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Hydrodynamic Theories for Flows of Active Liquid Crystals and the Generalized Onsager Principle

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Abstract: We articulate and apply the generalized Onsager principle to derive transport equations for active liquid crystals in a fixed domain as well as in a free surface domain adjacent to a passive fluid matrix. The Onsager principle ensures fundamental variational structure of the models as well as dissipative properties of the passive component in the models, irrespective of the choice of scale (kinetic to continuum) and of the physical potentials. Many popular models for passive and active liquid crystals in a fixed domain subject to consistent boundary conditions at solid walls, as well as active liquid crystals in a free surface domain with consistent transport equations along the free boundaries, can be systematically derived from the generalized Onsager principle. The dynamical boundary conditions are shown to reduce to the static boundary conditions for passive liquid crystals used previously.

Keywords: active liquid crystals; nonequilibrium thermodynamics; hydrodynamics; free surface boundary conditions

1. Introduction

Active matter systems are abundant in Nature and man-made materials. They include many familiar systems like a bacterial suspension, a flock of birds, a school of fish, an ensemble of catalytic nanomotors, photo-powered nanoparticles, and the cytoskeleton in a live cell [1]. They share a common feature: the fundamental active "particles" are motile and can move on their own with an energy input created either internally (metabolic processes or ATP-motor activity) or externally from magnetic or electric fields, photonic, chemical gradients, or catalysis. In these diverse examples, active matter systems exhibit anomalous density fluctuations at scales far removed from single particles and emergent collective behavior. Dynamic phase transitions, spatio-temporal structures and symmetry-breaking induced dynamic patterns are prominent phenomena commonly seen in such systems [1–3]. Here, we are interested in flows of active liquid crystals, where the individual particles are self-propelling. We consider both polar and apolar self-propelling particles, where the passive equilibrium is nematic above a critical particle concentration. We refer to [1–14] for further details, and close the introduction with selected contributions of particular relevance to this paper. The review by Marchetti *et al.* [1] is especially recommended, from which we recall key elements and distinctions of active nematic "fluids".

Models for "dry" active matter systems that do not conserve momentum have been explored by many, notably, by Chaté *et al.* [15–19] and Bertin *et al.* [20–22]. For wet active matter systems, a useful theoretical framework is a continuum model that generalizes liquid crystal hydrodynamics to include new features related to particle-scale activation [4]. For polar particles, continuum models employ a single vector to describe the broken head-tail symmetry; these polar vector models are identified as a low moment (zero and first) approximation of kinetic theory [1,2,23]. For apolar particles, models have employed either a single vector with imposed fore-aft symmetry (the nematic director) or a second order tensor (the nematic order tensor). For more general active liquid crystals whose active particles/molecules are primarily polar while the interactions may be dominated by apolar interactions, the first three moments (density, polarity vector, and the nematic order tensor) of the orientational distribution function are modeled either directly or by moment closures of the kinetic theory [3]. More generally, active liquid crystals are described by kinetic theories, generalizing the Doi-Edwards-Hess formalism for passive liquid crystals, *cf.* studies by Marchetti and Liverpool, Shelley, Saintillan *et al.* and Forest *et al.* [1,24–30]. In this formulation, microscopic symmetry is tacitly incorporated through the interaction potential, self-propelling velocity, as well as phenomenologically modeled active forces [31]. This formulation can unify all three types of continuum models, where any low moment model is recoverable from closure approximations. For further details, we refer to [1,2,4,32–34].

Joanny *et al.* derived a class of models for active polar liquid crystal gels using a formulation pioneered by Onsager for non-equilibrium thermodynamical systems [35]. In this paper, we extend the approach to more general hydrodynamic theories for active liquid crystal solutions and gels applicable to polar or apolar active matter systems [36]. We call this approach the generalized Onsager principle. First, we recall what is the Onsager theory for a matter system not far from equilibrium [37–39] and then define what we mean by the generalized Onsager principle.

We consider a matter system with a stable equilibrium at $\mathbf{0}$, in which the fluctuations of a set of coarse-grained variables $\mathbf{x} = (x_1, \cdots, x_n)^T$ are measured relative to their most probable (equilibrium) values $\mathbf{x} = \mathbf{0}$. The entropy of the system S, a function of $\mathbf{x}$, reaches its maximum value S_0 at equilibrium. Expanding the entropy function in a Taylor series about the equilibrium, it can be approximated by the quadratic form

$$S = S_0 + \Delta S(\mathbf{x}),$$

$$\Delta S = -\frac{1}{2}\mathbf{x}^T \cdot \mathbf{H} \cdot \mathbf{x},$$

(1)

where $\mathbf{H}$ is the Hessian, a symmetric, positive-definite matrix when S has continuous second order derivatives at a maximum. The probability density at state $\mathbf{x}$ near the equilibrium is related to $\Delta S(\mathbf{x})$ via the Boltzmann distribution $f(\mathbf{x}) = f_0 \, exp[\Delta S(\mathbf{x})/k_B T]$, with k_B the Boltzmann constant, T the absolute temperature and f_0 a normalization constant.

When the system deviates from equilibrium, spontaneous irreversible processes arise in response to the generalized thermodynamic force $\mathbf{X}$ conjugate to $\mathbf{x}$:

$$\mathbf{X} = (\frac{\partial \Delta S}{\partial \mathbf{x}}) = -\mathbf{H} \cdot \mathbf{x},$$

(2)

which is linear in $\mathbf{x}$ due to the quadratic form of $\Delta S(\mathbf{x})$ in Equation (1). Thus, entropy production (or change of entropy) is given by

$$\Delta S = \frac{1}{2}\mathbf{x}^T \cdot \mathbf{X}.$$

(3)

i.e., entropy production is determined by the inner product of the conjugate variable $\mathbf{X}$ and the original thermodynamic variable $\mathbf{x}$.

For a small deviation from equilibrium, the system is assumed in the linear response regime so that the state $\mathbf{x}(t)$ evolves according to the kinetic equation

$$\dot{\mathbf{x}} = \mathbf{L} \cdot \mathbf{X}, \tag{4}$$

or, equivalently,

$$\mathbf{X} = \mathbf{R} \cdot \dot{\mathbf{x}}, \tag{5}$$

where the kinetic coefficients (mobility) $\mathbf{L} = (L_{ij})$ form a symmetric matrix and so do the friction coefficients $\mathbf{R} = (R_{ij}) = \mathbf{L}^{-1}$, according to the Onsager reciprocal relation [37,40]. Off-diagonal entries of (L_{ij}) and (R_{ij}) are referred to as cross-coupling coefficients between different irreversible processes labeled by i and j. Under the condition that S is an even function of $\mathbf{x}$, Onsager derived the reciprocal relation [37,38]

$$L_{ij} = L_{ji}, \tag{6}$$

from the microscopic reversibility, that is for any $t > 0$ and τ,

$$\langle \mathbf{x}(t)\mathbf{x}^T(t + \tau) \rangle = \langle \mathbf{x}(t + \tau)\mathbf{x}^T(t) \rangle, \tag{7}$$

where the ensemble average is taken with respect to the probability density function $f(\mathbf{x}, t)$. We note that, for anisotropic and active matter systems, condition (7) may not be valid.

From the entropy function, we calculate the rate of entropy production as follows

$$\dot{S} = \dot{\mathbf{x}}^T \cdot \mathbf{X} = \mathbf{X}^T \cdot \mathbf{L} \cdot \mathbf{X}, \tag{8}$$

which is given as an inner product of a generalized flux $\dot{\mathbf{x}}$ and the generalized force $\mathbf{X}$. In order for entropy to increase when approaching the stable equilibrium in an irreversible process, $\mathbf{L}$ must be nonnegative definite. We next summarize the three key ingredients in the Onsager theory for nonequilibrium systems near a stable equilibrium:

(1) the kinetic Equation (4), which gives the governing system of equations for dynamics of the non-equilibrium system;
(2) the Onsager reciprocal relation (6);
(3) the nonnegative definiteness of $\mathbf{L}$ ensures entropy production while approaching the equilibrium in an irreversible process.

We term (1)–(3) the Onsager principle in place of the Onsager theory in this paper. This statement of the Onsager principle is equivalent to the Onsager maximum action principle for irreversible processes [37–40]. This is also equivalent to the minimum entropy production principle summarized by Prigogine for irreversible processes in stationary (or steady) states [41].

We next demonstrate that this is also equivalent to the statement on energy dissipation for nonequilibrium systems. Recall the first law of thermodynamics,

$$dE_k + dU = dQ - dW, \tag{9}$$

where dE_k is the increase of the kinetic energy of the matter system, dU is the increase of the internal energy of the matter system, dQ is the heat added to the system and dW is the work done to the surrounding by the system. We denote entropy S for the matter system as [42]

$$S = S_i + S_e, \tag{10}$$

where S_i is the entropy generated internally in the system and S_e is the entropy exchanged with the surrounding. The Helmholtz free energy F of the system is defined by

$$F = U - TS_i, \tag{11}$$

where T is the absolute temperature. So, it follows from Equation (9) that

$$dF = dU - dTS_i - TdS_i = -dE_k + dQ - S_i dT - TdS_i - dW. \tag{12}$$

For an irreversible process,

$$TdS_i = dQ + dQ', \tag{13}$$

where dQ' is the energy lost internally. Then,

$$dF + dE_k = -S_i dT - dW - dQ'. \tag{14}$$

For an isothermal system, $dT = 0$. So,

$$dF + dE_k = -(dW + dQ'), \tag{15}$$

This is known as the energy dissipation. Thus, the energy dissipation rate is given by

$$\frac{d}{dt}(E_k + F) = \frac{d(U + E_k)}{dt} - T\frac{dS_i}{dt} = -\frac{dW}{dt} - \frac{dQ'}{dt} = -T\mathbf{X}^T \cdot \mathbf{L} \cdot \mathbf{X}. \tag{16}$$

For a closed system, $\frac{dS_e}{dt} = 0$ and $\frac{d(U+E_k)}{dt} = 0$. So

$$\frac{d}{dt}(E_k + F) = -T\frac{dS}{dt} = -\frac{dW}{dt} - \frac{dQ'}{dt} = -T\mathbf{X}^T \cdot \mathbf{L} \cdot \mathbf{X}. \tag{17}$$

For an open system, $d(U + E_k) = -TdS_e$, where it is assumed that there is no work done during the exchange. So,

$$\frac{d}{dt}(E_k + F) = -T\frac{dS}{dt} = -\frac{dW}{dt} - \frac{dQ'}{dt} = -T\mathbf{X}^T \cdot \mathbf{L} \cdot \mathbf{X}. \tag{18}$$

This establishes the relation between the energy dissipation rate and the entropy production rate, which applies to both the closed and open system.

In this paper, we generalize the Onsager principle to a non-equilibrium system in which the source of external or chemical energy that gives rise to self-propulsion in the active matter is accounted for. Specifically, we consider the dissipation rate defined by the combination of the kinetic energy and the Helmholtz free energy. In [35], this combination is called the free energy, which indeed serves as the role of free energy in the nonequilibrium systems. We remove the symmetry constraint imposed on the mobility coefficient in the Onsager principle and abandon the non-negativeness of the mobility coefficient imposed for irreversible processes to allow reversible systems. This extension is important for anisotropic viscoelastic material systems including active matter systems, where both irreversible and reversible process can coexist. For these material systems, the mobility coefficient L can be decomposed into a symmetric and an antisymmetric part. The antisymmetric component, representing reversible dynamics, does not contribute to energy dissipation while the symmetric part does. The symmetric part, representing irreversible dynamics, is required to be nonnegative definite to ensure energy dissipation. We remark that the antisymmetric part corresponds to the Casimir principle while the symmetric part corresponds to the Onsager principle [42,43].

