k^2 + \ell_h^{-2})\widehat{\zeta\Delta\mu} - \left(k^2(k^2 + \ell_h^{-2}) + 4\tilde{\eta}_v^{2d}k_x^2k_y^2\right)\widehat{\zeta\Delta\mu Q}\\
&\quad + 2\tilde{\eta}_v^{2d}k_xk_y(k_x^2 - k_y^2)\widehat{\zeta\Delta\mu q} - \frac{\beta_1\beta_2}{2}(k_x^2 - k_y^2)(k^2 + \ell_h^{-2})\widehat{\lambda\Delta\mu}
\end{aligned} \tag{5.11}$$

$$\begin{aligned}
\eta d F[\partial_x v_y + \partial_y v_x] &= i\eta d(k_x\hat{v}_y + k_y\hat{v}_x)\\
&= \beta_1\chi\left[2\tilde{\eta}_v^{2d}(k_x^2 - k_y^2)k_xk_y\hat{Q} - \left(k^2\left(k^2 + \ell_h^{-2}\right) + \tilde{\eta}_v^{2d}(k_x^2 - k_y^2)^2\right)\hat{q}\right]\\
&\quad + \beta_1 L k^2\left[2\tilde{\eta}_v^{2d}(k_x^2 - k_y^2)k_xk_y\hat{Q} - \left(k^2\left(k^2 + \lambda_h^{-2}\right) + \eta_v^{2d}(k_x^2 - k_y^2)^2\right)\hat{q}\right]\\
&\quad - k_xk_y(k^2 + \ell_h^{-2})\widehat{\zeta\Delta\mu} + 2\tilde{\eta}_v^{2d}k_xk_y(k_x^2 - k_y^2)\widehat{\zeta\Delta\mu Q}\\
&\quad - \left(k^2(k^2 + \ell_h^{-2}) + \tilde{\eta}_v^{2d}(k_x^2 - k_y^2)^2\right)\widehat{\zeta\Delta\mu q} - \beta_1\beta_2k_xk_y(k^2 + \ell_h^{-2})\widehat{\lambda\Delta\mu}.
\end{aligned} \tag{5.12}$$

where

$$d = \left((1+\tilde{\eta}_v^{2d})k^2 + \ell_h^{-2}\right)\left(k^2 + \ell_h^{-2}\right), \tag{5.13}$$

the denominator in the expressions for the Fourier transforms of the velocity.

Note that we can solve for v_x and v_y by performing an inverse FFT on (5.9) and (5.10). Given these solutions and the expressions for the derivatives of the velocities in Fourier space, we can write (2.193) in Fourier space.

$$\begin{aligned}
\partial_t \hat{Q} = &-\frac{1}{\beta_2}\left(\chi + Lk^2\right)\hat{Q} \\
&- \frac{\beta_1^2}{2\eta d}\left(\chi + Lk^2\right)\left[\left(k^2\left(k^2+\ell_h^{-2}\right) + 4\tilde{\eta}_v^{2d}k_x^2k_y^2\right)\hat{Q} - 2\tilde{\eta}_v^{2d}(k_x^2-k_y^2)k_xk_y\hat{q}\right] \\
&- \frac{\beta_1}{2\eta d}\left[\frac{1}{2}(k_x^2-k_y^2)(k^2+\ell_h^{-2})\widehat{\zeta\Delta\mu} + \left(k^2(k^2+\ell_h^{-2}) + 4\tilde{\eta}_v^{2d}k_x^2k_y^2\right)\widehat{\zeta\Delta\mu Q}\right. \\
&\qquad\qquad \left. -2\tilde{\eta}_v^{2d}(k_x^2-k_y^2)k_xk_y\widehat{\zeta\Delta\mu q}\right] \\
&- \frac{\beta_1^2\beta_2}{4\eta d}(k_x^2-k_y^2)(k^2+\ell_h^{-2})\widehat{\lambda\Delta\mu} \\
&+ F\left[-(v_x\partial_x + v_y\partial_y)\tilde{Q} - q(\partial_x v_y - \partial_y v_x) + \lambda\Delta\mu\tilde{Q}\right],
\end{aligned} \tag{5.14}$$

where d is given by (5.13). Here, the first three lines are linear in $\hat{Q}$ and $\hat{q}$. The remaining terms are nonlinear. We can also write (2.194) in Fourier space.

