Active viscoelastic nematics with partial degree of order

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Continuum models of active nematic gels have proved successful to describe a number of biological systems consisting of a population of rod-like motile subunits in a fluid environment. However, to get a thorough understanding of the collective processes underlying the behaviour of active biosystems, the theoretical underpinnings of these models still need to be critically examined. To this end, we derive a minimal model based on a nematic elastomer energy, where the key parameters have a simple physical interpretation and the irreversible nature of activity emerges clearly. The interplay between viscoelastic material response and active dynamics of the microscopic constituents is accounted for by material remodelling. Partial degree of order and defect dynamics is included as a result of the kinematic coupling between the nematic elastomer shape-tensor and the orientational ordering tensor \( Q \). In a simple one-dimensional channel geometry, we use linear stability analysis to show that even in the isotropic phase, the interaction between flow-induced local nematic order and activity results in a spontaneous flow of particles.

1. Introduction

Active nematic gels are fluids or suspensions of orientable rod-like objects endowed with active dynamics. They are a recent physical paradigm used to represent the collective dynamics of many biological systems such as filaments of the cytoskeleton [1,2], dense bacterial suspensions [3–5], and, on a more macroscopic scale, also flocking of birds or fishes [6]. These systems are intrinsically out of equilibrium, because the particles continuously consume energy that is used for their active movement or to exert mechanical forces. The interplay between many of these active particles can lead to
very complex patterns of collective motion and self-organized structures [7–12], with features not observed in passive systems, such as internally generated flow patterns, large-scale collective motion, active turbulence and sustained oscillations.

These systems have very different microscopic interactions among their constituents; however, they share a number of qualitative features in their collective dynamics. This implies that it is possible to provide a macroscopic description that overlooks the fine microscopic details, and it is based only on very general principles such as compatibility with thermodynamics and the symmetry properties induced by the material symmetry of the microscopic constituents. However, these general principles still leave a lot of freedom in formulating a model and the relative importance of the many phenomenological parameters introduced have to be determined from experiments, which are difficult to perform and interpret [11,13].

To this end, it is important to carefully formulate simple models to advance our understanding of how the physics of the active matter is relevant in biological contexts. Continuum models based on nematic liquid crystal dynamics, namely, the Ericksen–Leslie theory if the orientational order is described by the director \( \mathbf{n} \) or the Beris–Edwards theory if the ordering tensor \( \mathbf{Q} \) is employed, seem to have been particularly successful in describing the rich physics of active matter [7,14–22], at least from a qualitative point of view. These active models typically add two key ingredients to the classic hydrodynamic equations of liquid crystals: a non-equilibrium stress term owing to activity, and a Maxwell relaxation time to account for the viscoelastic behaviour of most biological fluids.

The active contribution to the Cauchy stress tensor accounts for the chemical energy consumed by the microscopic constituents to generate macroscopic motion and is generally chosen to be proportional to the nematic ordering tensor, \( \sigma_{\text{active}} = -\zeta \mathbf{Q} \), where the sign of \( \zeta \) depends on whether the active particles generate contractile or extensile stresses [23,24]. Active nematics are characterized by a strong deviation from thermal equilibrium due to the environmental energy supply, and it is possible to observe complex dynamics, defects formation and active-driven turbulence [17,18,25,26]. Therefore, to investigate dynamic instabilities, defect formation and defect motion, it is important to use de Gennes’ \( \mathbf{Q} \)-tensor as an order descriptor in the model. We will consider for simplicity a dense single-phase material, although multiphase models have also been developed to describe cell separation mechanisms [21,27,28].

However, despite the many theoretical and numerical studies, the introduction of the active term, \( \sigma_{\text{active}} \), to the stress tensor, although attractive for its simplicity, is not completely satisfactory from a physical standpoint, and there are some critical points that can be raised against it. A first remark is related to the compatibility of \( \sigma_{\text{active}} \) with irreversible thermodynamics [29]. It is possible to use classical irreversible thermodynamics to derive a thermodynamically consistent coupled chemo-mechanical theory of active nematics, see [14,30]. However, \( \sigma_{\text{active}} \) appears in these models as a reactive, i.e. a time-reversible term. From a physical perspective, this implies that the transfer of chemical energy into macroscopic motion is a reversible process, so that it could be possible, in principle, to use particle locomotion to generate chemical fuel. However, it is natural to assume that the motile subunits could only consume chemical energy, so that activity should be introduced as an irreversible process.

It is interesting to note that a term of the type \( \sigma_{\text{active}} \mathbf{Q} \), proportional to \( \mathbf{Q} \), is indeed thermodynamically correct at first order. More precisely, it is possible to put forth a thermodynamically consistent theory of active nematics based on nematic elastomer energy and microscopic relaxation dynamics [31], where the activity is represented as an external remodelling force, which clearly distinguishes it from the commonly used time-reversible representation. When this latter theory is approximated under the assumption of fast material remodelling times and low activity, the first-order contribution to the stress tensor turns out to be proportional to \( \mathbf{Q} \), exactly as in the classical theories inspired by liquid crystal physics.

A second critical point is that the active stress power, \( \sigma_{\text{active}} \cdot \nabla \mathbf{v} \), vanishes in the absence of macroscopic motion. In turn, this implies that there is no chemical fuel consumption when \( \mathbf{v} = 0 \). However, chemical fuel (e.g. ATP molecules) can also be used for mesoscopic motion such as material reorganization at the microscale, or for polymer stiffening, without any visible
macroscopic velocity [31–33]. The transduction of chemical energy into mechanical work is thus internal to the material and is more related to the evolution of the physical cross-links and their reorganization rather than to the generation of macroscopic flow.

Viscoelastic effects are important to capture the types of slow dynamics that one might expect, e.g. in the cytoskeleton, which contains long-chain flexible polymers and other cytoplasmic components that have long intrinsic relaxation times. This feature is common to many biological tissues, but the standard continuum models of active matter, derived from liquid crystal physics, fail to capture this slow viscoelastic dynamics as they assume short local relaxation times. This is a major shortcoming because viscoelastic effects are expected to couple strongly with the active liquid-crystalline dynamics and thereby potentially radically modify the effects of activity. The interplay between viscoelasticity and active motion has been explored in a number of recent articles [20,34,35]. While the models in [20,34,35] introduce viscoelasticity by adding new terms to the free energy that account for the viscoelastic polymer and couple the nematic tensor $\mathbf{Q}$ with the polymeric conformation tensor, we here propose a theory that kinematically links the nematic-elastomer shape tensor (or step-length tensor), $\mathbf{L}$, with the ordering tensor, $\mathbf{Q}$. In so doing, viscoelastic features come out naturally from an active nematic elastomer model endowed with material relaxation. This latter feature is introduced by using a multiplicative decomposition of the deformation gradient, a classical technique in plasticity theory [36–38]. Similar ideas have been recently applied to describe viscoelastic soft solids with reinforcing fibres [39].

Starting from a classical nematic elastomer free energy, and adding material relaxation, active remodelling tensor, and linking the shape tensor to the nematic ordering tensor, we are able to propose a rather simple theory that is constructed on the basis of rational thermodynamics and accounts for defects formation, dynamics and viscoelastic effects, all of which seem to be essential ingredients for a sound description of active biological matter at the continuum scale.

This article is organized as follows. The model is presented in §2. In §3, we assume fast relaxation times and develop a fluid-like approximation that allows us to make a comparison with the existing theories. A linear stability analysis is performed in §3a to show that a spontaneous flow may arise even in the absence of any Landau-de Gennes potential that favours alignment. The opposite limit of nearly elastic behaviour is briefly explored in §4, where we show that activity can induce actuation in nematic elastomers. The conclusions are drawn in §5. Some technical derivations are given in the appendices for ease of reading.