In the active matter system, we consider the source of chemical energy (e.g., the one produced by ATP hydrolysis in myosin motors or through catalytic reaction) or external source converted chemical energy (e.g., energy due to photo induced chemical reactions or magnetic fields) as a source for an additional free energy. We first derive the governing system of equations in a domain with a fixed boundary together with the consistent boundary conditions that do not contribute to energy dissipation. Then, we extend it to a two-phase case in which the active liquid crystal system resides in a domain separated from a passive fluid matrix by free boundaries. In this case, we also consider the surface transport phenomena which may exist in such a matter system. In both cases, we let the active component of the free energy enters into the total stress through a reversible process and the dynamics of the internal variables (density, polarity vector, and nematic tensor) through irreversible processes. Then, the resultant theories of active matter systems may not respect energy dissipation anymore but their corresponding passive component, the limit when the activity is absent, must. This is the basic principle that we follow in the following derivation.

These models of complex active matter systems have applications to cell motility, a school of fish, a colony of bacteria in a viscous fluid bath, and the cortical layer in a live cell, guaranteeing that the system conserves momentum and the corresponding passive component satisfies the correct energy dissipation principle. In this way, the detailed physical and chemical processes of self-propulsion are determined specific to the active matter system and incorporated in the framework of the generalized Onsager principle. We proceed in this paper to illustrate this framework for active liquid crystals. We remark that there exist other approaches for developing extended hydrodynamic theories for complex fluid systems like the generalized Poisson bracket approach discussed in the book [44], the GENERIC formalism advocated in [45,46], and several more nonequilibrium thermodynamic frameworks reviewed by Sagis and others in [47–50]. All these approaches agree in principle on the fundamental mathematical structure of the non-equilibrium thermodynamic theory. In particular, the approach that has been used by Sagis *et al.* is especially close to what we are using in this paper [47–49]. However, our approach presented in this paper is simpler, constructive, and straight-forward in that it yields (derives or stipulates) the constitutive relations explicitly that warrants energy dissipation for the passive components for both the reversible and the irreversible nonequilibrium processes.

The rest of the paper is organized as follows. In Section 2, we derive the hydrodynamic model along with the boundary conditions in a fixed domain for an active liquid crystal system, closing the model on the first three moments of a probability distribution function. In Section 3, we present the model for an apolar active liquid crystal system. In Section 4, we extend the study to domains with free surfaces. Then we provide a closing remark.

2. A General Hydrodynamic Model for Active Liquid Crystals

We systemically derive a general hydrodynamic model for flows of active liquid crystals using the generalized Onsager principle at the continuum scale. We assume that the active liquid crystal system is composed of two components: the first component consists of the active anisotropic particles with a mass density ρ_1 and velocity $\mathbf{v}_1$ and the second component consists of the solvent which has a mass density ρ_2 with velocity $\mathbf{v}_2$. The corresponding mass conservation laws for the two components are given respectively by

$$\partial_t \rho_1 + \nabla \cdot (\rho_1 \mathbf{v}_1) = 0,$$

$$\partial_t \rho_2 + \nabla \cdot (\rho_2 \mathbf{v}_2) = 0.$$

Introducing the total mass density $\rho = \rho_1 + \rho_2$ and the mass-averaged center-of-mass velocity $\mathbf{v} = (\rho_1 \mathbf{v}_1 + \rho_2 \mathbf{v}_2)/\rho$, the total linear momentum density (or density flux) can be expressed as $\rho \mathbf{v}$. The total mass is conserved:

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{v}) = 0. \tag{19}$$

For the active particle component, we rewrite the current into a convective part moving with the center-of-mass velocity $\mathbf{v}$ and a diffusive part associated to the relative flux between the two components:

$$\partial_t \rho_1 + \nabla \cdot (\rho_1 \mathbf{v} + \hat{\mathbf{j}}) = 0, \tag{20}$$

where $\hat{\mathbf{j}} = \frac{\rho_1 \rho_2 (\mathbf{v}_1 - \mathbf{v}_2)}{\rho}$ is the diffusive current. In the following, we define the active particle number density as $c = \frac{\rho_1}{m_1}$, where m_1 is the mass of the active particle. We denote its flux as $\mathbf{j} = \frac{\hat{\mathbf{j}}}{m_1}$. The transport equation for c can then be written as

$$\partial_t c + \nabla \cdot (c\mathbf{v} + \mathbf{j}) = 0. \tag{21}$$

To describe the system's internal properties (or microstructure), a hierarchy of order parameters is necessary. A scalar concentration variable is needed to describe the density fluctuation in space and time. A vector order parameter is needed to describe the average polarity. A rank 2 tensor order parameter is needed to characterize the nematic order or the orientational correlation among the particles. So, the minimal number of order parameters in any viable model should be three: a scalar, a vector, and a second order tensor. We denote the polar order by a vector field $\mathbf{p}$ and the nematic order by a second order tensor field $\mathbf{Q}$, in addition to the density variable c.

Consider the active particle system as a discrete system with N particles located at $\mathbf{r}_n(t)$, n=1, $\cdots$, N, respectively, and each of the particles has a self-propelled velocity $\widehat{v}_n(t)$, $n = 1, \cdots, N$. We can normalize $\widehat{v}_n(t)$ as a unit vector to represent the direction of motion and describe speed fluctuations with a scalar, but we will not employ this normalization in this paper. We assume the domain of $\widehat{v}$, $\mathbf{V}$, is a compact domain in $\mathbf{R}^3$. The one-particle phase-space distribution $f_d(\mathbf{r}, \widehat{v}, t)$ is defined as follows:

$$f_d(\mathbf{r}, \widehat{v}, t) = \sum_n \delta(\mathbf{r} - \mathbf{r}_n(t)) \delta(\widehat{v} - \widehat{v}_n(t)). \tag{22}$$

The number density of active particles $c(\mathbf{r}, t)$ is the zeroth moment

$$c(\mathbf{r}, t) = \int_{\mathbf{V}} f_d(\mathbf{r}, \widehat{v}, t) d\widehat{v} = \sum_n \delta(\mathbf{r} - \mathbf{r}_n(t)). \tag{23}$$

The first moment of the distribution function is given by

$$c(\mathbf{r}, t)\mathbf{p}(\mathbf{r}, t) = \int_{\mathbf{V}} \widehat{v} f_d(\mathbf{r}, \widehat{v}, t) d\widehat{v} = \sum_n \widehat{v}_n(t) \delta(\mathbf{r} - \mathbf{r}_n(t)). \tag{24}$$

The polarization vector field $\mathbf{p}(\mathbf{r}, t)$ follows as a normalized first moment. The second moment is defined by

$$c(\mathbf{r}, t)\mathbf{Q}(\mathbf{r}, t) = \int_{\mathbf{V}} (\widehat{v}\widehat{v} - \frac{\|v\|^2}{d}) f_d(\mathbf{r}, \widehat{v}, t) d\widehat{v} = \sum_n (\widehat{v}_n(t)\widehat{v}_n(t) - \frac{\|\widehat{v}_n\|^2}{d}) \delta(\mathbf{r} - \mathbf{r}_n(t)), \tag{25}$$

where d is the system's dimensionality, from which a nematic order tensor $\mathbf{Q}(\mathbf{r}, t)$ can be defined as a normalized second moment. Notice that the tensor $\mathbf{Q}$ is traceless.

Often, one prefers the moments defined as primitive variables for developing multiphase models. In this context, the polarity vector and the nematic order tensor can then be defined as follows:

$$\mathbf{p}(\mathbf{r}, t) = \int_V \widehat{v} f_d(\mathbf{r}, \widehat{v}, t) d\widehat{v} = \sum_n \widehat{v}_n(t) \delta(\mathbf{r} - \mathbf{r}_n(t)),$$

$$\mathbf{Q}(\mathbf{r}, t) = \int_V (\widehat{v}\widehat{v} - \frac{\|v\|^2}{d}) f_d(\mathbf{r}, \widehat{v}, t) d\widehat{v} = \sum_n (\widehat{v}_n(t)\widehat{v}_n(t) - \frac{\|\widehat{v}_n\|^2}{d}) \delta(\mathbf{r} - \mathbf{r}_n(t)).$$

(26)

The free energy of the active particle system in volume element V must be prescribed in terms of the internal variables, in this case the first three moments of f_d and their gradients (*i.e.*, we assume weak non-locality for this paper):

$$F = F(c, \nabla c, \mathbf{p}, \nabla \mathbf{p}, \mathbf{Q}, \nabla \mathbf{Q}) = \int_V f(c, \nabla c, \mathbf{p}, \nabla \mathbf{p}, \mathbf{Q}, \nabla \mathbf{Q}) d\mathbf{x},$$

where f is the free energy density. At the boundary of the fixed material domain ∂V, we have an interfacial free energy

$$G = G(c, \mathbf{p}, \mathbf{Q}) = \int_{\partial V} g(c, \mathbf{p}, \mathbf{Q}) dS.$$

The active free energy in the active matter system is denoted as

$$A = \int_V R(\mathbf{x}, t) \widehat{\mu} d\mathbf{x},$$

where $R(\mathbf{x}, t)$ is the number density of the fundamental energy generating units in the active matter system and $\widehat{\mu}$ is the energy gain per fundamental unit at position $\mathbf{x}$, time t. For instance, $\widehat{\mu}$ is the energy gain per ATP molecule for F-actin filaments or microtubule in a live cell while $R(\mathbf{x}, t)$ is the number density of the ATP molecules. The sum of the kinetic and free energy of the system is called the total energy here or extended free energy in [35] given by

$$E^{total} = \int_V [\frac{\rho}{2} \|\mathbf{v}\|^2] d\mathbf{x} + F + G + A.$$

(27)

Since we are interested in an isothermal system, the temperature is assumed a constant and so the energy dissipation rate at a constant absolute temperature T is given by

$$\frac{dE^{total}}{dt} = \int_V d\mathbf{x} \{ \frac{1}{2} \frac{\partial(\rho \mathbf{v}^2)}{\partial t} + \frac{\partial f}{\partial t} - r\widehat{\mu} \} + \int_{\partial V} \frac{\partial g}{\partial t} dS.$$

(28)

There are four parts in the integration: the first and second parts are the rate changes of the kinetic energy and the active particle free energy, respectively, the third one is the energy reduction rate of the chemical energy, where $r = -\partial_t R$ is the consumption rate (the number of the fundamental energy producing units consumed per unit time and unit volume), the fourth is the rate of change of the surface free energy. The differential of the free energy density is given by

$$\frac{\partial f}{\partial t} = \frac{\partial f}{\partial c} \frac{\partial c}{\partial t} + \frac{\partial f}{\partial \mathbf{p}} \cdot \frac{\partial \mathbf{p}}{\partial t} + \frac{\partial f}{\partial \mathbf{Q}} : \frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial f}{\partial(\nabla c)} \cdot \frac{\partial(\nabla c)}{\partial t} + \frac{\partial f}{\partial(\nabla \mathbf{p})} : \frac{\partial(\nabla \mathbf{p})}{\partial t} + \frac{\partial f}{\partial(\nabla \mathbf{Q})} \vdots \frac{\partial(\nabla \mathbf{Q})}{\partial t}$$

$$= \mu \frac{\partial c}{\partial t} - \mathbf{h} \cdot \frac{\partial \mathbf{p}}{\partial t} - \mathbf{G} : \frac{\partial \mathbf{Q}}{\partial t} + \nabla \cdot (\frac{\partial f}{\partial(\nabla c)} \frac{\partial c}{\partial t} + \frac{\partial f}{\partial(\nabla \mathbf{p})} \cdot \frac{\partial \mathbf{p}}{\partial t} + \frac{\partial f}{\partial(\nabla \mathbf{Q})} : \frac{\partial \mathbf{Q}}{\partial t}).$$