$$\begin{aligned}
\partial_t \hat{q} = &-\frac{1}{\beta_2}(\chi + Lk^2)\hat{q} \\
&+ \frac{\beta_1^2}{2\eta d}\left(\chi + Lk^2\right)\left[2\tilde{\eta}_v^{2d}(k_x^2-k_y^2)k_xk_y\hat{Q} - \left(k^2\left(k^2+\ell_h^{-2}\right) + \tilde{\eta}_v^{2d}(k_x^2-k_y^2)^2\right)\hat{q}\right] \\
&- \frac{\beta_1}{2\eta d}\left[k_xk_y(k^2+\ell_h^{-2})\widehat{\zeta\Delta\mu} - 2\tilde{\eta}_v^{2d}k_xk_y(k_x^2-k_y^2)\widehat{\zeta\Delta\mu Q}\right. \\
&\qquad\qquad \left. + \left(k^2(k^2+\ell_h^{-2}) + \tilde{\eta}_v^{2d}(k_x^2-k_y^2)^2\right)\widehat{\zeta\Delta\mu q}\right] \\
&- \frac{\beta_1^2\beta_2}{2\eta d}\,k_xk_y(k^2+\ell_h^{-2})\widehat{\lambda\Delta\mu} \\
&+ F\left[-(v_x\partial_x + v_y\partial_y)q + \tilde{Q}(\partial_x v_y - \partial_y v_x) + \lambda\Delta\mu q\right]
\end{aligned} \tag{5.15}$$

Finally, we can write (4.24) in Fourier space, again with $\alpha_i = 0$.

$$\partial_t \hat{n}_i = -D_i k^2 \hat{n}_i + F\left[-\partial_x(n_i v_x) - \partial_y(n_i v_y) + \sum_k \nu_{ki} r_k\right]. \tag{5.16}$$

In this case, the first term is linear.

5.3 Implementation

To help reduce bugs, we introduce the following constants, recalling d, already defined in (5.13).

$$d = \left((1+\tilde{\eta}_v^{2d})k^2 + \ell_h^{-2}\right)\left(k^2 + \ell_h^{-2}\right) = a_0(a_0 + \tilde{\eta}_v^{2d}k^2) \tag{5.17}$$

$$a_0 = k^2 + \ell_h^{-2} \tag{5.18}$$

$$a_1 = \frac{\beta_1 \chi}{\eta} \tag{5.19}$$

$$a_2 = \frac{\beta_1 L}{\eta} k^2 \tag{5.20}$$

$$a_3 = \frac{\beta_1 \beta_2}{2\eta} \tag{5.21}$$

$$a_4 = \frac{k^2 + \tilde{\eta}_v^{2d} k_y^2 + \ell_h^{-2}}{d} \tag{5.22}$$

$$a_5 = \frac{k^2 + \tilde{\eta}_v^{2d} k_x^2 + \ell_h^{-2}}{d} \tag{5.23}$$

$$a_6 = \frac{\tilde{\eta}_v^{2d} k_x k_y}{d} \tag{5.24}$$

$$a_7 = \frac{1}{\beta_2}\left(\chi + Lk^2\right) \tag{5.25}$$

$$a_8 = \frac{\beta_1^2}{2\eta d}(\chi + Lk^2) \tag{5.26}$$

$$a_9 = a_0\, k^2 + 4\tilde{\eta}_v^{2d} k_x^2 k_y^2 \tag{5.27}$$

$$a_{10} = 2\tilde{\eta}_v^{2d}(k_x^2 - k_y^2)k_x k_y \tag{5.28}$$

$$a_{11} = a_0 k^2 + \tilde{\eta}_v^{2d}(k_x^2 - k_y^2)^2 \tag{5.29}$$

$$a_{12} = \frac{\beta_1}{2\eta d} \tag{5.30}$$

$$a_{13} = a_0 k_x k_y \tag{5.31}$$

$$a_{14} = \frac{a_0(k_x^2 - k_y^2)}{2} \tag{5.32}$$

$$a_{15} = \frac{\beta_1^2 \beta_2}{2\eta d} \tag{5.33}$$

$$a_{16} = k_x k_y\, a_0. \tag{5.34}$$

With these definitions, we have

$$\hat{f}_x = i\left[a_1(k_x\hat{Q} + k_y\hat{q}) + a_2(k_x\hat{Q} + k_y\hat{q}) + \frac{k_x}{2}\,\widehat{\zeta\Delta\mu} + k_x\widehat{\zeta\Delta\mu Q} + k_y\widehat{\zeta\Delta\mu q} + a_3k_x\widehat{\lambda\Delta\mu}\right] \tag{5.35}$$

$$\hat{f}_y = i\left[a_1(k_x\hat{q} - k_y\hat{Q}) + a_2(k_x\hat{q} - k_y\hat{Q}) + \frac{k_y}{2}\,\widehat{\zeta\Delta\mu} + k_x\widehat{\zeta\Delta\mu q} - k_y\widehat{\zeta\Delta\mu Q} + a_3k_y\widehat{\lambda\Delta\mu}\right] \tag{5.36}$$