2. Theory

After De Gennes introduced the ordering tensor $\mathbf{Q}$ to describe partial order in nematics, many authors have proposed general continuum theories of nematics with tensorial order. Among these, we would like to mention the works of Pereira Borgmeyer & Hess [40], Qian & Sheng [41] and Beris & Edwards [42], within the framework of irreversible thermodynamics, Sonnet et al. [43], who employ a new variational principle, and Stark & Lubensky [44], who use a general Poisson-bracket formalism. A critical account of these theories can be found in Refs. [43,45].

Here, we follow an alternative, and simpler, route by considering a theory based on a nematic elastomer free energy, material remodelling, kinematic (instead of energetic) coupling of the elastomer shape tensor and the nematic ordering tensor, and active external remodelling forcing. We try to present the theory in its simplest form, i.e. whenever possible, we choose the least number of phenomenological parameters (in the same spirit as the one constant approximation for Frank’s elastic energy in liquid crystal theory). However, at some places, we will indicate where a simple extension of the theory is possible.

To enforce a deformation of an elastic solid, like an elastomer, we must apply a load. As soon as the external forces are released, the material returns to its natural, unstressed configuration. At a microscopic level, during such process, the positions of the strained molecules are distorted without significant variations of their relative arrangement. By contrast, when a deformation is applied to a fluid, a further degree of freedom comes into play: molecular reorganization. Indeed, by suitably modifying the relative positions between material points, the system proves to
reduce and even eventually cancel the existing stresses just by adapting the natural configuration. This material remodelling, consisting basically in a relabelling of which molecules are the first neighbours of which, turns out to be able to reduce the stresses without making resort to any collective molecular motion. In other words, the relaxation process drives the natural, unstressed configuration closer to the present configuration. Nevertheless, experimental evidence suggests that not all the strains may be recovered by simply reorganizing the natural configuration. In particular, fluids are not able to relax density variations, as each fluid possesses a reference density dictated by the microscopic fact that each molecule occupies in average a well-defined volume. As a consequence, a necessary feature of a physically meaningful model of an accommodating fluid is that the energy cost of any density variation should not be compensated by the microscopic relaxation.

A now standard way to introduce material remodelling in a continuum theory is to use the Kröner–Lee–Rodriguez multiplicative decomposition \([46–48]\) for the deformation gradient \(F = F_e G\). The effective deformation tensor, \(F_e\), will measure the elastic response, from an evolving natural configuration, \(B_{\text{nat}}\) (figure 1). An alternative similar approach, which introduces metric degrees of freedom, has been recently used to describe active chiral viscoelastic materials \([49]\). The relaxing deformation tensor, \(G\), determines how this configuration locally departs from the reference configuration. Since the elastic response is determined by \(F_e\), only the effective deformation appears explicitly in the strain energy. By contrast, energy dissipation (entropy production) is only associated with the evolution of \(G\). The same multiplicative decomposition is now a standard tool in continuum theories to describe plastic behaviour or growth phenomena. It has also been recently applied to explain the hints of viscoelasticity that remain at the hydrodynamic level when a sound wave propagates inside a nematic crystal \([50–53]\).

For later convenience, we also define the inverse relaxing strain \(H = (G^T G)^{-1}\), so that the effective left-Cauchy–Green deformation tensor can be written as follows:

\[
B_e = F_e F_e^T = F G^{-1} G^{-T} F^T = F H F^T. \quad (2.1)
\]

For the sake of simplicity, we assume the standard energy of nematic elastomers, where the uniaxial symmetry of the constituents is reflected in the uniaxial symmetry of both the shape tensor \(L\) and the ordering tensor \(Q\). The free energy density per unit mass is taken to be,

\[
\sigma(\rho, F_e, L, Q, \nabla Q) = \sigma_0(\rho) + \frac{1}{2} \mu \left( \tr(L^{-1} F_e - I) - \log \det(L^{-1} F_e) \right) + \sigma_{\text{el}}(Q, \nabla Q), \quad (2.2)
\]
which comprises both the elastomer elastic energy, written in terms of \( L \), and the nematic energy, written in terms of \( Q \). At this stage, \( L \) and \( Q \) are still independent, but they will be kinematically related in the following. The first term in equation (2.2), \( \sigma_0(\rho) \) is a volumetric term that depends only on the density \( \rho \) and does not relax. By contrast, the second term, namely, the neo-Hookean nematic elastomer energy density \( [54] \), with shear modulus \( \rho\mu \), depends here only on the effective deformation tensor \( B_\nu \), and this is a signature that it undergoes a remodelling dynamics (which will be described by an equation for \( B_\nu \)). The third and fourth terms, \( \sigma_{ldG}(Q) \) and \( \sigma_{el}(Q, \nabla Q) \), are the standard Landau–de Gennes thermodynamic potential and nematic elastic energy. We will use the classical expressions:

\[
\sigma_{ldG}(Q) = \frac{1}{2} A \text{tr}(Q^2) - \frac{1}{3} B \text{tr}(Q^3) + \frac{1}{4} C \text{tr}(Q^2)^2
\]

and

\[
\sigma_{el}(Q, \nabla Q) = \frac{1}{2} k ||\nabla Q||^2,
\]

where, however, more complicated formulas can be used if, for instance, it is important to use different elastic constants. In terms of the director, \( n \), and the degree of order, \( S \), the tensors \( L \) and \( Q \) are typically written as follows:

\[
L = a(S)^2(n \otimes n) + a(S)^{-1}(I - n \otimes n)
\]

and

\[
Q = \frac{2}{3} S(n \otimes n) - \frac{1}{3} S(I - n \otimes n),
\]

where \( a \) is the material parameter\(^1\) that gives the amount of spontaneous elongation along \( n \) in an uniaxially ordered phase. The shape tensor is spherical, prolate or oblate, respectively, for \( a = 1 \), \( a > 1 \) and \( a < 1 \). The tensor \( L \) is symmetric and satisfies \( \det L = 1 \). By contrast, \( Q \) is symmetric and traceless.

It must be noted that in our theory, we do not assume \( L \) and \( Q \) as independent observables, so that equation (2.5) is not assumed to be valid \( a \) priori. We rather express \( L \) as a function of \( Q \). One simple strategy to relate the shape tensor \( L \) with the ordering tensor \( Q \) is to write [54–57] \( Q = f(L) = L - (1/3)\text{tr}(L)I \), so that \( Q \) is automatically traceless by construction. Despite its simplicity, this equation is not completely satisfactory. Firstly, we would like to express \( L \) as a function of \( Q \), but the inversion of the previous formula is not straightforward. More precisely, \( L \) is not uniquely defined by the inversion of \( Q = f(L) \), for a given \( Q \). It is uniquely defined only once we impose the additional condition \( \det L = 1 \), but the unit determinant property is not a consequence of the functional relation between \( Q \) and \( L \), i.e. it does not follow automatically from the properties of \( Q \). Furthermore, since \( S \) ranges in \([-1/2, 1]\), the maximum achievable value of the shape parameter is \( a_{\text{max}} \approx 1.32 \). This means that we need to introduce an additional material parameter, since otherwise it would not be possible to represent even moderate anisotropic situations, in contrast to the estimated value \( a \approx 2 \) found in [50,53].

There is, however, a unique functional relationship linking \( L \) to \( Q \) that verifies \( \text{tr}(Q) = 0 \) if and only if \( \det(L) = 1 \), and this is the exponential matrix. Therefore, it is natural to posit

\[
L = e^{bQ},
\]

where \( b \) is a material parameter that measures how much the nematic order given by \( Q \) affects the shape tensor \( L \). In particular, we find that \( a(S) = e^{bS/3} \).