(29)

Now we identify the conjugate variables to $c, \mathbf{p}$, and $\mathbf{Q}$ through variations of the free energy density f. The field conjugate to the density c is the chemical potential $\mu = \frac{\delta f}{\delta c} = \frac{\partial f}{\partial c} - \nabla \cdot \frac{\partial f}{\partial(\nabla c)}$, the field conjugate to the polarization $\mathbf{p}$ is the molecular field $\mathbf{h} = -\frac{\delta f}{\delta \mathbf{p}} = -\frac{\partial f}{\partial \mathbf{p}} + \nabla \cdot \frac{\partial f}{\partial(\nabla \mathbf{p})}$, and the field

conjugate to the nematic order $\mathbf{Q}$ is the variation $\mathbf{G} = -\frac{\delta f}{\delta \mathbf{Q}} = -\frac{\partial f}{\partial \mathbf{Q}} + \nabla \cdot \frac{\partial f}{\partial (\nabla \mathbf{Q})}$, another molecular field. If $\mathbf{Q}$ is traceless, $\mathbf{G} = -[\frac{1}{2}(\frac{\delta f}{\delta \mathbf{Q}} + \frac{\delta f}{\delta \mathbf{Q}}^T) - \frac{\mathbf{I}}{3} tr(\frac{\delta f}{\delta \mathbf{Q}})]$. We denote the product of two second order tensors as $\mathbf{A} : \mathbf{B} = A_{\alpha\beta} B_{\alpha\beta}$. So

$$\frac{dE^{total}}{dt} = \int_V d\mathbf{x} \{ \frac{1}{2} \frac{\partial(\rho \mathbf{v}^2)}{\partial t} + \mu \frac{\partial c}{\partial t} - \mathbf{h} \cdot \frac{\partial \mathbf{p}}{\partial t} - \mathbf{G} : \frac{\partial \mathbf{Q}}{\partial t} - r\hat{\mu} \} +$$

$$\int_{\partial V} dS \{ (\frac{\partial f}{\partial(\nabla c)} \frac{\partial c}{\partial t} + \frac{\partial f}{\partial(\nabla \mathbf{p})} \cdot \frac{\partial \mathbf{p}}{\partial t} + \frac{\partial f}{\partial(\nabla \mathbf{Q})} : \frac{\partial \mathbf{Q}}{\partial t}) \cdot \mathbf{n} \} + \int_{\partial V} dS \{ (\frac{\partial g}{\partial c} \frac{\partial c}{\partial t} + \frac{\partial g}{\partial \mathbf{p}} \cdot \frac{\partial \mathbf{p}}{\partial t} + \frac{\partial g}{\partial \mathbf{Q}} : \frac{\partial \mathbf{Q}}{\partial t}) \},$$

$$(30)$$

where ∂V is the surface of volume V and $\mathbf{n}$ is the external unit normal of ∂V. We assume the following so that the surface integral is zero, *i.e.*, the surface does not contribute to energy dissipation of the system:

$$\mathbf{n} \cdot \frac{\partial f}{\partial \nabla c} + \frac{\partial g}{\partial c} = 0,$$

$$\mathbf{n} \cdot \frac{\partial f}{\partial \nabla \mathbf{p}} + \frac{\partial g}{\partial \mathbf{p}} = 0,$$

$$\mathbf{n} \cdot \frac{\partial f}{\partial \nabla \mathbf{Q}} + \frac{\partial g}{\partial \mathbf{Q}} = 0.$$

$$(31)$$

These define the boundary conditions of the active matter system at the solid walls for the three internal variables $c, \mathbf{p}$ and $\mathbf{Q}$. From the previous discussion, the conservation laws of the active particle number, total system mass and system momentum are given by

$$\frac{\partial c}{\partial t} + \nabla \cdot (c\mathbf{v} + \mathbf{j}) = 0,$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0,$$

$$\frac{\partial(\rho \mathbf{v})}{\partial t} = \nabla \cdot (\sigma - \rho \mathbf{v}\mathbf{v}),$$

$$(32)$$

where $\mathbf{j}$ is the diffusive current of the active particles, σ is the momentum flux. Then, we have

$$\int_V d\mathbf{x} \{ \frac{1}{2} \frac{\partial(\rho \mathbf{v}^2)}{\partial t} + \mu \frac{\partial c}{\partial t} \} = \int_V d\mathbf{x} \{ -\partial_\beta v_\alpha \sigma_{\alpha\beta} + c v_\alpha \partial_\alpha \mu + j_\alpha \partial_\alpha \mu \} +$$

$$\int_{\partial V} dS \{ \mathbf{v} \cdot (-\frac{1}{2}\rho \mathbf{v}^2 \mathbf{I} - c\mu \mathbf{I} + \sigma) \cdot \mathbf{n} - \mu \mathbf{j} \cdot \mathbf{n} \}.$$

$$(33)$$

If we assume $\mathbf{v} = 0$ and $\mathbf{j} \cdot \mathbf{n} = 0$ at the boundary, the last surface integration is zero. Once again, the surface does not contribute to energy dissipation of the active matter system. These define additional boundary conditions for the velocity and the internal variables via the excessive flux. If the surface term is not assigned into zero, it will contribute to the energy dissipation. The latter case includes moving boundaries, which we will not pursue in this study.

We denote

$$D_{\alpha\beta} = \frac{1}{2}(\partial_\alpha v_\beta + \partial_\beta v_\alpha),$$

$$\Omega_{\alpha\beta} = \frac{1}{2}(\partial_\alpha v_\beta - \partial_\beta v_\alpha),$$

$$\dot{\mathbf{p}} = \partial_t \mathbf{p} + \mathbf{v} \cdot \nabla \mathbf{p} + \Omega \cdot \mathbf{p},$$

$$\overset{\square}{\mathbf{Q}} = \partial_t \mathbf{Q} + \mathbf{v} \cdot \nabla \mathbf{Q} + [\Omega \cdot \mathbf{Q} - \mathbf{Q} \cdot \Omega],$$

$$(34)$$

where $\mathbf{D}$ is the strain rate tensor, Ω is the vorticity tensor of the velocity field $\mathbf{v}$, $\overset{\Box}{\mathbf{p}}$ is the convected co-rotational derivative of vector $\mathbf{p}$, $\overset{\Box}{\mathbf{Q}}$ is the co-rotational derivative of tensor $\mathbf{Q}$. Then

$$-\mathbf{h} \cdot \frac{\partial \mathbf{p}}{\partial t} = -h_\alpha \dot{p}_\alpha + v_\alpha h_\gamma \partial_\alpha p_\gamma + \tfrac{1}{2}\partial_\beta v_\alpha (p_\alpha h_\beta - p_\beta h_\alpha),$$

$$-\mathbf{G} : \frac{\partial \mathbf{Q}}{\partial t} = -G_{\alpha\beta}\overset{\Box}{Q}_{\alpha\beta} + v_\alpha G_{\beta\gamma}\partial_\alpha Q_{\beta\gamma} + \partial_\beta v_\alpha (Q_{\alpha\gamma} G_{\gamma\beta} - G_{\alpha\gamma} Q_{\gamma\beta}),$$

(35)

where $\mathbf{G} : [\Omega \cdot \mathbf{Q} - \mathbf{Q} \cdot \Omega] = \partial_\beta v_\alpha (Q_{\alpha\gamma} G_{\gamma\beta} - G_{\alpha\gamma} Q_{\gamma\beta})$ due to symmetry of $\mathbf{Q}, \mathbf{G}$ and antisymmetry of Ω. We introduce the antisymmetric part of the stress σ^a and the Ericksen stress σ^e (Refer to Appendix A) respectively as follows:

$$\sigma^a_{\alpha\beta} = \tfrac{1}{2}(p_\alpha h_\beta - p_\beta h_\alpha) + (Q_{\alpha\gamma} G_{\gamma\beta} - G_{\alpha\gamma} Q_{\gamma\beta}),$$

$$\sigma^e_{\alpha\beta} = (f - c\mu)\delta_{\alpha\beta} - \frac{\partial f}{\partial(\partial_\beta c)}\partial_\alpha c - \frac{\partial f}{\partial(\partial_\beta p_\gamma)}\partial_\alpha p_\gamma - \frac{\partial f}{\partial(\partial_\beta Q_{\gamma\theta})}\partial_\alpha Q_{\gamma\theta},$$

(36)

$$\partial_\beta \sigma^e_{\alpha\beta} = -(c\partial_\alpha \mu + h_\gamma \partial_\alpha p_\gamma + G_{\beta\gamma}\partial_\alpha Q_{\beta\gamma}).$$

Then the energy dissipation is simplified into

$$\frac{dE^{total}}{dt} = \int_V d\mathbf{x}\{-\partial_\beta v_\alpha [\sigma_{\alpha\beta} - \sigma^e_{\alpha\beta} - \sigma^a_{\alpha\beta}] + j_\alpha \partial_\alpha \mu - h_\alpha \dot{p}_\alpha - G_{\alpha\beta}\overset{\Box}{Q}_{\alpha\beta} - r\widehat{\mu}\} - \int_V d\mathbf{x}\partial_\beta(v_\alpha \sigma^e_{\alpha\beta}).$$

(37)

From the vanishing surface terms, we summarize the boundary conditions as follows

$$\mathbf{v}|_{\partial V} = 0, \quad \frac{\partial f}{\partial(\nabla c)} \cdot \mathbf{n} + \frac{\partial g}{\partial c} = 0, \quad \mathbf{j} \cdot \mathbf{n} = 0, \quad \frac{\partial f}{\partial(\nabla \mathbf{p})} \cdot \mathbf{n} + \frac{\partial g}{\partial \mathbf{p}} = 0, \quad \frac{\partial f}{\partial(\nabla \mathbf{Q})} \cdot \mathbf{n} + \frac{\partial g}{\partial \mathbf{Q}} = 0.$$

(38)

For $c, \mathbf{p}, \mathbf{Q}$, the boundary conditions (BCs) are mixed (Robin). There are two boundary conditions for c due to the nature of the transport (the Cahn-Hilliard equation) of c. We remark that if we do not postulate the transport equation of c in a conservative form (e.g., we use an Allen–Cahn type equation to describe the transport of c), the boundary condition on $\mathbf{j}$ will not be necessary. If the surface energy density dominates, we arrive at the Dirichlet BCs (or the anchoring boundary condition) for the internal variables:

$$\frac{\partial g}{\partial c} = 0, \frac{\partial g}{\partial \mathbf{p}} = 0, \frac{\partial g}{\partial \mathbf{Q}} = 0.$$

(39)