$$\hat{v}_x = a_4\hat{f}_x - a_6\hat{f}_y \tag{5.37}$$

$$\hat{v}_y = a_5\hat{f}_y - a_6\hat{f}_x \tag{5.38}$$

$$\begin{aligned}\partial_t\hat{Q} = {} & -a_7\hat{Q} - a_8\left(a_9\hat{Q} - a_{10}\hat{q}\right) - a_{12}\left(a_{14}\widehat{\zeta\Delta\mu} + a_9\widehat{\zeta\Delta\mu Q} - a_{10}\widehat{\zeta\Delta\mu q}\right) - a_{15}\,a_{14}\widehat{\lambda\Delta\mu} \\ & + F\left[-(v_x\partial_x + v_y\partial_y)\tilde{Q} - q(\partial_x v_y - \partial_y v_x) + \lambda\Delta\mu\tilde{Q}\right]\end{aligned} \tag{5.39}$$

$$\begin{aligned}\partial_t\hat{q} = {} & -a_7\hat{q} + a_8\left(a_{10}\hat{Q} - a_{11}\hat{q}\right) - a_{12}\left(a_{13}\widehat{\zeta\Delta\mu} - a_{10}\widehat{\zeta\Delta\mu Q} + a_{11}\widehat{\zeta\Delta\mu q}\right) - a_{15}\,a_{16}\widehat{\lambda\Delta\mu} \\ & + F\left[-(v_x\partial_x + v_y\partial_y)q + \tilde{Q}(\partial_x v_y - \partial_y v_x) + \lambda\Delta\mu q\right]\end{aligned} \tag{5.40}$$

$$\partial_t\hat{n}_i = -D_ik^2\hat{n}_i + F\left[-\left(\partial_x(n_iv_x) + \partial_y(n_iv_y)\right) + \tau\sum_k \nu_{ki}r_k\right]. \tag{5.41}$$

To write the IMEX scheme, we make the following definitions

$$\begin{aligned}\hat{f}_Q(\hat{Q},\hat{q},\hat{n}_i) \equiv {} & -a_{12}\left(a_{14}\widehat{\zeta\Delta\mu} + a_9\widehat{\zeta\Delta\mu Q} - a_{10}\widehat{\zeta\Delta\mu q}\right) - a_{15}\,a_{14}\widehat{\lambda\Delta\mu} \\ & + F\left[-(v_x\partial_x + v_y\partial_y)\tilde{Q} - q(\partial_x v_y - \partial_y v_x) + \lambda\Delta\mu\tilde{Q}\right]\end{aligned} \tag{5.42}$$

$$\begin{aligned}\hat{f}_q(\hat{Q},\hat{q},\hat{n}_i) \equiv {} & -a_{12}\left(a_{13}\widehat{\zeta\Delta\mu} - a_{10}\widehat{\zeta\Delta\mu Q} + a_{11}\widehat{\zeta\Delta\mu q}\right) - a_{15}\,a_{16}\widehat{\lambda\Delta\mu} \\ & + F\left[-(v_x\partial_x + v_y\partial_y)q + \tilde{Q}(\partial_x v_y - \partial_y v_x) + \lambda\Delta\mu q\right]\end{aligned} \tag{5.43}$$

$$\hat{f}_{n_i}(\hat{Q},\hat{q},\hat{n}_i) \equiv F\left[-\left(\partial_x(n_iv_x) + \partial_y(n_iv_y)\right) + \tau\sum_k \nu_{ki}r_k\right] \tag{5.44}$$

$$b_{11} \equiv -a_7 - a_8a_9 \tag{5.45}$$

$$b_{12} = b_{21} \equiv a_8a_{10} \tag{5.46}$$

$$b_{22} \equiv -a_7 - a_8a_{11}, \tag{5.47}$$

and rewrite the above equations as

$$\partial_t\hat{Q} = b_{11}\hat{Q} + b_{12}\hat{q} + \hat{f}_Q(\hat{Q},\hat{q},\hat{n}_i) \tag{5.48}$$

$$\partial_t\hat{q} = b_{21}\hat{Q} + b_{22}\hat{q} + \hat{f}_q(\hat{Q},\hat{q},\hat{n}_i) \tag{5.49}$$

$$\partial_t\hat{n}_i = -D_ik^2\hat{n}_i + \hat{f}_n(\hat{Q},\hat{q},\hat{n}_i) \tag{5.50}$$

Note that in practice, we set the zero mode in d to be unity when $\gamma = 0$ to avoid divide by zero errors when computing the other constants. This is of no consequence because in the velocity calculations, we intentionally set the zero modes of $\hat{f}_x$ and $\hat{f}_y$ to be zero, and in all other cases, the zero modes are multiplied by a zero wave number in all expressions.