We base the derivation of the equations of motion on the free energy imbalance for mechanical theories [58,59]: the power expended by the external forces on a convecting spatial region \( \mathcal{P}_t \) must be greater than or equal to the temporal increase in kinetic and free energy of \( \mathcal{P}_t \). The difference

\(^1\)In nematic elastomer theory, the shape parameter \( a \) is usually denoted with \( \ell_1 \), and called effective step-length along the direction parallel to \( n \). However, we prefer to use \( a \) since our theory, in the limit of fast relaxation times, also applies to liquid crystals where the concept of step-length, which is closely related to polymer physics, is not clearly defined.
being the power dissipated in irreversible processes. Specifically, for any isothermal process, for any portion \( \mathcal{P}_i \) of the body at all times, we require

\[
\mathcal{D} := \mathcal{W}^{\text{ext}} - \dot{\mathcal{F}} \geq 0,
\]

where \( \mathcal{W}^{\text{ext}} \) is the power expended by the external forces, \( \dot{\mathcal{F}} \) is the rate of change of the kinetic energy, \( \dot{\mathcal{F}} \) is the rate of change of the free energy and the dissipation \( \mathcal{D} \) is a positive quantity that represents the energy loss due to irreversible processes (entropy production). Here, an overdot indicates the material time derivative. Furthermore, we assume that no positive dissipation is associated with a rigid rotation of the whole body. A final key assumption is that positive dissipation is only associated to the evolution of the natural or stress-free configuration of the body, i.e. entropy is produced only when microscopic reorganization occurs.

The equations of motions can now be derived following the thermodynamic procedure outlined in [31]. The details of this derivation when the tensor \( \mathbf{Q} \) is employed are reported in appendix A. We simply report the main equations here. The dissipation is derived in appendix A, see equations (A 10) and (A 11), and it is reported here below for ease of reading. Specifically, for any isothermal process, for any test field. More precisely, we gather:

\[\int_{\mathcal{A}} \left( \rho \frac{\partial \mathbf{e}}{\partial \mathbf{Q}} \right) \cdot \dot{\mathbf{Q}} \, d\alpha + \int_{\mathcal{S}} \left( \mathbf{v} \cdot \mathbf{Q} \right) \cdot \mathbf{Q} \cdot d\mathbf{a} \]

where \( \mathbf{B} \) is the external body force, \( \mathbf{T} \) is the Cauchy stress tensor (as defined in (A 8)), \( \mathbf{h} \) is the molecular field (as defined in (A 9)), \( \mathbf{T}_a \) is the activity tensor. The co-deformational time derivative is defined as \( \mathbf{B}_c^e := (\mathbf{B}_e) - (\nabla \mathbf{v}) \mathbf{B}_e - \mathbf{B}_e (\nabla \mathbf{v})^T \). Since \( \mathbf{B}_e(t, \mathbf{x}) \) is a spatial tensor field, the Cartesian components of \( \mathbf{B}_c^e \) are explicitly calculated as follows:

\[
[B_c^e]_{ij} = \frac{\partial[B_e]_{ij}}{\partial t} + \sum_{k=1}^3 \left( \frac{\partial[B_e]_{ij}}{\partial x_k} v_k - \frac{\partial v_i}{\partial x_k} [B_e]_{kj} - [B_e]_{ik} \frac{\partial v_j}{\partial x_k} \right).
\]

It is important to remark that this time derivative comes out naturally from our mathematical setting, and it is a correct representation of the modelling dynamics. Indeed, from equation (A 3), we gather \( \mathbf{B}_c^e = \mathbf{FHF}^T \); thus, \( \mathbf{B}_c^e \) vanishes if and only if no material remodelling occurs (\( \mathbf{H} = 0 \) implies elastic, time-reversible, deformations).

When the free energy (2.2) is used, we find (see appendix B for more details on the ordering tensor equation) the following explicit expressions for the pressure, the Cauchy stress tensor and the molecular field

\[
p(\rho) = \rho^2 \frac{\partial \sigma_0}{\partial \rho},
\]

\[
\mathbf{T} = -p(\rho) \mathbf{I} + \rho \mu (e^{-b \mathbf{Q}} \mathbf{B}_e - \mathbf{I}) - \rho k(\nabla \mathbf{Q}) \odot (\nabla \mathbf{Q})
\]

and

\[
\mathbf{h} = \rho \left( \frac{\partial \sigma_{\text{LdG}}}{\partial \mathbf{Q}} \right) - \text{div}(\rho k \nabla \mathbf{Q}) - \frac{1}{2} \rho \mu b \int_0^1 e^{a b \mathbf{Q}} (e^{-b \mathbf{Q}} \mathbf{B}_e) e^{-a b \mathbf{Q}} \, d\alpha.
\]

There are two types of governing equations. The first set of equations comprises balance laws that do not imply dissipation of energy. These, and the corresponding boundary conditions, are derived from the vanishing of the first four integrals in (2.9), for any test field. More precisely, we assume the local conservation of mass (2.14a) and derive the remaining balance equations from (2.9), so that the equations for the density \( \rho \), the velocity field \( \mathbf{v} \) and the ordering tensor \( \mathbf{Q} \) are as follows:

\[
\dot{\rho} + \rho \text{div} \mathbf{v} = 0, \tag{2.14a}
\]

\[
\rho \dot{\mathbf{v}} = \mathbf{b} + \text{div} \mathbf{T} \tag{2.14b}
\]

and

\[
\mathbf{h}^* = 0, \tag{2.14c}
\]

where \( \mathbf{h}^* = (\mathbf{h} + \mathbf{h}^T)/2 - (1/3) \text{tr}(\mathbf{h}) \mathbf{I} \) is the traceless symmetric part of \( \mathbf{h} \).
On the portion of the boundary where the traction is specified, we have \( T_v = t_{(w)} \), where \( v \) is the outer unit normal. When no magnetic couple stress acts on the boundary, we read from (2.9) the natural boundary condition for \( Q \):

\[
\left( \frac{\partial \sigma}{\partial \nabla Q} \right)^* = 0.
\]  

(2.15)

The second type of equations is associated with irreversible processes and follow from linear irreversible thermodynamics principles. These equations describe how the effective strain tensor \( B_e \) relaxes in time given the two competing effects: natural (viscous-like) relaxation towards the natural state dictated by \( L \) and the external remodelling force given by the activity tensor \( T_a \). The simplification of equation (A 12) leads to the following remodelling equation:

\[
\tau B_e^\dagger - B_e^{-1} = T_a - e^{-bQ},
\]

(2.16)

with \( \tau \) a characteristic relaxation time. Equation (2.16) guarantees that the dissipation (2.9) is always greater or equal to zero, so that the second principle of thermodynamics is satisfied.

When \( \tau \gg 1 \), i.e. for very long relaxation times, the material response is elastic, there is no dissipation of energy and, to leading order, (2.16) becomes \( B_e^\dagger = 0 \). This is the condition to impose if we want to reproduce an elastic, non-dissipative, response in our theory. By contrast, when \( \tau \ll 1 \), i.e. for very short relaxation times compared with the characteristic times of the macroscopic motion (measured by \( 1/||\nabla v|| \)), the tensor \( B_e \) quickly relaxes to a new stationary state. In such a case, we reproduce ideal and viscous flow behaviours. This approximation will be explored in more detail in §3. In intermediate regimes, we recover a viscoelastic material response.

Unlike classical theoretical models of plasticity, the evolution equation (2.16) is written in terms of the spatial (Eulerian) tensor field \( B_e \). In so doing, we regard \( B_e \) as a state variable that characterizes the stress state of the material (via equation (2.12)) and eliminate from the theory the arbitrariness due to the choices of reference and natural configuration [59–61].