There are two issues to be addressed in order to complete the derivation through the generalized Onsager principle. One is to derive the Gibbs–Duhem relation to identify the Ericksen stress $\sigma^e_{\alpha\beta}$. The other one is to prove that the stress σ^s, given by

$$\sigma^s_{\alpha\beta} = \sigma_{\alpha\beta} - \sigma^e_{\alpha\beta} - \sigma^a_{\alpha\beta},$$

(40)

is in fact symmetric. We address these two issues in Appendix A to keep the presentation flowing. For the time being, we assume both are true. Then, we rewrite the energy dissipation functional as follows

$$\frac{dE^{total}}{dt} = -\int_V d\mathbf{x}\{D_{\alpha\beta}\sigma^s_{\alpha\beta} + j_\alpha(-\partial_\alpha \mu) + h_\alpha \dot{p}_\alpha + G_{\alpha\beta}\overset{\Box}{Q}_{\alpha\beta} + r\widehat{\mu}\}.$$

(41)

The generalized fluxes and the corresponding generalized forces, identified from the energy dissipation, are listed below

$$
\begin{array}{ccc}
\text{Flux} & \longleftrightarrow & \text{Force} \\
\sigma^s_{\alpha\beta} & \longleftrightarrow & D_{\alpha\beta} \\
\overset{\square}{Q}_{\alpha\beta} & \longleftrightarrow & G_{\alpha\beta} \\
\dot{p}_\alpha & \longleftrightarrow & h_\alpha \\
j_\alpha & \longleftrightarrow & -\partial_\alpha \mu \\
r & \longleftrightarrow & \widehat{\mu}.
\end{array}
\tag{42}
$$

Note that, the generalized forces have different signatures under time inversion. While **D** changes sign, the other forces do not. Therefore we distinguish between the components of the fluxes that show the same behavior under time inversion as the dissipative conjugated forces or fluxes, and those that show the opposite behavior called reactive conjugated forces or fluxes. We denote the various components by superscripts *d* and *r*, respectively.

The phenomenological equations for the dissipative currents can be written as

$$
\begin{pmatrix}
\sigma^{s,d}_{\alpha\beta} \\
\overset{\square d}{Q}_{\alpha\beta} \\
\dot{p}^d_\alpha \\
j^d_\alpha \\
r^d
\end{pmatrix}
=
\begin{pmatrix}
A_0 & 0 & 0 & 0 & 0 \\
0 & \frac{1}{\gamma_2}\delta_{\alpha k}\delta_{\beta l} & \frac{\chi_1}{2}A_{\alpha\beta k} & \frac{\chi_2}{2}A_{\alpha\beta k} & A_{5,\alpha\beta} \\
0 & \frac{\chi_1}{2}A^T_{\alpha kl} & \frac{1}{\gamma_1}\delta_{\alpha k} & \lambda\delta_{\alpha k} & B_\alpha \\
0 & \frac{\chi_2}{2}A^T_{\alpha kl} & \lambda\delta_{\alpha k} & \gamma\delta_{\alpha k} & (\kappa+\omega_0 c)p_\alpha \\
0 & A_{5,kl} & B_k & (\kappa+\omega_0 c)p_k & \Lambda
\end{pmatrix}
\begin{pmatrix}
D_{kl} \\
G_{kl} \\
h_k \\
-\partial_k\mu \\
\widehat{\mu}
\end{pmatrix},
\tag{43}
$$

where

$$
\begin{aligned}
&A_{\alpha\beta k} = (p_\alpha\delta_{\beta k} + p_\beta\delta_{\alpha k}) - \tfrac{2}{3}\delta_{\alpha\beta}p_l\delta_{lk}, \\
&A^T_{\alpha kl} = 2(p_\beta\delta_{\alpha k}\delta_{\beta l} - \tfrac{p_\beta}{3}\delta_{\alpha\beta}\delta_{kl}), \\
&A_0 = 2\eta\delta_{\alpha k}\delta_{\beta l} + (\bar{\eta} - \tfrac{2}{3}\eta)\delta_{\alpha\beta}\delta_{kl} + \alpha_1(Q_{\alpha k}\delta_{\beta l} + \delta_{\alpha k}Q_{\beta l}) \\
&\quad+\alpha_2 Q_{kl}Q_{\alpha\beta} + \alpha_3(p_\alpha p_k\delta_{\beta l} + \delta_{\alpha k}p_\beta p_l) + \alpha_4 p_k p_l p_\alpha p_\beta, \\
&B_\alpha = \lambda_1 p_\alpha - \omega\mathbf{p}\cdot\nabla p_\alpha - \omega p_\alpha\nabla\cdot\mathbf{p}, \\
&A_5 = \zeta_1(\mathbf{pp} - \tfrac{\|\mathbf{p}\|^2}{3}\mathbf{I}) + (\zeta_2 - \omega_2\nabla\cdot\mathbf{p} - \omega_2\mathbf{p}\cdot\nabla)\mathbf{Q}.
\end{aligned}
\tag{44}
$$

It is easy to show that the coefficient matrix is symmetric. We insist the passive limit of the active matter system is a dissipative system. Then, the left upper submatrix is nonnegative definite. So, the diagonal parameters $\eta, \gamma, \gamma_1, \gamma_2$ are nonnegative together with a set of constraints on the model parameters independent of $\hat{\mu}$. The reactive terms can be written as

$$
\begin{pmatrix}
\sigma^{s,r}_{\alpha\beta} \\
\overset{\square r}{Q}_{\alpha\beta} \\
\dot{p}^r_\alpha \\
j^r_\alpha \\
r^r
\end{pmatrix}
=
\begin{pmatrix}
0 & -A_1 & -A_2 & -A_3 & A_4 \\
A_1 & 0 & 0 & 0 & 0 \\
A'_2 & 0 & 0 & 0 & 0 \\
A'_3 & 0 & 0 & 0 & 0 \\
-A'_4 & 0 & 0 & 0 & 0
\end{pmatrix}
\begin{pmatrix}
D_{kl} \\
G_{kl} \\
h_k \\
-\partial_k\mu \\
\widehat{\mu}
\end{pmatrix},
\tag{45}
$$

where

$$
\begin{aligned}
A_1 &= \nu_0 \delta_{\alpha k}\delta_{\beta l} + a[Q_{\alpha k}\delta_{\beta l} + \delta_{\alpha k}Q_{\beta l}] - a(Q_{kl}(Q_{\alpha\beta} + \tfrac{1}{3}\delta_{\alpha\beta})) + \theta_1\delta_{kl}\delta_{\alpha\beta}, \\
A_2 &= \tfrac{\nu_1}{2}(p_\beta\delta_{\alpha k} + p_\alpha\delta_{\beta k}) + \theta_2 p_k\delta_{\alpha\beta}, \\
A_2' &= \nu_1 p_\beta\delta_{\alpha k}\delta_{\beta l} + \theta_2 p_\alpha\delta_{kl}, \\
A_3 &= \tfrac{\nu_2}{2}(p_\beta\delta_{\alpha k} + p_\alpha\delta_{\beta k}) + \theta_3 p_k\delta_{\alpha\beta}, \\
A_3' &= \nu_2 p_\beta\delta_{\alpha k}\delta_{\beta l} + \theta_3 p_\alpha\delta_{kl}, \\
A_4 &= \zeta p_\alpha p_\beta + \zeta_0 Q_{\alpha\beta} + \beta_1(\partial_\alpha p_\beta + \partial_\beta p_\alpha) + \beta_2 \mathbf{p}\cdot\nabla Q_{\alpha\beta} + \beta_3\nabla^2 Q_{\alpha\beta} - (\zeta_2 + \zeta_3 p_\alpha p_\alpha)\delta_{\alpha\beta}, \\
A_4' &= A_4\delta_{\alpha k}\delta_{\beta l}.
\end{aligned}
\tag{46}
$$

For the reactive fluxes, the coefficient matrix is antisymmetric, implying $\text{Flux}^r \cdot \text{Force} = 0$; so, the reactive processes do not contribute to energy dissipation.

We summarize the equations in the following

$$
\partial_t c + \nabla \cdot ((\mathbf{v} + \omega_0\hat{\mu}\mathbf{p})c) = -\nabla \cdot (-\gamma\nabla\mu + \chi_2 \mathbf{G}\cdot\mathbf{p} - \tfrac{\chi_2}{3}tr(\mathbf{G})\mathbf{p} + \lambda\mathbf{h} + \kappa\mathbf{p}\hat{\mu} + \nu_2\mathbf{D}\cdot\mathbf{p} + \theta_3 D_{\gamma\gamma}\mathbf{p}),
$$

$$
\partial_t\mathbf{p} + \nabla \cdot ((\mathbf{v} + \omega\hat{\mu}\mathbf{p})\mathbf{p}) - \nabla\cdot\mathbf{vp} + \Omega\cdot\mathbf{p} = \tfrac{1}{\gamma_1}\mathbf{h} + \chi_1\mathbf{G}\cdot\mathbf{p} - \tfrac{\chi_1}{3}tr(\mathbf{G})\mathbf{p} - \lambda\nabla\mu + \lambda_1\hat{\mu}\mathbf{p} + \nu_1\mathbf{D}\cdot\mathbf{p} + \theta_2 D_{\gamma\gamma}\mathbf{p},
$$

$$
\begin{aligned}
\frac{\partial\mathbf{Q}}{\partial t} + \nabla \cdot ((\mathbf{v} + \omega_2\hat{\mu}\mathbf{p})\mathbf{Q}) - \nabla\cdot\mathbf{vQ} + \Omega\cdot\mathbf{Q} - \mathbf{Q}\cdot\Omega - a[\mathbf{Q}\cdot\mathbf{D} + \mathbf{D}\cdot\mathbf{Q}] &= \tfrac{1}{\gamma_2}\mathbf{G} + \tfrac{\chi_1}{2}(\mathbf{ph} + \mathbf{hp}) \\
- \tfrac{\chi_2}{2}(\mathbf{p}\nabla\mu + \nabla\mu\mathbf{p}) + \zeta_1\hat{\mu}\mathbf{pp} + \nu_0\mathbf{D} - a(\mathbf{Q}:\mathbf{D})\mathbf{Q} + (\theta_1 D_{\gamma\gamma} - \tfrac{a\mathbf{Q}:\mathbf{D}}{3} - \tfrac{\chi_1\mathbf{p}\cdot\mathbf{h}}{3} + \tfrac{\chi_2\mathbf{p}\cdot\nabla\mu}{3} - \tfrac{\hat{\mu}\zeta_1\|\mathbf{p}\|^2}{3})\mathbf{I} &+ \zeta_2\hat{\mu}\mathbf{Q},
\end{aligned}
$$

$$
\partial_t\rho + \nabla\cdot(\rho\mathbf{v}) = 0,
$$

$$
\partial_t(\rho\mathbf{v}) + \nabla\cdot(\rho\mathbf{vv}) = \nabla\cdot\sigma,
\tag{47}
$$

$$
\sigma = \sigma^s + \sigma^e + \sigma^a,
$$

$$
\begin{aligned}
\sigma_{\alpha\beta}^e &= (f - c\mu)\delta_{\alpha\beta} - \frac{\partial f}{\partial(\partial_\beta c)}\partial_\alpha c - \frac{\partial f}{\partial(\partial_\beta p_\gamma)}\partial_\alpha p_\gamma - \frac{\partial f}{\partial(\partial_\beta Q_{\gamma\theta})}\partial_\alpha Q_{\gamma\theta}, \\
\nabla\cdot\sigma^e &= -(c\nabla\mu + \nabla\mathbf{p}\cdot\mathbf{h} + \nabla\mathbf{Q}:\mathbf{G}), \\
\sigma^a &= \tfrac{1}{2}(\mathbf{ph} - \mathbf{hp}) + (\mathbf{Q}\cdot\mathbf{G} - \mathbf{G}\cdot\mathbf{Q}),
\end{aligned}
$$