5.3.1 CNAB2 implementation

We can write the expressions for the CNAB2 scheme. We abbreviate $\hat{f}_Q(\hat{Q}^n, \hat{q}^n, \hat{n}_i^n)$ as $f_Q(U^n)$, with similar abbreviations for $\hat{f}_q$ and $\hat{f}_{n_i}$.

$$\frac{\hat{Q}^{n+2} - \hat{Q}^{n+1}}{k_{n+1}} = \left(1 + \frac{\omega}{2}\right) \hat{f}_Q(U^{n+1}) - \frac{\omega}{2} \hat{f}_Q(U^n) + \frac{1}{2}\left(b_{11}(\hat{Q}^{n+2} + \hat{Q}^{n+1}) + b_{12}(\hat{q}^{n+2} + \hat{q}^{n+1})\right) \tag{5.51}$$

$$\frac{\hat{q}^{n+2} - \hat{q}^{n+1}}{k_{n+1}} = \left(1 + \frac{\omega}{2}\right) \hat{f}_q(U^{n+1}) - \frac{\omega}{2} \hat{f}_q(U^n) + \frac{1}{2}\left(b_{21}(\hat{Q}^{n+2} + \hat{Q}^{n+1}) + b_{22}(\hat{q}^{n+2} + \hat{q}^{n+1})\right) \tag{5.52}$$

$$\frac{\hat{n}_i^{n+2} - \hat{n}_i^{n+1}}{k_{n+1}} = \left(1 + \frac{\omega}{2}\right) \hat{f}_{n_1}(U^{n+1}) - \frac{\omega}{2} \hat{f}_{n_i}(U^n) \frac{\tilde{D}_i k^2}{2} \left(\hat{n}_i^{n+2} + \hat{n}_i^{n+1}\right). \tag{5.53}$$

Rearrangement of these equations yields

$$\left(\frac{1}{k_{n+1}} - \frac{b_{11}}{2}\right) \hat{Q}^{n+2} - \frac{b_{12}}{2} \hat{q}^{n+2} = \left(1 + \frac{\omega}{2}\right) \hat{f}_Q(U^{n+1}) - \frac{\omega}{2} \hat{f}_Q(U^n) + \left(\frac{1}{k_{n+1}} + \frac{b_{11}}{2}\right) \hat{Q}^{n+1} + \frac{b_{12}}{2} \hat{q}^{n+1} \tag{5.54}$$

$$-\frac{b_{21}}{2} \hat{Q}^{n+2} + \left(\frac{1}{k_{n+1}} - \frac{b_{22}}{2}\right) \hat{q}^{n+2} = \left(1 + \frac{\omega}{2}\right) \hat{f}_q(U^{n+1}) - \frac{\omega}{2} \hat{f}_q(U^n) + \frac{b_{21}}{2} \hat{Q}^{n+1} + \left(\frac{1}{k_{n+1}} + \frac{b_{22}}{2}\right) \hat{q}^{n+1} \tag{5.55}$$

$$\left(\frac{1}{k_{n+1}} + \frac{\tilde{D}_i k^2}{2}\right) \hat{n}_i^{n+2} = \left(1 + \frac{\omega}{2}\right) \hat{f}_{n_1}(U^{n+1}) - \frac{\omega}{2} \hat{f}_{n_i}(U^n) + \left(\frac{1}{k_{n+1}} - \frac{\tilde{D}_i k^2}{2}\right) \hat{n}_i^{n+1}. \tag{5.56}$$

We can now solve for the values of $\hat{Q}^{n+2}$, $\hat{q}^{n+2}$, and $\hat{n}_i^{n+2}$. We define rhs_Q and rhs_q as the right hand side of the top two equations. Then, we have

$$\hat{Q}^{n+2} = \frac{1}{\left(\frac{1}{k_{n+1}} - \frac{b_{11}}{2}\right)\left(\frac{1}{k_{n+1}} - \frac{b_{22}}{2}\right) - \frac{b_{12} b_{21}}{4}} \left[\left(\frac{1}{k_{n+1}} - \frac{b_{22}}{2}\right) \text{rhs}_Q + \frac{b_{12}}{2} \text{rhs}_q\right] \tag{5.57}$$