### 3. Active fluid approximation

When the relaxation time \( \tau \) is very short compared with the characteristic times of deformation, measured by \( 1/||\nabla v|| \), the material effectively behaves as an ordinary fluid since the material reorganization is much faster than the deformation. Hence, our theory reduces to that of an active liquid crystal. For a simpler comparison with existing theories, we also assume low activity. Specifically, we assume that \( B_e \) is just a small correction of its equilibrium value in the passive case

\[
B_e = L + B_1, \quad \text{with} \quad ||B_1|| = O(\varepsilon), \quad ||T_a|| = O(\varepsilon),
\]

(3.1)

where \( \varepsilon = \tau ||\nabla v|| \), and we recall that \( L = e^Q \). The substitution of equation (3.1) into equation (2.16) yields, to first order,

\[
L^{-1}B_e = I + (T_a - \tau L^\dagger)L + O(\varepsilon^2).
\]

(3.2)

Equation (3.2) can be inserted in equation (2.12), so that the stress tensor for the active fluid reads

\[
T = -p(\rho)I + \rho \mu (T_a - \tau L^\dagger)L - \rho k(\nabla Q) \odot (\nabla Q),
\]

(3.3)

which actually shows an active term, \( \rho \mu T_a L \), that can be chosen to share the nematic symmetry with \( Q \), in agreement with the classical active liquid crystal theories. The passive term, \( -\rho \mu \tau L^\dagger L \), generates the nematic liquid crystal viscous stress and allows us to identify the Leslie viscosity coefficients in terms of the material parameters \( \rho \), \( \mu \), \( a \) and \( \tau \) [53], and their dependence on the degree of order \( S \). It is worth noticing that no previous knowledge of the viscous terms compatible with nematic symmetry is required to construct the stress tensor. The correct dependence on the director and its derivatives appear naturally in the expansion as a consequence of the calculations.

Likewise, no integrity bases of scalar invariants constructed from \( Q \) and its derivatives are needed to find the evolution equation for the ordering tensor \( Q \). This is particularly interesting since, in a traditional approach, there is in principle no limitation on the number of times \( Q \) can
Figure 2. Schematic representation of the channel geometry. Translational invariance along the x-axis ensures that all the unknown fields only depend on the transverse variable y, and that $v_y = 0$. We assume no-slip walls at $y = 0$, $y = L$, and planar boundary conditions for the nematic director. We set $S = S_{pr}$ at the boundary.

appear in the ordering tensor equation [45]. By contrast, in our case, the only terms appearing in this equation are those coming from the derivatives of the free energy density.

For all practical purposes, it is probably more convenient to use the integral formula (2.13) to calculate the molecular field. However, in order to see what combinations of $Q$ (and its derivatives) appear in the ordering tensor equation, and for a more transparent comparison with the existing theories, it is helpful to recast $L^V$ in terms of $Q$ and its derivatives. This is possible if we further assume that $b \ll 1$, i.e. there is a weak coupling between orientational order and natural strain. In such a case, we have $L = e^{bQ} \approx I + bQ$, which still yields $\det L = 1$ to first order in $b$. Hence, we recover the classical linear functional dependence of $L$ on $Q$ (see the discussion on pp. 59–61 of [54]).

The integral in the molecular field equation (2.13) can be calculated explicitly under this assumption, as reported in appendix C. The ordering tensor equation (2.14) now reads

$$\rho \left( \frac{\partial \sigma_\text{LdG}}{\partial Q} \right)^* - \text{div} (\rho k \nabla Q) - \frac{1}{2} \rho \mu b (T_a + 2\tau D + b \frac{1}{2} (Q T_a + T_a Q) + 2\beta (Q D + D Q) - \beta Q^\diamond) = 0,$$

so that we recover the same combination of terms ($D$, $Q D + D Q$, and $Q^\diamond$) that is traditionally obtained when the dissipation function is truncated at second degree in $Q$, $Q^\diamond$ [22,41,42] (see [43,45] for a fuller discussion). It is worth noticing that the activity remodelling tensor $T_a$ is explicitly included also in the ordering tensor equation (3.4).

(a) Active spontaneous flow in the isotropic phase

A distinguishing feature of active nematics is that they have a natural tendency to flow when the activity parameter overcomes a typical critical value [7,8,26,53,62,63]. It is then natural to test our model against such a prediction and, in particular, to investigate the interplay between activity and preferred order. To this end, we study the spontaneous flow of an active nematic fluid in a simple channel geometry. We consider here only high-dense suspensions, where density variations are negligible, and the material is nearly incompressible. Therefore, we neglect the important effect of particle concentration at the boundaries that is observed for low-dense active suspensions [64]. For simplicity, we consider a system with translational invariance along x, and we assume that the unknown fields, $v_x$, $Q_{xx}$ and $Q_{xy}$, depend only on the transverse variable $y$ (figure 2). We recall that in our two-dimensional example $Q$ and $h^*$ are $2 \times 2$ symmetric and traceless matrices, so that $Q_{yx} = Q_{xy}$, $Q_{yy} = -Q_{xx}$, $h^*_{yx} = h^*_{xy}$ and $h^*_{yy} = -h^*_{xx}$. The degree of order, $S$, and the director, $n$, are then derived from the eigenvalues and eigenvectors of $Q$.

The nematic degree of order in the active system is governed by a Landau–de Gennes potential, whose minimum is denoted with $S_{pr}$, the preferred value of the degree of order $S$. In our thin
channel geometry, we posit

$$\sigma_{l, anticipating}(Q) = \frac{1}{2} \text{tr}(Q^2) + \frac{1}{2} \text{tr}(Q^2) = \frac{k}{\xi^2} S^2(S^2 - 2S_{pr}),$$

(3.5)

where we have parametrized $\sigma_{l, anticipating}(Q)$ using the nematic coherence length $\xi = \sqrt{4k/C}$, and the preferred degree of order is $S_{pr} = \sqrt{-2A/C}$. The nematic coherence length compares the strength of the elastic and thermodynamic contributions with the free energy. It characterizes the size of the domains, where the degree of orientation may be different from the preferred value $S_{pr}$. We have omitted the cubic term in equation (3.5) since we are using the two-dimensional ordering tensor $Q$, which has only one quadratic invariant. In the nematic phase, the Landau–de Gennes potential has two symmetric minima in $S = +S_{pr}$ and $S = -S_{pr}$, and a maximum in $S = 0$. The isotropic phase corresponds to $S = 0$. To see the effect of preferred order on the flow, we perform the linear analysis using a generic value for $S_{pr}$. The isotropic case will be discussed by setting $S_{pr} = 0$ in the final formulas.

The equations of motions are given as in (2.14b) and (2.14c), where the Cauchy stress tensor and the molecular field are given as in the active fluid approximation described in §3. It is worth mentioning that (2.14a) is automatically satisfied due to incompressibility. Furthermore, due to stationarity and translational invariance along the channel, equations (2.14b) and (2.14c) simply read $\partial T_{xy}/\partial y = 0$, $\partial T_{yy}/\partial y = 0$ and $h^*_x = 0$, $h^*_y = 0$. We also assume no-slip boundary conditions for the velocity field $v_x(y)$, tangential conditions for the director and $S(0) = S_{pr}$, $S(L) = S_{pr}$ at the channel walls.

The momentum balance equation (2.14b), in the stationary case and with $T$ as given in (3.3), yields

$$4b\tau Q_{xx}'' v_x' + b\xi Q_{xy}' + 2\tau(2bQ_{xx} - 1)v_x'' = 0$$

(3.6a)

and

$$\rho Q_{xy}'(b\mu \tau v_x' - 4kQ_{xy}'') + \frac{1}{2}\rho Q_{xx}'(b\xi \mu - 8kQ_{xx}'') + b\mu \rho Q_{xy} v_x'' - p' = 0.$$  

(3.6b)

In agreement with the active fluid approximation of §3, we have used $L \approx I + bQ$ and retained only terms up to first order in $b$. Translational invariance implies that the unknown fields, namely, $v_x, Q_{xx}$ and $Q_{xy}$, are functions only of the transverse variable $y$. We have chosen the simplest form for the activity tensor, i.e. $T_a = -(1/2)\xi I$. Equation (3.6b) can be used to find the pressure function $p(y)$, but it will not be used in the rest of the article.