$$
\begin{aligned}
\sigma^s &= -\Pi\mathbf{I} + 2\eta\mathbf{D} + \alpha_1(\mathbf{Q}\cdot\mathbf{D} + \mathbf{D}\cdot\mathbf{Q}) + \alpha_2(\mathbf{Q}:\mathbf{D})\mathbf{Q} + \alpha_3(\mathbf{pp}\cdot\mathbf{D} + \mathbf{D}\cdot\mathbf{pp}) + \alpha_4(\mathbf{pp}:\mathbf{D})\mathbf{pp} \\
&\quad - a(\mathbf{Q}\cdot\mathbf{G} + \mathbf{G}\cdot\mathbf{Q}) - \nu_0\mathbf{G} + a(\mathbf{Q}:\mathbf{G})\mathbf{Q} - \tfrac{\nu_1}{2}(\mathbf{ph} + \mathbf{hp}) + \tfrac{\nu_2}{2}(\mathbf{p}\nabla\mu + \nabla\mu\mathbf{p}) \\
&\quad + \zeta\hat{\mu}\mathbf{pp} + \zeta_0\hat{\mu}\mathbf{Q} + \beta_1\hat{\mu}(\nabla\mathbf{p} + \nabla\mathbf{p}^T) + \beta_2\hat{\mu}\mathbf{p}\cdot\nabla\mathbf{Q} + \beta_3\hat{\mu}\nabla^2\mathbf{Q},
\end{aligned}
$$

where $\Pi = -(\bar{\eta} - \tfrac{2}{3}\eta)D_{\gamma\gamma} - \tfrac{aQ_{kl}G_{kl}}{3} + \theta_1 G_{\gamma\gamma} + \theta_2 p_\gamma h_\gamma - \theta_3 p_\gamma\partial_\gamma\mu + (\zeta_2 + \zeta_3 p_\gamma p_\gamma)\hat{\mu}$ is the pressure. If we assume the total density $\rho = \rho_0$ is constant, that means the fluid is incompressible, $\nabla\cdot\mathbf{v} = 0$, $D_{\gamma\gamma} = 0$. Then we can drop the parameters $\theta_i, i = 1, 2, 3$ and Π is the hydrostatic pressure. The boundary conditions are given by Equation (38).

All the terms related to $\hat{\mu}$ are active energy contributions in the system. If the active energy is removed from the system, the system is reduced to the traditional passive liquid crystal system, and our model recovers the usual liquid crystal hydrodynamics model [5,51,52].

3. Hydrodynamic Model for Apolar Active Liquid Crystal Systems

For the apolar system, we assume the polar vector $\mathbf{p} = \mathbf{0}$ and only consider the tensor order parameter $\mathbf{Q}$ and concentration c. Then, the model reduces to the following.

$$\partial_t c + \nabla \cdot (\mathbf{v}c) = \nabla \cdot (\gamma \nabla \mu),$$

$$\partial_t \mathbf{Q} + \mathbf{v} \cdot \nabla \mathbf{Q} + \Omega \cdot \mathbf{Q} - \mathbf{Q} \cdot \Omega - a[\mathbf{Q} \cdot \mathbf{D} + \mathbf{D} \cdot \mathbf{Q}] = \frac{1}{\gamma_2}\mathbf{G} + \nu_0 \mathbf{D} - a(\mathbf{Q} : \mathbf{D})(\mathbf{Q} + \frac{\mathbf{I}}{3}) + \zeta_2 \hat{\mu} \mathbf{Q},$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0,$$

$$\partial_t(\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v}\mathbf{v}) = \nabla \cdot (\sigma^s + \sigma^e + \sigma^a), \tag{48}$$

$$\sigma^e_{\alpha\beta} = (f - c\mu)\delta_{\alpha\beta} - \frac{\partial f}{\partial(\partial_\beta c)}\partial_\alpha c - \frac{\partial f}{\partial(\partial_\beta Q_{\gamma\theta})}\partial_\alpha Q_{\gamma\theta}, \quad \nabla \cdot \sigma^e = -(c\nabla\mu + \nabla\mathbf{Q} : \mathbf{G}),$$

$$\sigma^a = (\mathbf{Q} \cdot \mathbf{G} - \mathbf{G} \cdot \mathbf{Q}),$$

$$\sigma^s = -\Pi\mathbf{I} + 2\eta\mathbf{D} + \alpha_1(\mathbf{Q} \cdot \mathbf{D} + \mathbf{D} \cdot \mathbf{Q}) + \alpha_2(\mathbf{Q} : \mathbf{D})\mathbf{Q}$$
$$-a(\mathbf{Q} \cdot \mathbf{G} + \mathbf{G} \cdot \mathbf{Q}) - \nu_0\mathbf{G} + a(\mathbf{Q} : \mathbf{G})\mathbf{Q} + \zeta_0\hat{\mu}\mathbf{Q} + \beta_3\hat{\mu}\nabla^2\mathbf{Q}.$$

where $\Pi = -\frac{aQ_{kl}G_{kl}}{3} + \zeta_2\hat{\mu}$.

The free energy functional is given by [1]

$$F = \int_{\mathbf{r}}\{\frac{\alpha(c)}{2}\mathbf{Q} : \mathbf{Q} + \frac{\beta(c)}{3}tr(\mathbf{Q}^3) + \frac{\gamma(c)}{4}(\mathbf{Q} : \mathbf{Q})^2 + \frac{K(c)}{2}(\nabla\mathbf{Q} \vdots \nabla\mathbf{Q}) + \frac{L(c)}{2}\|\nabla \cdot \mathbf{Q}\|^2 +$$

$$C(c)\mathbf{Q} : \nabla\nabla\frac{\delta c}{c_0} + \frac{A(c)}{2}(\frac{\delta c}{c_0})^2 + \frac{B(c)}{2}\|\nabla c\|^2\}. \tag{49}$$

The system is nematic at equilibrium if $\alpha < 0$ and $\gamma > 0$. K is the Frank elasticity coefficient, the C term is the bilinear coupling of $\mathbf{Q}$ and c. A is the compression modulus of density fluctuations $\delta c = c - c_0$. We can generalize $\frac{A(c)}{2}\delta c^2$ into a function of c: $h(c)$.

The conjugate fields are given by

$$\mu = \frac{\delta F}{\delta c} = \frac{\alpha'(c)}{2}\mathbf{Q} : \mathbf{Q} + \frac{\beta'(c)}{3}tr(\mathbf{Q}^3) + \frac{\gamma'(c)}{4}(\mathbf{Q} : \mathbf{Q})^2 + \frac{K'(c)}{2}(\nabla\mathbf{Q}\vdots\nabla\mathbf{Q}) + \frac{L'(c)}{2}\|\nabla \cdot \mathbf{Q}\|^2 + C'(c)\mathbf{Q} : \nabla\nabla\frac{\delta c}{c_0} +$$

$$\frac{A'(c)}{2}(\frac{\delta c}{c_0})^2 + \frac{B'(c)}{2}\|\nabla c\|^2 + \frac{C}{c_0}\nabla\nabla : \mathbf{Q} + \frac{A\delta c}{c_0^2} - \nabla \cdot (B\nabla c),$$

$$G_{\alpha\beta} = -\frac{\delta F}{\delta\mathbf{Q}_{\alpha\beta}} = -[\alpha\mathbf{Q} + \beta(\mathbf{Q}^2 - \mathbf{Q} : \mathbf{Q}\frac{\mathbf{I}}{3}) + \gamma\mathbf{Q} : \mathbf{Q}\mathbf{Q} - \nabla \cdot (K\nabla\mathbf{Q}) - (\frac{1}{2}\nabla_\alpha(L\nabla_i Q_{i\beta}) + \frac{1}{2}\nabla_\beta(L\nabla_i Q_{i\alpha}) - \tag{50}$$

$$\frac{\nabla_\alpha(L\nabla_i \mathbf{Q}_{i\alpha})}{3}\mathbf{I}) + \frac{C}{c_0}(\nabla\nabla c - tr(\nabla\nabla c)\frac{\mathbf{I}}{3})].$$

4. Hydrodynamic Model for Free Surface Flows of Active Matter Systems

4.1. Models for Passive Liquid Crystals

We first consider a mixture of *passive liquid crystals* in which a free surface separates the liquid crystal from the other fluids. We denote the total energy of the liquid crystal system in a given material domain V by

$$E = \int_V [\frac{\rho}{2}\|\mathbf{v}\|^2 + f(c, \nabla c, \mathbf{p}, \nabla\mathbf{p}, \mathbf{Q}, \nabla\mathbf{Q})]d\mathbf{x} + \int_\Gamma [\frac{\rho_s}{2}\|\mathbf{v}\|^2 + g(c_s, \nabla_s c_s, \mathbf{p}_s, \nabla_s \mathbf{p}_s, \mathbf{Q}_s, \nabla_s \mathbf{Q}_s)]ds, \quad (51)$$

where f is the bulk free energy density, g is the "excessive" [53,54] surface free energy density at a material interface Γ within domain V, defined by $\Phi(\mathbf{x}, t) = 0$, ρ_s is the surface excessive mass density, c_s is the surface excessive active liquid crystal concentration, $\mathbf{p}_s$ and $\mathbf{Q}_s$ are the polarity vector and nematic tensor on the surface, and $\nabla_s = \mathbf{I}_s \cdot \nabla$ is the surface gradient operator, where $\mathbf{I}_s = \mathbf{I} - \mathbf{nn}$, $\mathbf{n}$ is the unit normal of the interfacial surface, given by $\mathbf{n} = \frac{\nabla \Phi}{\|\nabla \Phi\|}$. Here, we assume the excessive free energy density g on the free surface depends on the gradients of the order parameters as well. We assume the velocity across the interface is continuous so that

$$(\partial_t + \mathbf{v} \cdot \nabla)\Phi = 0. \tag{52}$$

The bulk conservation laws are the mass, active species and momentum conservation:

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{v}) = 0,$$

$$\partial_t (\rho \mathbf{v}) = \nabla \cdot (\sigma - \rho \mathbf{vv}) + \mathbf{F}_e, \tag{53}$$

$$\partial_t c + \nabla \cdot (c\mathbf{v} + \mathbf{j}) = 0,$$

where σ is the bulk stress tensor, $\mathbf{F}_e$ is the bulk elastic force and $\mathbf{j}$ is the diffusive flux for the liquid crystal.