$$\hat{q}^{n+2} = \frac{1}{\left(\frac{1}{k_{n+1}} - \frac{b_{11}}{2}\right)\left(\frac{1}{k_{n+1}} - \frac{b_{22}}{2}\right) - \frac{b_{12} b_{21}}{4}} \left[\frac{b_{21}}{2} \text{rhs}_Q + \left(\frac{1}{k_{n+1}} - \frac{b_{11}}{2}\right) \text{rhs}_q\right] \tag{5.58}$$

$$\hat{n}_i^{n+2} = \frac{1}{\frac{1}{k_{n+1}} + \frac{\tilde{D}_i k^2}{2}} \left[\left(1 + \frac{\omega}{2}\right) \hat{f}_{n_1}(U^{n+1}) - \frac{\omega}{2} \hat{f}_{n_i}(U^n) + \left(\frac{1}{k_{n+1}} - \frac{\tilde{D}_i k^2}{2}\right) \hat{n}_i^{n+1}\right]. \tag{5.59}$$

Note that this solution requires that the matrix

$$\begin{pmatrix} \frac{1}{k_{n+1}} - \frac{b_{11}}{2} & -\frac{b_{12}}{2} \\ -\frac{b_{12}}{2} & \frac{1}{k_{n+1}} - \frac{b_{22}}{2} \end{pmatrix} \tag{5.60}$$

is nonsingular. We can show this is the case by considering its determinant. The determinant is

$$\left(\frac{1}{k_{n+1}}-\frac{b_{11}}{2}\right)\left(\frac{1}{k_{n+1}}-\frac{b_{22}}{2}\right)-\frac{b_{12}^2}{4}=\text{positive terms}+\frac{b_{11}b_{22}}{4}\left(1-\frac{b_{12}^2}{b_{11}b_{22}}\right). \tag{5.61}$$

Since the product $b_{11}b_{22}$ is positive, we have only to show that the ratio

$$\frac{b_{12}^2}{b_{11}b_{22}}<1 \tag{5.62}$$

to prove that the determinant is positive and the matrix therefore nonsingular. Evaluating the ratio,

$$\frac{b_{12}^2}{b_{11}b_{22}}=\frac{a_8^2a_{10}^2}{\text{positive terms}+a_8^2a_9a_{11}}<\frac{a_{10}^2}{a_9a_{11}}=\frac{a_{10}^2}{\text{positive terms}+a_{10}^2}<1. \tag{5.63}$$

Therefore, the determinant is positive and the matrix is nonsingular.

5.3.2 SBDF2 implementation

The formulae for the SBDF2 method are derived analogously.

$$\left(\frac{1+2\omega}{k_{n+1}(1+\omega)}-b_{11}\right)\hat{Q}^{n+2}-b_{12}\hat{q}^{n+2}=(1+\omega)\hat{f}_Q(U^{n+1})-\omega\hat{f}_Q(U^n)+\frac{1}{k_{n+1}}\left((1+\omega)\hat{Q}^{n+1}-\frac{\omega^2}{1+\omega}\hat{Q}^n\right) \tag{5.64}$$

$$-b_{21}\hat{q}^{n+2}+\left(\frac{1+2\omega}{k_{n+1}(1+\omega)}-b_{22}\right)\hat{q}^{n+2}=(1+\omega)\hat{f}_q(U^{n+1})-\omega\hat{f}_q(U^n)+\frac{1}{k_{n+1}}\left((1+\omega)\hat{q}^{n+1}-\frac{\omega^2}{1+\omega}\hat{q}^n\right) \tag{5.65}$$

$$\left(\frac{1+2\omega}{k_{n+1}(1+\omega)}+\tilde{D}_ik^2\right)\hat{n}_i^{n+2}=(1+\omega)\hat{f}_{n_i}(U^{n+1})-\omega\hat{f}_{n_i}(U^n)+\frac{1}{k_{n+1}}\left((1+\omega)\hat{n}_i^{n+1}-\frac{\omega^2}{1+\omega}\hat{n}_i^n\right). \tag{5.66}$$

Again, defining rhs_Q as the right hand side of the first equation, etc., we have

$$\hat{Q}^{n+2}=\frac{1}{\left(\frac{1+2\omega}{k_{n+1}(1+\omega)}-b_{11}\right)\left(\frac{1+2\omega}{k_{n+1}(1+\omega)}-b_{22}\right)-b_{12}b_{21}}\left[\left(\frac{1+2\omega}{k_{n+1}(1+\omega)}-b_{22}\right)\text{rhs}_Q+b_{12}\,\text{rhs}_q\right] \tag{5.67}$$

$$\hat{q}^{n+2}=\frac{1}{\left(\frac{1+2\omega}{k_{n+1}(1+\omega)}-b_{11}\right)\left(\frac{1+2\omega}{k_{n+1}(1+\omega)}-b_{22}\right)-b_{12}b_{21}}\left[b_{21}\,\text{rhs}_Q+\left(\frac{1+2\omega}{k_{n+1}(1+\omega)}-b_{11}\right)\text{rhs}_q\right] \tag{5.68}$$

$$\hat{n}_i^{n+2}=\frac{\text{rhs}_{n_i}}{\frac{1+2\omega}{k_{n+1}(1+\omega)}+\tilde{D}_ik^2}. \tag{5.69}$$

We can show that the system of equations always has a solution in a similar manner as we did for the CNAB2 case.