Two more scalar equations are obtained from the order tensor equation equation (2.14c) (or, more directly, equation (3.4)), which, to order $O(b)$, reads

$$kQ_{xx}'' + \frac{2kQ_{xx}(S_{pr}^2 - 4Q_{xy}^2)}{\xi^2} - \frac{8kQ_{xx}^3}{\xi^2} = 0$$

(3.7a)

and

$$kQ_{xy}'' + \frac{2kQ_{xy}(S_{pr}^2 - 4Q_{xx}^2)}{\xi^2} - \frac{8kQ_{xy}^3}{\xi^2} + \frac{1}{2} b\mu \tau v_x' = 0.$$  

(3.7b)

Equations (3.6a), (3.7a) and (3.7b) are three nonlinear equations in the unknowns $v_x, Q_{xx}$ and $Q_{xy}$, respectively, that are in general difficult to solve. However, it is straightforward to check that $Q_{xx} = S_{pr}/2, Q_{xy} = 0$ and $v_x = 0$ is always a trivial solution, for any value of the parameters. Furthermore, above a critical threshold for the activity parameter $\xi$, a bifurcation occurs, and the trivial solution is no longer unique.

The critical condition is found by performing a linear stability analysis about the trivial solution. To find the linear equations, we perturb the trivial solution and set $Q_{xx} = S_{pr}/2 + \delta Q_{xx},$
Q\textsubscript{xy} = \delta Q\textsubscript{xy} and v\textsubscript{x} = \delta v\textsubscript{x}. To first order, equations (3.6a), (3.7a) and (3.7b) yield
\begin{equation}
\delta Q\textsubscript{xy}' = b\zeta \delta Q\textsubscript{xy} + 2\tau (bS\textsubscript{pr} - 1) \delta v\textsubscript{y}'' = 0,
\end{equation}
\begin{equation}
\delta Q\textsubscript{xx}'' - \frac{4S\textsubscript{pr}^2 \delta Q\textsubscript{xx}}{b^2} = 0
\end{equation}
and
\begin{equation}
k \delta Q\textsubscript{xy}'' + \frac{1}{2} b\mu \tau \delta v\textsubscript{x}' = 0.
\end{equation}
Equation (3.8b) is decoupled from the other two equations and can be solved immediately: the only solution that satisfies both boundary conditions is \(\delta Q\textsubscript{xx} = 0\). By contrast, it is easy to show that equations (3.8a) and (3.8c) admit real non-trivial solutions whenever \(\zeta / (1 - bS\textsubscript{pr}) > 0\), and the following critical condition is satisfied
\begin{equation}
\sqrt{\frac{\zeta \mu}{4k} \frac{bL}{\sqrt{1 - bS\textsubscript{pr}}}} = 2\pi n,
\end{equation}
where \(n\) is a non-vanishing integer. The condition \(\zeta / (1 - bS\textsubscript{pr}) > 0\) implies that we can investigate spontaneous flow even in the absence of a Landau–de Gennes potential, i.e. when \(S\textsubscript{pr} = 0\), provided that \(\zeta > 0\).

Furthermore, for every \(n\), we find that the null space of the linear operator is two-dimensional, so that there are two possible modes of bifurcations in agreement with the linear stability analysis given in [53] and the numerical studies of [16,65].

\begin{equation}
\delta Q\textsubscript{xy} = 2\pi n\alpha \sin \left(\frac{2\pi ny}{L}\right) - \frac{16\pi^2 n^2 (1 - bS\textsubscript{pr})}{b\zeta} \beta \sin^2 \left(\frac{\pi ny}{L}\right)
\end{equation}
and
\begin{equation}
\delta v\textsubscript{x} = \frac{L}{\tau} \left[ \frac{b\zeta}{1 - bS\textsubscript{pr}} \alpha \sin^2 \left(\frac{\pi ny}{L}\right) + 2n\pi \beta \sin \left(\frac{2\pi ny}{L}\right) \right],
\end{equation}
where \(\alpha\) and \(\beta\) are the two arbitrary mode amplitudes that cannot be determined from this simple linear analysis. By using equations (3.10) and (3.11), it is possible to derive the qualitative behaviour of \(S\), \(v\), and the angle \(\theta\) as a function of \(y\) (for an approximate quantitative analysis, we need to know the amplitudes \(\alpha\) and \(\beta\)).

By contrast, other works [7,8,21,35,62] only predict a single bifurcation mode, i.e. a sinusoidal modulation with a node at the centre of the channel. The tumbling parameter does not play a significant role in our theory, while a key parameter is the coupling constant \(b\). This is again a difference with respect to the models inspired by the Beris–Edwards theory of liquid crystals (see, for instance [13,18,21,35]).

For extensile materials, with \(\zeta > 0\), it is possible to find a critical activity also when the preferred nematogens alignment is isotropic (\(S\textsubscript{pr} = 0\)). To analyse this case, we plot in figure 3 the critical activity, \(\zeta_c\) as given in (3.9) with \(n = 1\), as a function of the preferred degree of orientation, \(S\textsubscript{pr}\), for different values of the coupling parameter \(b\). As expected, \(\zeta_c\) increases with decreasing \(b\) and diverges when \(b \to 0\). In physical terms, this means that if there is no coupling between orientational order and natural strain, then no spontaneous flow arises. However, it is interesting to observe that even in the absence of any preferred orientation, when \(S\textsubscript{pr} = 0\), and the material is naturally isotropic, the critical activity is still finite, so that it is possible to observe an activity-induced spontaneous flow even when \(\sigma\textsubscript{LdG} = 0\). This is in agreement with some recent results [21,66,67], which study the instability in the Beris–Edwards theory of active nematic liquid crystals or flocking dynamics with Toner–Tu theory.

4. Activity-induced actuation

Our model can in principle describe a range of viscoelastic behaviours that are present in a number of polymeric and biological materials including entangled protein filaments and biological and artificial muscles. To encompass this diversity, the relaxation time, \(\tau\), may vary
Figure 3. Critical activity, $\zeta_c$, as a function of the preferred degree of order, $S_{pr}$, as given in equation (3.9) with $n = 1$, for different values of the coupling parameter $b$. There is a finite $\zeta_c$ even when $S_{pr} = 0$, so that the preferred phase is isotropic.

from $\tau \ll 1$ where the polymeric dynamics are rapid and only contribute to the viscosity of the fluid, to $\tau \to +\infty$, where the polymer effectively acts as an elastomeric solid.

In §3, we discussed the first approximation. Here, we briefly explore one simple consequence of the active elastic approximation, namely, the spontaneous stretch induced by an active term. In general, it is more difficult to study the elastic limit. In fact, $B_e^{\nabla_e}$ becomes vanishingly small, while $\tau \to +\infty$, so that $\tau ||B_e^{\nabla_e}|| = O(1)$. This means that all the terms in (2.16) are of the same order, and no dominant balance argument can be applied to simplify the equation. A possible simplification is to use a small displacement approximation and write

$$B_e = L + B_1.$$  (4.1)

This is similar to the assumption (3.1) in §3; however, this is now not due to a fast remodelling that makes $B_e$ always close to the natural configuration $L$, but rather to a small displacement approximation, which may be due to a small active contribution. This may not be valid at large times since soft matter materials usually undergo large deformations and $B_e$ can in principle be large in the elastic regime (despite $B_e^{\nabla_e}$ being small).