The surface conservation laws are surface excessive mass, active species conservation and surface momentum conservation:

$$\partial_t \rho_s + \nabla_s \cdot (\rho_s \mathbf{v}) = 0,$$

$$\partial_t (\rho_s \mathbf{v}) = \nabla_s \cdot (\sigma_s - \rho_s \mathbf{vv}) + \mathbf{F}_s, \tag{54}$$

$$\partial_t c_s + \nabla_s \cdot (c_s \mathbf{v} + \mathbf{j}_s) = j_c,$$

where σ_s is the excessive surface stress, $\mathbf{F}_s$ is the excessive surface elastic force and $\mathbf{j}_s$ is the excessive surface diffusive flux for liquid crystals. We note that $\mathbf{v}(\mathbf{x}, t)|_{\Gamma} = \mathbf{v}(\mathbf{x}_s, t)$ because the surface is a material surface. We assume $\mathbf{v}|_{\partial V} = 0$ in the following derivation and define

$$\Omega_s = \tfrac{1}{2}[\nabla_s \mathbf{v} \cdot \mathbf{I}_s - \mathbf{I}_s \cdot \nabla_s \mathbf{v}^T], \quad \mathbf{D}_s = \tfrac{1}{2}[\nabla_s \mathbf{v} \cdot \mathbf{I}_s + \mathbf{I}_s \cdot (\nabla_s \mathbf{v})^T]. \tag{55}$$

We define the invariant derivatives on the surface as follows

$$\tfrac{d_s}{dt} c_s = \partial_t c_s + \mathbf{v} \cdot \nabla_s c_s,$$

$$\tilde{\mathbf{p}}_s = \partial_t \mathbf{p}_s + \mathbf{v} \cdot \nabla_s \mathbf{p}_s + \Omega_s \cdot \mathbf{p}_s, \tag{56}$$

$$\hat{\mathbf{Q}}_s = \partial_t \mathbf{Q}_s + \mathbf{v} \cdot \nabla_s \mathbf{Q}_s + \Omega_s \cdot \mathbf{Q}_s \cdot \mathbf{I}_s - \mathbf{I}_s \cdot \mathbf{Q}_s \cdot \Omega_s.$$

In the following, we give a simple proof for the invariant derivative: $\tilde{\mathbf{p}}_s$. If both the background moving surface and the director $\mathbf{p}_s$ on the surface rotate around the normal $\mathbf{n}$ at the same angular velocity θ. Then the surface velocity $\mathbf{v}_s = \mathbf{I}_s \cdot (\theta \times \mathbf{r})$, and $\Omega_s \cdot \mathbf{p}_s = -\mathbf{I}_s \cdot (\theta \times \mathbf{p}_s)$. At time t,

the director at location $\mathbf{r}$ is $\mathbf{p}_s(\mathbf{r}, t)$. After a small time Δt, at time $t + \Delta t$, the director at the location $\mathbf{r} + \mathbf{I}_s \cdot (\theta \times \mathbf{r})\Delta t$ is $\mathbf{p}_s(\mathbf{r} + \mathbf{I}_s \cdot (\theta \times \mathbf{r})\Delta t, t + \Delta t) = \mathbf{p}_s(\mathbf{r}, t) + \mathbf{I}_s \cdot (\theta \times \mathbf{p}_s(\mathbf{r}, t))\Delta t + O(\Delta t^2)$,

$$
\begin{aligned}
\frac{\partial \mathbf{p}_s}{\partial t} &= \lim_{\Delta t \to 0} \frac{\mathbf{p}_s(\mathbf{r}, t+\Delta t) - \mathbf{p}_s(\mathbf{r}, t)}{\Delta t} \\[2mm]
&= \lim_{\Delta t \to 0} \frac{\mathbf{p}_s(\mathbf{r}, t+\Delta t) - \mathbf{p}_s(\mathbf{r} + \mathbf{I}_s \cdot (\theta \times \mathbf{r})\Delta t, t+\Delta t) + \mathbf{p}_s(\mathbf{r} + \mathbf{I}_s \cdot (\theta \times \mathbf{r})\Delta t, t+\Delta t) - \mathbf{p}_s(\mathbf{r}, t)}{\Delta t} \\[2mm]
&= \lim_{\Delta t \to 0} \frac{-\mathbf{I}_s \cdot (\theta \times \mathbf{r}) \cdot \nabla \mathbf{p}_s(\mathbf{r} + \mathbf{I}_s \cdot (\theta \times \mathbf{r}) a \Delta t, t+\Delta t)\Delta t + \mathbf{I}_s \cdot (\theta \times \mathbf{p}_s(\mathbf{r}, t))\Delta t}{\Delta t}, \qquad a \in (0,1) \\[2mm]
&= -\mathbf{I}_s \cdot (\theta \times \mathbf{r}) \cdot \nabla \mathbf{p}_s(\mathbf{r}, t) + \mathbf{I}_s \cdot (\theta \times \mathbf{p}_s) \\[2mm]
&= -\mathbf{v} \cdot \nabla_s \mathbf{p}_s - \Omega_s \cdot \mathbf{p}_s.
\end{aligned}
\tag{57}
$$

So, $\tilde{\mathbf{p}}_s = \partial_t \mathbf{p}_s + \mathbf{v} \cdot \nabla_s \mathbf{p}_s + \Omega_s \cdot \mathbf{p}_s = 0$ under a pure rotation on the tangent plane, which is equivalent to say that $\tilde{\mathbf{p}}_s$ is an invariant derivative. For tensor $\mathbf{Q}_s$, we can show its rotational invariance in the tangent plane analogously using its definition.

Then the energy dissipation rate is calculated as follows.

$$
\begin{aligned}
\frac{dE}{dt} =& \int_V [-(\nabla \mathbf{v})^T : (\sigma) + \mathbf{v} \cdot \mathbf{F}_e + \frac{\delta f}{\delta c}\frac{\partial c}{\partial t} + \frac{\delta f}{\delta \mathbf{p}} \cdot \frac{\partial \mathbf{p}}{\partial t} + \frac{\delta f}{\delta \mathbf{Q}} : \frac{\partial \mathbf{Q}}{\partial t} + \nabla \cdot (\mathbf{v} f)] d\mathbf{x} + \\[2mm]
& \int_\Gamma [[\frac{\partial f}{\partial \nabla_i \mathbf{p}_j} \partial_t \mathbf{p}_j n_i + \frac{\partial f}{\partial \nabla_i \mathbf{Q}_{jk}} \partial_t \mathbf{Q}_{jk} n_i + \frac{\partial f}{\partial \nabla_i c} \partial_t c n_i + \mathbf{v} n : \sigma]] ds + \\[2mm]
& \int_\Gamma [\frac{\partial g}{\partial c_s} \partial_t c_s + \frac{\partial g}{\partial \mathbf{p}_s} \cdot \partial_t \mathbf{p}_s + \frac{\partial g}{\partial \mathbf{Q}_s} : \partial_t \mathbf{Q}_s + \frac{\partial g}{\partial \nabla_s c_s} \cdot \partial_t (\nabla_s c_s) + \frac{\partial g}{\partial \nabla_s \mathbf{p}_s} : \partial_t (\nabla_s \mathbf{p}_s) + \frac{\partial g}{\partial \nabla_s \mathbf{Q}_s} \vdots \partial_t (\nabla_s \mathbf{Q}_s) + \nabla_s \cdot (\mathbf{v} g)] ds + \\[2mm]
& \int_\Gamma [\mathbf{v} \cdot (\nabla_s \cdot \sigma_s + \mathbf{F}_s)] ds \\[4mm]
=& \int_V [-(\nabla \mathbf{v})^T : (\sigma - \sigma^a - \sigma^e) + \mathbf{v} \cdot \mathbf{F}_e + \mathbf{j} \cdot \nabla \mu - \mathbf{h} \cdot \dot{\mathbf{p}} - \mathbf{G} : \overset{\square}{\mathbf{Q}}] d\mathbf{x} + \\[2mm]
& \int_\Gamma [[\frac{\partial f}{\partial \nabla_i \mathbf{p}_j} \partial_t \mathbf{p}_j n_i + \frac{\partial f}{\partial \nabla_i \mathbf{Q}_{jk}} \partial_t \mathbf{Q}_{jk} n_i + \frac{\partial f}{\partial \nabla_i c} \partial_t c n_i + \mathbf{v} n : \sigma - \mu(c v_i + \mathbf{j}_i) n_i - v_i \sigma^e_{ij} n_j + f v_i n_i]] ds + \\[2mm]
& \int_\Gamma [\frac{\partial g}{\partial c_s}\frac{d_s c_s}{dt} + \frac{\partial g}{\partial \mathbf{p}_s} \cdot \frac{d_s \mathbf{p}_s}{dt} + \frac{\partial g}{\partial \mathbf{Q}_s} : \frac{d_s \mathbf{Q}_s}{dt} + \frac{\partial g}{\partial \nabla_s c_s} \cdot \partial_t (\nabla_s c_s) + \frac{\partial g}{\partial \nabla_s \mathbf{p}_s} : \partial_t (\nabla_s \mathbf{p}_s) + \frac{\partial g}{\partial \nabla_s \mathbf{Q}_s} \vdots \partial_t (\nabla_s \mathbf{Q}_s) + \frac{\partial g}{\partial \nabla_s c_s} \cdot \mathbf{v} \cdot \nabla_s (\nabla_s c_s) + \\[2mm]
& \frac{\partial g}{\partial \nabla_s \mathbf{p}_s} : (\mathbf{v} \cdot \nabla_s)(\nabla_s \mathbf{p}_s) + \frac{\partial g}{\partial \nabla_s \mathbf{Q}_s} \vdots (\mathbf{v} \cdot \nabla_s)(\nabla_s \mathbf{Q}_s) + g \nabla_s \cdot \mathbf{v} + \nabla_s \cdot (\mathbf{v} \cdot \sigma_s)] ds + \int_\Gamma [(\nabla_s \mathbf{v})^T : (-\sigma_s) + \mathbf{v} \cdot \mathbf{F}_s] ds.
\end{aligned}
\tag{58}
$$

Here, the notation $[[\cdot]]$ denotes the jump of the variable $\{\cdot\}$ across the free surface. For simplicity, we assume the surface energy is short-ranged: $g = g(c_s, \mathbf{p}_s, \mathbf{Q}_s)$,

$$
\begin{aligned}
\frac{dE}{dt} =& \int_V [-(\nabla \mathbf{v})^T : (\sigma - \sigma^a - \sigma^e) + \mathbf{v} \cdot \mathbf{F}_e + \mathbf{j} \cdot \nabla \mu - \mathbf{h} \cdot \dot{\mathbf{p}} - \mathbf{G} : \overset{\square}{\mathbf{Q}}] d\mathbf{x} + \\[2mm]
& \int_\Gamma [[\frac{\partial f}{\partial \nabla_i c} \partial_t c n_i + \frac{\partial f}{\partial \nabla_i \mathbf{p}_j} \partial_t \mathbf{p}_j n_i + \frac{\partial f}{\partial \nabla_i \mathbf{Q}_{jk}} \partial_t \mathbf{Q}_{jk} n_i + \mathbf{v} n : \sigma - \mu(c v_i + \mathbf{j}_i) n_i - v_i \sigma^e_{ij} n_j + f v_i n_i]] ds + \\[2mm]
& \int_\Gamma [\frac{\partial g}{\partial c_s}\frac{d_s c_s}{dt} + \frac{\partial g}{\partial \mathbf{p}_s} \cdot \tilde{\mathbf{p}}_s + \frac{\partial g}{\partial \mathbf{Q}_s} : \hat{\mathbf{Q}}_s - \frac{\partial g}{\partial \mathbf{p}_s} \cdot (\Omega_s \cdot \mathbf{p}_s) - \frac{\partial g}{\partial \mathbf{Q}_s} : (\Omega_s \cdot \mathbf{Q}_s \cdot \mathbf{I}_s - \mathbf{I}_s \cdot \mathbf{Q}_s \cdot \Omega_s) + g \nabla_s \cdot \mathbf{v} + \nabla_s \cdot (\mathbf{v} \cdot \sigma_s)] ds + \\[2mm]
& \int_\Gamma [(\nabla_s \mathbf{v})^T : (-\sigma_s) + \mathbf{v} \cdot \mathbf{F}_s] ds.
\end{aligned}
\tag{59}
$$