Appendix: Helpful relations

$A_{\alpha\beta}$ and $B_{\alpha\beta}$ are second order tensors. u_α and v_α are vectors. f is a scalar valued function.

Indicial and vector notation

$$u_\alpha \, v_\alpha = u \cdot v = u^T \, v \tag{5.70}$$

$$u_\alpha \, v_\beta = uv = u \otimes v \tag{5.71}$$

$$\epsilon_{\alpha\beta\gamma} \, u_\beta \, v_\gamma = \mathbf{u} \times \mathbf{v} \tag{5.72}$$

$$A_{\alpha\beta} \, v_\beta = A \cdot v \tag{5.73}$$

$$A_{\alpha\beta} \, v_\alpha = A^T \cdot v \tag{5.74}$$

$$A_{\alpha\beta} \, B_{\beta\gamma} = A \cdot B \tag{5.75}$$

$$A_{\alpha\beta} \, B_{\gamma\beta} = A \cdot B^T \tag{5.76}$$

$$A_{\alpha\beta} \, B_{\alpha\gamma} = A^T \cdot B \tag{5.77}$$

$$A_{\alpha\beta} \, B_{\alpha\beta} = A : B = \mathrm{Tr}\left(A^T \cdot B\right) \tag{5.78}$$

$$A_{\alpha\beta} \, B_{\beta\alpha} = A : B^T = \mathrm{Tr}\left(A^T \cdot B^T\right) \tag{5.79}$$

$$A_{\alpha\beta} \, B_{\alpha\beta} = A_{\alpha\beta} \, B_{\beta\alpha} \text{ for symmetric } A \tag{5.80}$$

$$A_{\alpha\alpha} = A_{\alpha\beta}\delta_{\alpha\beta} = \mathrm{Tr}(A) \tag{5.81}$$

$$A_{\alpha\mu} B_{\beta\nu} C_{\alpha\beta} = A^T \cdot C \cdot B \tag{5.82}$$

$$\partial_\alpha f = \nabla f = \mathrm{grad}\, f \tag{5.83}$$

$$\partial_\alpha \, v_\alpha = \nabla \cdot v = \mathrm{div}\ v \tag{5.84}$$

$$\epsilon_{\alpha\beta\gamma} \, \partial_\alpha \, v_\beta = \nabla \times \mathbf{v} = \mathrm{curl}\, \mathbf{v} \tag{5.85}$$

$$\partial_\alpha \, v_\beta = \nabla v = \nabla \otimes v \tag{5.86}$$

$$\partial_\beta \, A_{\alpha\beta} = \nabla \cdot A \tag{5.87}$$

$$\partial_\alpha \, A_{\alpha\beta} = \nabla \cdot A^T \tag{5.88}$$

$$\partial_\alpha \left(v_\alpha v_\beta\right) = \partial_\beta \left(v_\alpha v_\beta\right) = v_\alpha \partial_\beta v_\beta + v_\beta \partial_\beta v_\alpha = \left(\nabla \cdot v\right) v + v \cdot \nabla v \tag{5.89}$$

$$|A_{\alpha\beta}| = \epsilon_{i_1 i_2 \cdots i_n} A_{1 i_1} A_{2 i_1} \cdots A_{n i_n} = \det \mathbf{A} \tag{5.90}$$

$$\delta_{\alpha\beta}\delta_{\alpha\beta} = 3 \tag{5.91}$$

Properties of the Levi-Civita symbol

(Some of these properties are repeated below.) A tensor $A_{\alpha\beta}$ may be split into a symmetric part $A^s_{\alpha\beta}$ and an antisymmetric part $A^a_{\alpha\beta}$. We denote an antisymmetric tensor with an a superscript and a symmetric tensor with an s superscript. $A^s_{\alpha\beta}$ may be made traceless by simply subtracting a third of the trace from the diagonal, $\mathring{A}^s_{\alpha\beta} = A^s_{\alpha\beta} - \delta_{\alpha\beta} A_{\gamma\gamma}/3$.