We consider a homogeneous infinite material (i.e. we are not concerned with boundary conditions) at rest and explore the effect of activity on its equilibrium configuration. Within the small displacement approximation, the zeroth-order remodelling equation (2.16) simply yields $L^\nabla = 0$, which is automatically satisfied for homogeneous equilibrium states (i.e. with constant $Q$ and $v = 0$). To find the contribution of activity, we must proceed to the next order of approximation, which gives

$$\tau B_1^{\nabla_e} + L^{-1}B_1L^{-1} = T_a.$$  (4.2)

Therefore, in the elastic case, an active equilibrium configuration with $v = 0$ is possible only if $B_1 = LT_aL$. We need to check whether this solution is compatible with the balance of linear momentum, $\text{div}T = 0$ and the director equation. To first order, the Cauchy stress tensor (2.12) becomes

$$T = -p(\rho)I + \rho \mu L^{-1}B_1 = -p(\rho)I + \rho \mu T_aL,$$  (4.3)

where, as usual in nematic elastomers, we have neglected the contribution of the Ericksen stress tensor (which, anyway, vanishes in a homogeneous state). We also take $S = \text{constant}$ and write
\( n = (\cos \theta(y), \sin \theta(y), 0) \). For concreteness, we choose the active tensor along a specific axis: \( T_a = -\frac{1}{2} \zeta e_x \otimes e_x \). After some algebra, the equilibrium equation \( \text{div} T = 0 \) and the director equation require

\[
\frac{a^3}{2a} - \frac{1}{2a} \zeta \mu \rho' \cos(2\theta(y)) = 0, \quad p'(y) = 0, \quad \sin(2\theta(y)) = 0. \tag{4.4}
\]

Hence, a homogenous stationary solution is possible with either \( \theta = 0 \) or \( \theta = \pi/2 \), i.e. \( n = e_x \) or \( n \perp e_x \). In the first case, we have the natural deformation

\[
B_e(n = e_x) = a^2(1 - a^2 \zeta / 2) e_x \otimes e_x + \frac{1}{a}(I - e_x \otimes e_x), \tag{4.5}
\]

while in the second,

\[
B_e(n = e_y) = \left( \frac{1}{a} - \frac{\zeta}{2a^2} \right) e_x \otimes e_x + a^2(e_y \otimes e_y) + \frac{1}{a}(e_z \otimes e_z). \tag{4.6}
\]

In the presence of activity, both the director and the elastic matrix evolve in agreement with the activity tensor. There are homogeneous equilibrium solutions, which have residual stress and are stretched or contracted, with respect to the natural state \( B_e = L \), according to the action of the activity tensor.

## 5. Conclusion

Many continuum theories seem to effectively describe out of equilibrium dynamics of active nematics in terms of a large number of phenomenological parameters. Furthermore, such parameters are difficult to determine from microscopic information or experimental data, in particular in active systems where energy is injected at the microscopic units. Most active nematic responses depend on the competition between active stresses that promote director or velocity gradients and viscoelastic stresses that resist them. As a consequence of this interplay, experimental measurements often access only non-trivial combinations of hydrodynamic parameters, and it is very difficult to assess the importance of each single parameter. Even direct measurements that rely on controlled flow experiments are difficult to devise if the underlying flows are chaotic. As a result, there is still no consensus on which macroscopic description is the most physically sound.

In this article, we have presented a minimal continuum theory with few, but not fewer, key parameters having a clear physical interpretation. The model we propose is based on a kinematic coupling between nematic elastomer shape-tensor and de Gennes ordering tensor, and material remodelling dynamics. Hence, it is able to account for viscoelastic effects, partial degree of nematic order and defect dynamics. To explore the first implications of the theory, we studied the dynamical properties of thin films of active nematic fluids confined in a channel geometry. Above a critical activity, a rich variety of complex behaviours is observed. In particular, it is possible to observe a spontaneous flow of particles even in the absence of any thermodynamic potential that could favour the alignment of the rod-like units. Therefore, activity itself can give rise to local flows, which in turn gives rise to the nematic order, and this enhances the effect of activity and the flows itself. This effect is important to explain the origin of nematic order in active systems and hence the physics of biological matter. In fact, most theoretical models assume the presence of nematic order by prescribing a Landau–de Gennes potential, but it is not clear what could be the microscopic origin of this potential, especially since many active systems do not maintain nematic order when the activity magnitude tends to zero.

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**Authors’ contributions.** S.S.T.: conceptualization, formal analysis, investigation, methodology, supervision, writing—original draft and writing—review and editing.

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Appendix A. Derivation of the governing equations

Let us first state two lemmas that will be used to simplify the calculations and which we state without proof.

**Lemma A.1.** Let \( f \) be a function depending only on \( F_e \) (or \( B_e \)). Then,

1. \( (\partial f/\partial F)F^T = (\partial f/\partial F_e)F_e^T + 2(\partial f/\partial B_e)B_e \)
2. \( F^{-T}(\partial f/\partial H)F^{-1} = \partial f/\partial B_e \)

**Lemma A.2.** Let \( f = f(\rho) \) be a function of \( \rho \) only. Then, \( (\partial f/\partial F)F^T = -\rho(\partial f(\rho)/\partial \rho)I \).

Let us define the expended power by the external forces, the kinetic energy and the free energy as follows:

\[
W^{(\text{ext})} := \int_{P_1} b \cdot v \, dv + \int_{\partial P_1} t_{(v)} \cdot v \, dt + \int_{P_e} E \cdot \dot{Q} \, dv + \int_{P_e} E_{(v)} \cdot \dot{Q} \, dt + \int_{P_1} T_a \cdot B_e^\nabla \, dv,
\]

\[
K + F := \int_{P_1} \left( \frac{1}{2} \rho \dot{v}^2 + \rho \sigma(\rho, B_e, Q, \nabla Q) \right) \, dv,
\]

where \( v \) is the velocity field, \( P_1 \) is a spatial region that convects with the body and

\[
B_e^{\nabla} := (B_e)^\cdot - (\nabla v) B_e - B_e (\nabla v)^T = F H F^T
\]

is the co-deformational derivative [58,68], a frame-indifferent time derivative of \( B_e \) relative to a convected coordinate system that moves and deforms with the flowing body. The unit vector \( v \) is the external unit normal to the boundary \( \partial P_1 \), \( b \) is the external body force and \( t_{(v)} \) is the external traction on the bounding surface \( \partial P_1 \). The tensor fields \( E \) and \( E_{(v)} \) are the generalized body and contact force densities conjugate to the microstructure: they have to be included, e.g. in the presence of an external magnetic field, but for simplicity, they will be set to zero in the following derivations. The last term in equation (A1) represents the power expended by the remodelling generalized force \( T_a \) [31]. It must be noted that \( T_a \) is the only term conjugate to the remodelling velocity field \( B_e^{\nabla} \). By contrast, the classical active stress \( \sigma_{\text{active}} = -\varepsilon Q \) is paired with the macroscopic velocity gradient \( \nabla v \). It is clear from the identity \( B_e^{\nabla} = F H F^T \) that \( B_e^{\nabla} \) has the right properties to represent the kinematics of reorganization: (1) it is frame-invariant, (2) it vanishes whenever the deformation is purely elastic, i.e. \( B_e^{\nabla} = 0 \) if and only if \( H = 0 \). The same derivative also appears in the three-dimensional models for Maxwell viscoelastic fluids [68].