We note that the one-sided limit of the internal variables, assuming they are defined globally, can be related to the surface value via the adsorption coefficients as follows:

$$c_\pm|_\Gamma = K_{c,\pm}c_s,$$

$$\mathbf{p}_\pm|_\Gamma = K_{p,\pm}\mathbf{p}_s, \tag{60}$$

$$\mathbf{Q}_\pm|_\Gamma = K_{Q,\pm}\mathbf{Q}_s,$$

where $K_{i,\pm}, i = c, p, Q$ are the adsorption coefficients from the $+$ and $-$ side of the surface. In the following, we consider one side $(-)$ of the surface as an isotropic viscous fluid where $K_{i,-} = 0$, we only need one absorption coefficient, that is $K_{i,+} = K_i$. Hence, we drop the subscript $\pm$ on the $K's$. These define the relations between the internal variables on the surface and the ones in the bulk. With these assumptions, the energy dissipation reduces to

$$\frac{dE}{dt} = \int_V [-(\nabla\mathbf{v})^T : (\sigma - \sigma^a - \sigma^e) + \mathbf{v}\cdot\mathbf{F}_e + \mathbf{j}\cdot\nabla\mu - \mathbf{h}\cdot\dot{\mathbf{p}} - \mathbf{G} : \overset{\square}{\mathbf{Q}}]d\mathbf{x}+$$

$$\int_\Gamma[[\mathbf{vn} : (\sigma - \sigma^e) - \mu(c\mathbf{v}+\mathbf{j})\cdot\mathbf{n} - \mathbf{n}\cdot\frac{\partial f}{\partial\nabla\mathbf{p}}\cdot(\mathbf{v}\cdot\nabla_s)\mathbf{p} - \mathbf{n}\cdot\frac{\partial f}{\partial\nabla\mathbf{Q}} : (\mathbf{v}\cdot\nabla_s)\mathbf{Q} - \mathbf{n}\cdot\frac{\partial f}{\partial\nabla c}(\mathbf{v}\cdot\nabla_s)c + f\mathbf{v}\cdot\mathbf{n}]]ds+$$

$$\int_\Gamma[(\frac{\partial g}{\partial c_s} + K_c\mathbf{n}\cdot\frac{\partial f}{\partial\nabla c})\frac{d_s c_s}{dt} + (\frac{\partial g}{\partial\mathbf{p}_s} + K_p\mathbf{n}\cdot\frac{\partial f}{\partial\nabla\mathbf{p}})\cdot\tilde{\mathbf{p}}_s + (\frac{\partial g}{\partial\mathbf{Q}_s} + K_Q\mathbf{n}\cdot\frac{\partial f}{\partial\nabla\mathbf{Q}}) : \hat{\mathbf{Q}}_s - (\frac{\partial g}{\partial\mathbf{p}_s} + K_p\mathbf{n}\cdot\frac{\partial f}{\partial\nabla\mathbf{p}})\cdot(\Omega_s\cdot\mathbf{p}_s)-$$

$$(\frac{\partial g}{\partial\mathbf{Q}_s} + K_Q\mathbf{n}\cdot\frac{\partial f}{\partial\nabla\mathbf{Q}}) : (\Omega_s\cdot\mathbf{Q}_s\cdot\mathbf{I}_s - \mathbf{I}_s\cdot\mathbf{Q}_s\cdot\Omega_s) + g\nabla_s\cdot\mathbf{v} + \nabla_s\cdot(\mathbf{v}\cdot\sigma_s)]ds + \int_\Gamma[(\nabla_s\mathbf{v})^T : (-\sigma_s) + \mathbf{v}\cdot\mathbf{F}_s]ds. \tag{61}$$

It follows from the transport equation for c_s that $\frac{d_s c_s}{dt} = -\nabla_s\cdot\mathbf{v}c_s - \nabla_s\cdot\mathbf{j}_s + j_c$, where j_c is an excessive surface density growth rate. The energy dissipation reduces to

$$\frac{dE}{dt} = \int_V [-(\nabla\mathbf{v})^T : (\sigma - \sigma^a - \sigma^e) + \mathbf{v}\cdot\mathbf{F}_e + \mathbf{j}\cdot\nabla\mu - \mathbf{h}\cdot\dot{\mathbf{p}} - \mathbf{G} : \overset{\square}{\mathbf{Q}}]d\mathbf{x}+$$

$$\int_\Gamma[[\mathbf{vn} : (\sigma - \sigma^e) - \mu(c\mathbf{v}+\mathbf{j})\cdot\mathbf{n} - \mathbf{n}\cdot\frac{\partial f}{\partial\nabla\mathbf{p}}\cdot(\mathbf{v}\cdot\nabla_s)\mathbf{p} - \mathbf{n}\cdot\frac{\partial f}{\partial\nabla\mathbf{Q}} : (\mathbf{v}\cdot\nabla_s)\mathbf{Q} - \mathbf{n}\cdot\frac{\partial f}{\partial\nabla c}(\mathbf{v}\cdot\nabla_s)c + f\mathbf{v}\cdot\mathbf{n}]]ds+$$

$$\int_\Gamma[-(\frac{\partial g}{\partial c_s} + K_c\mathbf{n}\cdot\frac{\partial f}{\partial\nabla c})(\nabla_s\cdot\mathbf{v}c_s + \nabla_s\cdot(\mathbf{I}_s\cdot\mathbf{j}_s) - j_c) + (\frac{\partial g}{\partial\mathbf{p}_s} + K_p\mathbf{n}\cdot\frac{\partial f}{\partial\nabla\mathbf{p}})\cdot\tilde{\mathbf{p}}_s + (\frac{\partial g}{\partial\mathbf{Q}_s} + K_Q\mathbf{n}\cdot\frac{\partial f}{\partial\nabla\mathbf{Q}}) : \hat{\mathbf{Q}}_s - \tag{62}$$

$$(\frac{\partial g}{\partial\mathbf{p}_s} + K_p\mathbf{n}\cdot\frac{\partial f}{\partial\nabla\mathbf{p}})\cdot(\Omega_s\cdot\mathbf{p}_s) - (\frac{\partial g}{\partial\mathbf{Q}_s} + K_Q\mathbf{n}\cdot\frac{\partial f}{\partial\nabla\mathbf{Q}}) : (\Omega_s\cdot\mathbf{Q}_s\cdot\mathbf{I}_s - \mathbf{I}_s\cdot\mathbf{Q}_s\cdot\Omega_s) + g\nabla_s\cdot\mathbf{v} + \nabla_s\cdot(\mathbf{v}\cdot\sigma_s)]ds+$$

$$\int_\Gamma[(\nabla_s\mathbf{v})^T : (-\sigma_s) + \mathbf{v}\cdot\mathbf{F}_s]ds,$$

where we have used the assumption $\mathbf{j}_s = \mathbf{I}_s\cdot\mathbf{j}_s$. The integral term consists of

$$\int_\Gamma \nabla_s\cdot(\mathbf{v}\cdot\sigma_s)ds = \int_\Gamma(\nabla_s\cdot(\mathbf{I}_s\cdot\mathbf{v}\cdot\sigma_s) - 2\kappa\mathbf{v}\cdot\sigma_s\cdot\mathbf{n})ds = \int_{\partial\Gamma}\mathbf{v}\cdot\sigma_s\cdot\mathbf{dL} + \int_\Gamma -2\kappa\mathbf{v}\cdot\sigma_s\cdot\mathbf{n}ds, \tag{63}$$

where $\kappa = \frac{1}{2}(\kappa_1 + \kappa_2)$ is the mean surface curvature, κ_1, κ_2 are the principal curvatures of the surface. The first term is assumed 0 because if $\partial\Gamma \in \partial V$ it is true automatically, otherwise, Γ is a closed surface so that $\partial\Gamma = \{\phi\}$. Then, the second term is added to $\mathbf{F}_s$.

From Equation (62), we define $\mu_s = \frac{\partial g}{\partial c_s} + K_c \mathbf{n} \cdot \frac{\partial f}{\partial \nabla c}$, $\mathbf{h}_s = -(\frac{\partial g}{\partial \mathbf{p}_s} + K_p \mathbf{n} \cdot \frac{\partial f}{\partial \nabla \mathbf{p}})$, $\mathbf{G}_s = -(\frac{\partial g}{\partial \mathbf{Q}_s} + K_Q \mathbf{n} \cdot \frac{\partial f}{\partial \nabla \mathbf{Q}})$, which are the chemical potential, molecular field and the corresponding variation field to $\mathbf{Q}_s$ on the surface. We then define the following

$$\sigma^s = \sigma - \sigma^a - \sigma^e,$$

$$\sigma_s^s = \sigma_s - (g - c_s \mu_s)\mathbf{I}_s - \tfrac{1}{2}\mathbf{I}_s \cdot (\mathbf{p}_s \mathbf{h}_s - \mathbf{h}_s \mathbf{p}_s) - (\mathbf{I}_s \cdot \mathbf{Q}_s \cdot \mathbf{I}_s \cdot \mathbf{G}_s - \mathbf{I}_s \cdot \mathbf{G}_s \cdot \mathbf{I}_s \cdot \mathbf{Q}_s),$$

$$\mathbf{F}_s + [[(\sigma - \sigma^e)]] \cdot \mathbf{n} + [[f - \mu c]]\mathbf{n} - K_c(\mathbf{n} \cdot \tfrac{\partial f}{\partial \nabla c})\nabla_s c_s - K_p \nabla_s \mathbf{p}_s \cdot (\mathbf{n} \cdot \tfrac{\partial f}{\partial \nabla \mathbf{p}}) -$$

$$K_Q \nabla_s \mathbf{Q}_s : (\mathbf{n} \cdot \tfrac{\partial f}{\partial \nabla \mathbf{Q}}) - 2\kappa \sigma_s \cdot \mathbf{n} = 0,$$

$$-[[\mu \mathbf{j}]] \cdot \mathbf{n} + j_c \mu_s \leq 0,$$

$$\mathbf{F}_e = 0.$$

(64)

The energy dissipation reduces to

$$\tfrac{dE}{dt} \leq \int_V [-(\nabla \mathbf{v})^T : \sigma^s + \mathbf{j} \cdot \nabla \mu - \mathbf{h} \cdot \dot{\mathbf{p}} - \mathbf{G} : \overset{\square}{\mathbf{Q}}]d\mathbf{x} + \int_\Gamma [-(\nabla_s \mathbf{v})^T : \sigma_s^s + \mathbf{j}_s \cdot \nabla_s \mu_s - \mathbf{h}_s \cdot \tilde{\mathbf{p}}_s - \mathbf{G}_s : \hat{\mathbf{Q}}_s]ds. \quad (65)$$

Here we drop the term $\int_\Gamma \nabla_s \cdot (\mathbf{I}_s \cdot \mathbf{j}_s \mu_s)ds$, which is a line integral assumed to be 0. This formulation allows us to apply the generalized Onsager principle to obtain the constitutive relations. Since the passive liquid crystal system is a special limit of the more general active liquid crystal system, we will focus on the constitutive equations for the active liquid crystal.