$$\epsilon_{\alpha\beta\gamma} = \begin{cases} 1 & \text{if } \alpha\beta\gamma = 123, 231, 312 \\ -1 & \text{if } \alpha\beta\gamma = 321, 213, 132 \\ 0 & \text{otherwise} \end{cases} . \tag{5.92}$$

$$\epsilon_{abc}\epsilon_{123} = \delta_{a1}(\delta_{b2}\delta_{c3} - \delta_{b3}\delta_{c2}) - \delta_{a2}(\delta_{b1}\delta_{c3} - \delta_{b3}\delta_{c1}) + \delta_{a3}(\delta_{b1}\delta_{c2} - \delta_{b2}\delta_{c1}) \tag{5.93}$$

$$\epsilon_{\alpha\beta\gamma}\,\epsilon_{\alpha\delta\mu} = \delta_{\beta\delta}\delta_{\gamma\mu} - \delta_{\beta\mu}\delta_{\gamma\delta}, \text{ or } \epsilon_{abc}\epsilon_{a23} = \delta_{b2}\delta_{c3} - \delta_{b3}\delta_{c2} \tag{5.94}$$

$$\epsilon_{\alpha\beta\gamma}\epsilon_{\alpha\beta\delta} = 2\delta_{\gamma\delta}, \text{ or } \epsilon_{abc}\epsilon_{ab3} = 2\delta_{c3} \tag{5.95}$$

$$\epsilon_{\alpha\beta\gamma}\epsilon_{\alpha\beta\gamma} = 6 \tag{5.96}$$

$$\frac{1}{2}\epsilon_{\alpha\beta\gamma}\epsilon_{\delta\mu\gamma}A_{\delta\mu} = A^a_{\alpha\beta} = \frac{1}{2}(A_{\alpha\beta} - A_{\beta\alpha}) \tag{5.97}$$

$$\epsilon_{\alpha\beta\gamma}A^a_{\beta\gamma} = 2(A^a_{23}, -A^a_{31}, A^a_{12})^T \tag{5.98}$$

$$\epsilon_{\alpha\beta\gamma}a_\gamma = \begin{pmatrix} 0 & a_3 & -a_2 \\ -a_3 & 0 & a_1 \\ a_2 & -a_1 & 0 \end{pmatrix} . \tag{5.99}$$

Transformation of tensors under arbitrary rotation

Let $T_\alpha\beta\gamma\cdots$ be a rank n tensor and $R_{\alpha\beta}$ denote an arbitrary rotation tensor. The transformed tensor undergoing rotation is

$$T'_{\mu\nu\rho\cdots} = (R_{\mu\alpha}R_{\nu\beta}R_{\rho\gamma}\cdots)T_{\alpha\beta\gamma} \equiv \mathsf{R}T_{\alpha\beta\gamma\cdots}. \tag{5.100}$$

The following properties hold for an arbitrary rotation.

$$R_{\mu\alpha}R_{\nu\alpha} = \delta_{\mu\nu} \tag{5.101}$$

$$\delta'_{\mu\nu} = R_{\mu\alpha}R_{\nu\beta}\delta_{\alpha\beta} = R_{\mu\beta}R_{\nu\beta} = \delta_{\mu\nu} \tag{5.102}$$

$$\epsilon'_{\mu\nu\rho} = R_{\mu\alpha}R_{\nu\beta}R_{\rho\gamma}\epsilon_{\alpha\beta\gamma} = \epsilon_{\mu\nu\rho}|R_{\alpha\beta}| = \epsilon_{\mu\nu\rho} \tag{5.103}$$

Integration by parts

We consider integrations of functions (which may have different tensorial order) $u(x)$ and $v(x)$, when x is a vector. We introduce the notation below.

$$\int_\Omega dx = \text{integral over volume } \Omega \tag{5.104}$$

$$\int_{\partial\Omega} dx = \text{integral over surface } \partial\Omega \tag{5.105}$$

$$\nu = \text{outward unit normal from the surface } \partial\Omega \tag{5.106}$$

Useful integrals:

$$\int_\Omega dx\, f\, \partial_\alpha v_\alpha = \int_{\partial\Omega} dx\, f v_\alpha \nu_\alpha - \int_\Omega dx\, v_\alpha \partial_\alpha f \tag{5.107}$$

$$\int_\Omega dx\, v_\alpha\, \partial_\alpha f = \int_{\partial\Omega} dx\, f v_\alpha \nu_\alpha - \int_\Omega dx\, f \partial_\alpha v_\alpha \tag{5.108}$$

$$\int_\Omega dx\, v_\alpha\, \partial_\beta A_{\alpha\beta} = \int_{\partial\Omega} dx\, A_{\alpha\beta}\, v_\beta\, \nu_\alpha - \int_\Omega dx\, A_{\alpha\beta}\, \partial_\alpha v_\beta \tag{5.109}$$

$$\int_\Omega dx\, v^2\, \partial_\alpha v_\alpha = \int_{\partial\Omega} dx\, v^2\, v_\alpha \nu_\alpha - 2 \int_\Omega dx\, v_\alpha v_\beta\, \partial_\alpha v_\beta \tag{5.110}$$