To calculate the dissipation, we first calculate the material time derivative of \( K + F \):

\[
\dot{K} + \dot{F} = \int_{P_1} \left( \rho \dot{v} \cdot v + \rho \frac{\partial \sigma}{\partial F} \cdot \dot{F} + \rho \frac{\partial \sigma}{\partial H} \cdot \dot{H} + \rho \frac{\partial \sigma}{\partial Q} \cdot \dot{Q} + \rho \frac{\partial \sigma}{\partial \nabla Q} \cdot (\nabla Q) \right) \, dv = \int_{P_1} \left( \rho \dot{v} \cdot v + \rho \frac{\partial \sigma}{\partial F} F^T \cdot \nabla v + \rho \frac{\partial \sigma}{\partial B_e} B_e^\nabla + \rho \frac{\partial \sigma}{\partial Q} Q + \rho \frac{\partial \sigma}{\partial \nabla Q} \cdot (\nabla Q) \right) \, dv,
\]

where, to simplify the calculations, we have implicitly used the local conservation of mass \( \dot{\rho} + \rho \text{div} v = 0 \). The last term in the integral is simplified by using the following identities (with \( F_k =

\[2\] Also known as upper-convected time derivative, upper-convected rate or contravariant rate.
\[ (\nabla \mathbf{Q})_{\alpha \beta \gamma} = \frac{\partial}{\partial t} \left( \frac{\partial \mathbf{Q}_{\alpha \beta}}{\partial x_{\gamma}} \right) \]

\[ = (\nabla \dot{\mathbf{Q}})_{\alpha \beta \gamma} + \frac{\partial \mathbf{Q}_{\alpha \beta}}{\partial x_{\gamma}} (-F^{-1} \nabla \mathbf{v})_{\delta \gamma} = \left[ \nabla \mathbf{Q} - (\nabla \mathbf{Q})(\nabla \mathbf{v}) \right]_{\alpha \beta \gamma} \]

(A5)

and

\[ \rho \frac{\partial \sigma}{\partial \nabla \mathbf{Q}} \cdot (\nabla \mathbf{Q}) = \rho \frac{\partial \sigma}{\partial \nabla \mathbf{Q}} \cdot (\nabla \dot{\mathbf{Q}}) - \rho \frac{\partial \sigma}{\partial \nabla \mathbf{Q}} \cdot (\nabla \mathbf{Q})(\nabla \mathbf{v}) \]

\[ = \rho \frac{\partial \sigma}{\partial \mathbf{Q}_{\alpha \beta \gamma}} \dot{\mathbf{Q}}_{\alpha \beta \gamma} - \rho \frac{\partial \sigma}{\partial \mathbf{Q}_{\alpha \beta \gamma}} Q_{\alpha \beta \gamma \delta \gamma} v_{\delta \gamma} \]

\[ = \left( \rho \frac{\partial \sigma}{\partial \mathbf{Q}_{\alpha \beta \gamma}} \dot{\mathbf{Q}}_{\alpha \beta \gamma} \right) - \left( \rho \frac{\partial \sigma}{\partial \mathbf{Q}_{\alpha \beta \gamma}} \dot{\mathbf{Q}}_{\alpha \beta \gamma} - \rho Q_{\alpha \beta \gamma \delta \gamma} \frac{\partial \sigma}{\partial \mathbf{Q}_{\alpha \beta \gamma}} v_{\delta \gamma} \right) \]

\[ = \text{div} \left( \rho \dot{\mathbf{Q}} \odot \frac{\partial \sigma}{\partial \nabla \mathbf{Q}} \right) - \text{div} \left( \rho \frac{\partial \sigma}{\partial \nabla \mathbf{Q}} \right) \cdot \dot{\mathbf{Q}} - \left( \rho (\nabla \mathbf{Q}) \odot \frac{\partial \sigma}{\partial \nabla \mathbf{Q}} \right) \cdot \nabla \mathbf{v}, \] (A6)

where, following [43], the circled dot means the contraction of the first two indexes, so, for instance \((\nabla \mathbf{Q} \odot \nabla \mathbf{Q})_{jk} = Q_{hi,j}Q_{hi,k}\). Hence, we obtain

\[ \dot{K} + \dot{\mathcal{F}} = \int_{\mathcal{P}_1} \left( \rho \dot{\mathbf{v}} \cdot \mathbf{v} + \mathbf{T} \cdot \nabla \mathbf{v} + \rho \frac{\partial \sigma}{\partial \mathbf{B}_e} \cdot \mathbf{B}_e + \mathbf{h} \cdot \dot{\mathbf{Q}} \right) \, dV + \int_{\partial \mathcal{P}_1} \left( \rho \frac{\partial \sigma}{\partial \nabla \mathbf{Q}} \right) \cdot \dot{\mathbf{Q}} \, dA, \] (A7)

where we have defined the Cauchy stress tensor and the molecular field as follows:

\[ \mathbf{T} = \rho \frac{\partial \sigma}{\partial \mathbf{F}} \mathbf{F}^T - \rho (\nabla \mathbf{Q}) \odot \frac{\partial \sigma}{\partial \nabla \mathbf{Q}} = -\rho^2 \frac{\partial \sigma}{\partial \rho} \mathbf{I} + \rho \frac{\partial \sigma}{\partial \mathbf{F}_e} \mathbf{F}_e^T - \rho (\nabla \mathbf{Q}) \odot \frac{\partial \sigma}{\partial \nabla \mathbf{Q}} \] (A8)

and

\[ \mathbf{h} = \rho \frac{\partial \sigma}{\partial \nabla \mathbf{Q}} - \text{div} \left( \rho \frac{\partial \sigma}{\partial \nabla \mathbf{Q}} \right). \] (A9)

A further simplification using divergence theorem yields the final expression for the dissipation

\[ \mathcal{D} = \mathcal{W}^{(\text{ext})} - \dot{K} - \dot{\mathcal{F}} = \int_{\mathcal{P}_1} (\mathbf{b} - \rho \dot{\mathbf{v}} + \text{div} \, \mathbf{T}) \cdot \mathbf{v} \, dV \]

\[ + \int_{\partial \mathcal{P}_1} (t_{\mathbf{v}} - \mathbf{T} \cdot \mathbf{v}) \cdot \mathbf{v} \, dA - \int_{\mathcal{P}_1} \mathbf{h} \cdot \dot{\mathbf{Q}} \, dV \]

\[ - \int_{\partial \mathcal{P}_1} \left( \rho \frac{\partial \sigma}{\partial \nabla \mathbf{Q}} \right) \cdot \dot{\mathbf{Q}} \, dA + \int_{\mathcal{P}_1} \left( \mathbf{T}_a - \rho \frac{\partial \sigma}{\partial \mathbf{B}_e} \right) \cdot \mathbf{B}_e^\gamma \, dV, \] (A10)

where we have used \( \mathbf{E} = 0 \) and \( \mathbf{E}_{\text{ext}} = 0 \). The key assumption of our derivation is that only the last integral in (A10) can be responsible of a positive dissipation. In physical terms, positive dissipation is uniquely associated with material remodelling. Hence, balance equations (2.14) (and corresponding boundary terms) are obtained by setting to zero the terms conjugate to the arbitrary kinematic fields \( \mathbf{v} \) and \( \dot{\mathbf{Q}} \). Furthermore, since \( \dot{\mathbf{Q}} \) is symmetric and traceless, \( \mathbf{h} \cdot \dot{\mathbf{Q}} = h^* \cdot \dot{\mathbf{Q}} \), where \( h^* = (\mathbf{h} + \mathbf{h}^T)/2 - (1/3) \text{tr}(\mathbf{h}) \mathbf{I} \) is the symmetric traceless part of \( \mathbf{h} \), so that it is sufficient to posit \( h^* = 0 \) to derive the balance equation.