Symmetry properties of 2nd order tensors

A tensor $A_{\alpha\beta}$ may be split into a symmetric part $A^s_{\alpha\beta}$ and an antisymmetric part $A^a_{\alpha\beta}$. We denote an antisymmetric tensor with an a superscript and a symmetric tensor with an s superscript. $A^s_{\alpha\beta}$ may be made traceless by simply subtracting a third of the trace from the diagonal, $\mathring{A}^s_{\alpha\beta} = A^s_{\alpha\beta} - \delta_{\alpha\beta} A_{\gamma\gamma}/3$.

$$A_{\alpha\beta} = A^s_{\alpha\beta} + A^a_{\alpha\beta} = \mathring{A}^s_{\alpha\beta} + A^a_{\alpha\beta} + \delta_{\alpha\beta} A_{\gamma\gamma}/3 \tag{5.111}$$

$$A^s_{\alpha\beta} = \frac{1}{2}(A_{\alpha\beta} + A_{\beta\alpha}) \tag{5.112}$$

$$A^a_{\alpha\beta} = \frac{1}{2}(A_{\alpha\beta} - A_{\beta\alpha}) = \frac{1}{2}\epsilon_{\alpha\beta\gamma}\epsilon_{\delta\mu\gamma} A_{\delta\mu} \tag{5.113}$$

$$\delta_{\alpha\beta} \mathring{A}^s_{\alpha\beta} = 0 \tag{5.114}$$

$$\delta_{\alpha\beta} A^a_{\alpha\beta} = 0 \tag{5.115}$$

$$\delta_{\alpha\beta} A_{\alpha\beta} = A_{\alpha\alpha} \tag{5.116}$$

$$A^s_{\alpha\beta} = A^s_{\beta\alpha} \tag{5.117}$$

$$A^a_{\alpha\beta} = -A^a_{\beta\alpha} \;\Rightarrow \text{diagonal elements of } A^a_{\alpha\beta} = 0 \tag{5.118}$$

$$A_{\alpha\alpha} = A^s_{\alpha\alpha} \tag{5.119}$$

$$A^a_{\alpha\beta} B^s_{\alpha\beta} = 0 \tag{5.120}$$

$$A^a_{\alpha\beta} \mathring{B}^s_{\alpha\beta} = 0 \tag{5.121}$$

$$A^a_{\alpha\beta} B^a_{\alpha\beta} = \frac{1}{2}(A_{\alpha\beta} B_{\alpha\beta} - A_{\alpha\beta} B_{\beta\alpha}) \tag{5.122}$$

$$A^s_{\alpha\beta} B^s_{\alpha\beta} = \frac{1}{2}(A_{\alpha\beta} B_{\alpha\beta} + A_{\alpha\beta} B_{\beta\alpha}) \tag{5.123}$$

$$\mathring{A}^s_{\alpha\beta}\mathring{B}^s_{\alpha\beta} = \frac{1}{2}(A_{\alpha\beta}B_{\alpha\beta} + A_{\alpha\beta}B_{\beta\alpha}) - \frac{1}{3}A_{\alpha\alpha}B_{\beta\beta} \tag{5.124}$$

$$\epsilon_{\alpha\beta\gamma}A^s_{\alpha\beta} = \epsilon_{\alpha\beta\gamma}A^s_{\beta\gamma} = 0 \tag{5.125}$$

$$\epsilon_{\alpha\beta\gamma}A^a_{\alpha\beta} = \epsilon_{\alpha\beta\gamma}A^a_{\beta\gamma} = 2(A^a_{23}, -A^a_{31}, A^a_{12})^T \tag{5.126}$$

If $C_{\alpha\beta} = A_{\alpha\gamma}B_{\beta\gamma}$, then

$$C^s_{\alpha\beta} = \frac{1}{2}(A_{\alpha\gamma}B_{\beta\gamma} + A_{\beta\gamma}B_{\alpha\gamma}) \tag{5.127}$$

$$C^a_{\alpha\beta} = \frac{1}{2}(A_{\alpha\gamma}B_{\beta\gamma} - A_{\beta\gamma}B_{\alpha\gamma}). \tag{5.128}$$