After inserting equations (2.14) in (A10), the dissipation simplifies to

\[ \mathcal{D} = \int_{\mathcal{P}_1} \left( \mathbf{T}_a - \rho \frac{\partial \sigma}{\partial \mathbf{B}_e} \right) \cdot \mathbf{B}_e^\gamma \, dV, \] (A11)

and its positivity is guaranteed if we take the evolution equation (2.16). More generally, it is sufficient to take

\[ \mathcal{D}(\mathbf{B}_e^\gamma) = \mathbf{T}_a - \rho \frac{\partial \sigma}{\partial \mathbf{B}_e}, \] (A12)
where $\mathbb{D}$ is a positive-definite fourth-rank tensor with the major symmetries, i.e. such that $A \cdot \mathbb{D} A > 0$ for any symmetric $A \neq 0$. See [53] for a more detailed discussion about the structure of the tensor $\mathbb{D}$ and the possible relaxation times. The evolution equation given in the text is the simplest possible choice with only one relaxation time, after the substitution of

$$
\rho \frac{\partial \sigma}{\partial B_e} = \frac{1}{2} \mu (L^{-1} - B_e^{-1}) = \frac{1}{2} \mu (e^{-bQ} - B_e^{-1}).
$$

(A 13)

**Appendix B. Ordering tensor equation**

To find $h^\star$, we use equations (2.3) and (2.4) to calculate the following Fréchet derivatives:

$$
\frac{\partial \sigma_{\text{LdG}}(Q)}{\partial Q} = AQ - BQ^2 + C \text{tr}(Q^2)Q,
$$

$$
\left( \frac{\partial \sigma_{\text{LdG}}(Q)}{\partial Q} \right)^\star = AQ - B\left(Q^2 - \frac{1}{3} \text{tr}(Q^2)I\right) + C \text{tr}(Q^2)Q,
$$

$$
\frac{\partial \sigma_{\text{el}}(Q, \nabla Q)}{\partial \nabla Q} = k(\rho)\nabla Q.
$$

More involved is the calculation of the derivative of the neo-Hookean term $g(Q) = \frac{1}{2} \mu (e^{-bQ} \cdot B_e)$. We will use Feynman's formula for the derivative of the matrix exponential (eqn (6), [69,70])

$$
(D \exp(A))[B] = \frac{\partial}{\partial \varepsilon} \exp(A + \varepsilon B) \bigg|_{\varepsilon=0} = \int_0^1 e^{(1-\alpha)bQ} B e^{a\varepsilon} d\alpha,
$$

(B 1)

where $A$ and $B$ are two arbitrary second-rank tensors. In our case, we have, for any $X$,

$$
\frac{\partial (L^{-1} \cdot B_e)}{\partial Q} \cdot X = \frac{\partial}{\partial \varepsilon} \bigg|_{\varepsilon=0}^{1} e^{-b(Q+\varepsilon X) \cdot B_e} = -b \int_0^1 e^{-(1-\alpha)bQ} X e^{-\alpha bQ} \cdot B_e d\alpha
$$

$$
= -bX \cdot \int_0^1 e^{-(1-\alpha)bQ} B e e^{-\alpha bQ} d\alpha
$$

$$
= -bX \cdot \int_0^1 e^{a\varepsilon bQ (L^{-1} B_e) e^{-\alpha bQ}} d\alpha,
$$

(B 2)

where we have used $L^{-1} = e^{-bQ}$ and the fact that $L^{-1}$ commutes with $e^{a\varepsilon bQ}$. Therefore, the derivative of the neo-Hookean term with respect to $Q$ is

$$
\frac{\partial}{\partial Q} \text{tr}(L^{-1} B_e) = -b \int_0^1 e^{a\varepsilon bQ (L^{-1} B_e) e^{-\alpha bQ}} d\alpha,
$$

(B 3)

so that the evolution of the tensor $Q$ is governed by

$$
h^\star = \rho \left( AQ - B\left(Q^2 - \frac{1}{3} \text{tr}(Q^2)I\right) + C \text{tr}(Q^2)Q \right)
$$

$$
- \frac{1}{2} \rho \mu b \int_0^1 e^{a\varepsilon bQ (L^{-1} B_e) e^{-\alpha bQ}} \bigg| d\alpha - \text{div} (\rho k \nabla Q) = 0.
$$

(B 4)

A useful special case of equation (B 1) that it is worth reporting is

$$
(e^{bQ(x,t)})^\cdot = b \int_0^1 e^{(1-\alpha)bQ} Q e^{a\varepsilon bQ} d\alpha.
$$

(B 5)
We can try to simplify equation (B 3) by using equation (2.6) and the Cayley–Hamilton theorem to write

\[ e^{a b Q} = a_1(S, \alpha)Q + a_2(S, \alpha)Q^2, \quad (B 6) \]

\[ a_1(S, \alpha) = \frac{(1/2)e^{abS/3} - 2e^{-abS/3}}{S} \quad (B 7) \]

and

\[ a_2(S, \alpha) = 3((1/2)e^{abS/3} + e^{-abS/3})/S^2. \quad (B 8) \]

When inserted in equation (B 3), the integral is then reduced to the calculations of the integrals of the products \( a_1(S, \alpha)a_1(S, -\alpha) \), \( a_1(S, \alpha)a_2(S, -\alpha) \), \( a_2(S, \alpha)a_1(S, -\alpha) \) and \( a_2(S, \alpha)a_2(S, -\alpha) \). The result is most conveniently written in terms of the tensor \( N = n \otimes n - \frac{1}{3}I \). After some algebra, not reported for brevity, we find

\[
\left( \frac{\partial}{\partial Q} \operatorname{tr}(L^{-1}B_\alpha) \right)^* = c_1 NB_\alpha N + c_2(NB_\alpha N^2 + N^2B_\alpha N) + c_3 N^2B_\alpha N^2 + \frac{b}{3} \operatorname{tr}(L^{-1}B_\alpha)I, \quad (B 9a) \]

\[ c_1 = -4be^{bS/3} - \frac{1}{4}be^{-2bS/3} + 2(e^{bS/3} - e^{-2bS/3})/S, \quad (B 9b) \]

\[ c_2 = 6be^{bS/3} - \frac{3}{4}be^{-2bS/3} + 3(e^{bS/3} - e^{-2bS/3})/(2S), \quad (B 9c) \]

and

\[ c_3 = -9be^{bS/3} - \frac{9}{4}be^{-2bS/3} - 9(e^{bS/3} - e^{-2bS/3})/S. \quad (B 9d) \]

Equation (B 4) then reads

\[
AQ - B\left( Q^2 - \frac{1}{3} \operatorname{tr}(Q^2) I \right) + C \operatorname{tr}(Q^2)Q - \frac{1}{2} \mu b \int_0^1 [e^{a b Q}(L^{-1}B_\alpha)e^{-abQ}]^* d\alpha - k\Delta Q = 0. \quad (B 11) \]

In many situations, the material is nearly incompressible, so that a good approximation the density \( \rho \) is constant. Hence, we can write (B 4) as follows:

\[
AQ - B\left( Q^2 - \frac{1}{3} \operatorname{tr}(Q^2) I \right) + C \operatorname{tr}(Q^2)Q - \frac{1}{2} \mu b \int_0^1 [e^{a b Q}(L^{-1}B_\alpha)e^{-abQ}]^* d\alpha - k\Delta Q = 0. \quad (B 11) \]

**Appendix C. Ordering tensor equation for the active fluid approximation**

When \( b \ll 1 \), we approximate the shape tensor as \( L \approx I + bQ \) so that \( L^\top \approx I^\top + bQ^\top = -2D + bQ^\top \). We can now use this approximation and equation (3.2) to simplify the integral in equation (2.13). Let us define \( X := T_a - \tau L^\top \) and consider its expansion in \( b \): \( X = X_0 + bX_1 + o(b) = T_a + 2bD - b\tau Q^\top + o(b) \). In construction with the usual presentations in this context, we introduce the co-rotational time derivative \( Q^\tau := Q - WQ + QW \), with \( W = (\nabla v - (\nabla v^\top))/2 \), so that we can write the co-deformational time derivative as follows:

\[
Q^\tau = Q^\tau - DQ - QD. \quad (C 1) \]

Finally, the integral in equation (2.13) simplifies to

\[
\int_0^1 e^{a b Q}(L^{-1}B_\alpha)e^{-abQ} d\alpha = I + \int_0^1 e^{a b Q}(T_a - \tau L^\top)e^{(1-a)bQ} d\alpha
\]

\[
= I + \int_0^1 (I + \alpha bQ)(X_0 + bX_1)(I + (1 - \alpha)bQ) d\alpha
\]

\[
= I + T_a + 2bD + \frac{b}{2}(QT_a + T_aQ) + 2b\tau(QD + DQ) - b\tau Q^\tau. \quad (C 2) \]
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