4.2. Models for Active Liquid Crystals

For active liquid crystals, we need to add the active energy contribution $r\hat{\mu}$ to the total free energy functional. Namely,

$$\tfrac{dE}{dt} \leq \int_V [-(\nabla \mathbf{v})^T : \sigma^s + \mathbf{j} \cdot \nabla \mu - \mathbf{h} \cdot \dot{\mathbf{p}} - \mathbf{G} : \overset{\square}{\mathbf{Q}} - r\hat{\mu}]d\mathbf{x} +$$
$$\int_\Gamma [-(\nabla_s \mathbf{v})^T : \sigma_s^s + \mathbf{j}_s \cdot \nabla_s \mu_s - \mathbf{h}_s \cdot \tilde{\mathbf{p}}_s - \mathbf{G}_s : \hat{\mathbf{Q}}_s - r_s \hat{\mu}_s]ds, \quad (66)$$

where r is the active energy consumption rate and $\hat{\mu}$ is the active energy potential in the bulk, r_s and $\hat{\mu}_s$ are the corresponding quantities on the moving interface. In the bulk, we have proved that σ^s is symmetry (see Appendix A), so that

$$(\nabla \mathbf{v})^T : \sigma^s = \mathbf{D} : \sigma^s. \quad (67)$$

On the surface, we assume that $\sigma_s^s = \mathbf{I}_s \cdot \sigma_s^s \cdot \mathbf{I}_s$ and it is symmetry, such that

$$(\nabla_s \mathbf{v})^T : \sigma_s^s = \mathbf{D}_s : \sigma_s^s. \quad (68)$$

Then, we can apply the generalized Onsager principle to arrive at the constitutive relations. We denote the generalized flux as $\mathcal{F} = (\sigma^s, \overset{\square}{\mathbf{Q}}, \dot{\mathbf{p}}, \mathbf{j}, r, \sigma_s^s, \hat{\mathbf{Q}}_s, \tilde{\mathbf{p}}_s, \mathbf{j}_s, r_s)$ and the generalized force as $\mathcal{U} = (\mathbf{D}, \mathbf{G}, \mathbf{h}, -\nabla \mu, \hat{\mu}, \mathbf{D}_s, \mathbf{G}_s, \mathbf{h}_s, -\nabla_s \mu_s, \hat{\mu}_s)$. We find that the bulk free energy also gives a contribution to the surface generalized forces in $\mathbf{G}_s, \mathbf{h}_s, -\nabla_s \mu_s$. The generalized Onsager principle states that

$$\mathcal{F} = (D_{sym} + D_{anti}) \cdot \mathcal{U}, \quad (69)$$

where

$$D_{sym} = \begin{pmatrix} D^b_{sym} & \mathbf{0} \\ \mathbf{0} & D^s_{sym} \end{pmatrix},$$

$$D_{anti} = \begin{pmatrix} D^b_{anti} & \mathbf{0} \\ \mathbf{0} & D^s_{anti} \end{pmatrix},$$

(70)

D^b_{sym}, D^s_{sym} are 5×5 symmetric matrices and D^b_{anti}, D^s_{anti} are 5×5 antisymmetric matrices, respectively. We use subscripts $\alpha\beta$ for tensors and α for vectors in $\mathcal{F}$ and use subscripts kl for tensors and k for vectors in $\mathcal{U}$. Then, the corresponding coefficients can be written as follows. First, the coefficients in the bulk are given by

$$D^b_{sym} = \begin{pmatrix} A_0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{\gamma_2}\delta_{\alpha k}\delta_{\beta l} & \frac{\chi_1}{2}A_{\alpha\beta k} & \frac{\chi_2}{2}A_{\alpha\beta k} & A_{5,\alpha\beta} \\ 0 & \frac{\chi_1}{2}A^T_{\alpha kl} & \frac{1}{\gamma_1}\delta_{\alpha k} & \lambda\delta_{\alpha k} & B_\alpha \\ 0 & \frac{\chi_2}{2}A^T_{\alpha kl} & \lambda\delta_{\alpha k} & \gamma\delta_{\alpha k} & (\kappa + \omega_0 c)p_\alpha \\ 0 & A_{5,kl} & B_k & (\kappa + \omega_0 c)p_k & \Lambda \end{pmatrix},$$

(71)

$$D^b_{anti} = \begin{pmatrix} 0 & -A_1 & -A_2 & -A_3 & A_4 \\ A_1 & 0 & 0 & 0 & 0 \\ A'_2 & 0 & 0 & 0 & 0 \\ A'_3 & 0 & 0 & 0 & 0 \\ -A'_4 & 0 & 0 & 0 & 0 \end{pmatrix},$$

where

$$A_{\alpha\beta k} = (p_\alpha\delta_{\beta k} + p_\beta\delta_{\alpha k}) - \frac{2}{3}\delta_{\alpha\beta}p_l\delta_{lk},$$
$$A^T_{\alpha kl} = 2(p_\beta\delta_{\alpha k}\delta_{\beta l} - \frac{p_\beta}{3}\delta_{\alpha\beta}\delta_{kl}),$$
$$A_0 = 2\eta\delta_{\alpha k}\delta_{\beta l} + (\bar{\eta} - \frac{2}{3}\eta)\delta_{\alpha\beta}\delta_{kl} + \alpha_1(Q_{\alpha k}\delta_{\beta l} + \delta_{\alpha k}Q_{\beta l})$$
$$+\alpha_2 Q_{kl}Q_{\alpha\beta} + \alpha_3(p_\alpha p_k\delta_{\beta l} + \delta_{\alpha k}p_\beta p_l) + \alpha_4 p_k p_l p_\alpha p_\beta,$$
$$B_\alpha = \lambda_1 p_\alpha - \omega\mathbf{p}\cdot\nabla p_\alpha - \omega p_\alpha\nabla\cdot\mathbf{p},$$
$$A_1 = \nu_0\delta_{\alpha k}\delta_{\beta l} + a[Q_{\alpha k}\delta_{\beta l} + \delta_{\alpha k}Q_{\beta l}] - a(Q_{kl}(Q_{\alpha\beta} + \frac{1}{3}\delta_{\alpha\beta})) + \theta_1\delta_{kl}\delta_{\alpha\beta},$$
$$A_2 = \frac{\nu_1}{2}(p_\beta\delta_{\alpha k} + p_\alpha\delta_{\beta k}) + \theta_2 p_k\delta_{\alpha\beta},$$
$$A'_2 = \nu_1 p_\beta\delta_{\alpha k}\delta_{\beta l} + \theta_2 p_\alpha\delta_{kl},$$
$$A_3 = \frac{\nu_2}{2}(p_\beta\delta_{\alpha k} + p_\alpha\delta_{\beta k}) + \theta_3 p_k\delta_{\alpha\beta},$$
$$A'_3 = \nu_2 p_\beta\delta_{\alpha k}\delta_{\beta l} + \theta_3 p_\alpha\delta_{kl},$$
$$A_4 = \zeta p_\alpha p_\beta + \zeta_0 Q_{\alpha\beta} + \beta_1(\partial_\alpha p_\beta + \partial_\beta p_\alpha) + \beta_2\mathbf{p}\cdot\nabla Q_{\alpha\beta} + \beta_3\nabla^2 Q_{\alpha\beta} - (\zeta_2 + \zeta_3 p_\alpha p_\alpha)\delta_{\alpha\beta},$$
$$A'_4 = A_4\delta_{\alpha k}\delta_{\beta l},$$
$$A_5 = \zeta_1(\mathbf{pp} - \frac{\|\mathbf{p}\|^2}{3}\mathbf{I}) + (\zeta_2 - \omega_2\nabla\cdot\mathbf{p} - \omega_2\mathbf{p}\cdot\nabla)\mathbf{Q}.$$

(72)

Similarly, the coefficients of the matrices defined on the surface terms are given by

$$
D_{sym}^s = \begin{pmatrix}
A_0^s & 0 & 0 & 0 & 0 \\
0 & \frac{1}{\gamma_2^s}\delta_{\alpha k}\delta_{\beta l} & \frac{\chi_1^s}{2}A_{\alpha\beta k}^s & \frac{\chi_2^s}{2}A_{\alpha\beta k}^s & A_{5,\alpha\beta}^s \\
0 & \frac{\chi_1^s}{2}A_{\alpha kl}^{s,T} & \frac{1}{\gamma_1^s}\delta_{\alpha k} & \lambda^s\delta_{\alpha k} & B_\alpha^s \\
0 & \frac{\chi_2^s}{2}\mathbf{I}_s\cdot A_{\alpha kl}^{s,T} & \lambda^s\mathbf{I}_{s,\alpha k} & \gamma^s\mathbf{I}_{s,\alpha k} & (\kappa^s+\omega_0^s c_s)\mathbf{I}_{s,\alpha\beta}p_\beta \\
0 & A_{5,kl}^s & B_k^s & (\kappa^s+\omega_0^s c_s)p_k & \Lambda^s
\end{pmatrix},
$$

$$
D_{anti}^s = \begin{pmatrix}
0 & -A_1^s & -A_2^s & -A_3^s & A_4^s \\
A_1^s & 0 & 0 & 0 & 0 \\
A_2^{s'} & 0 & 0 & 0 & 0 \\
A_3^{s'} & 0 & 0 & 0 & 0 \\
-A_4^{s'} & 0 & 0 & 0 & 0
\end{pmatrix},
\tag{73}
$$

where

$$
\begin{aligned}
&A_{\alpha\beta k}^s = (p_{s,\alpha}\delta_{\beta k}+p_{s,\beta}\delta_{\alpha k})-\tfrac{2}{3}\delta_{\alpha\beta}p_{s,l}\delta_{lk},\\
&A_{\alpha kl}^{s,T}=2(p_{s,\beta}\delta_{\alpha k}\delta_{\beta l}-\tfrac{p_{s,\beta}}{3}\delta_{\alpha\beta}\delta_{kl})\\
&A_0^s=2\eta^s\mathbf{I}_{s,\alpha k}\mathbf{I}_{s,\beta l}+(\bar\eta^s-\tfrac{2}{3}\eta^s)\delta_{kl}\mathbf{I}_{s,\alpha\beta}+\alpha_1^s(\mathbf{I}_{s,\alpha j}Q_{s,jk}\mathbf{I}_{s,\beta l}+\mathbf{I}_{s,\alpha k}Q_{s,jl}\mathbf{I}_{s,\beta j})\\
&\quad+\alpha_2^s Q_{s,kl}\mathbf{I}_{s,\alpha i}Q_{s,ij}\mathbf{I}_{s,\beta j}+\alpha_3^s(\mathbf{I}_{s,\alpha i}p_{s,i}p_{s,k}\mathbf{I}_{s,\beta l}+\mathbf{I}_{s,\alpha k}p_{s,l}p_{s,j}\mathbf{I}_{s,\beta j})+\alpha_4^s p_{s,k}p_{s,l}\mathbf{I}_{s,\alpha i}p_{s,i}p_{s,j}\mathbf{I}_{s,\beta j},\\
&B_\alpha^s=\lambda_1^s p_{s,\alpha}-\omega\mathbf{p}_s\cdot\nabla_s p_{s,\alpha}-\omega p_{s,\alpha}\nabla_s\cdot\mathbf{p}_s,\\
&A_1^s=v_0^s\mathbf{I}_{s,\alpha k}\mathbf{I}_{s,\beta l}+a^s[\mathbf{I}_{s,\alpha j}Q_{s,jk}\mathbf{I}_{s,\beta l}+\mathbf{I}_{s,\alpha k}Q_{s,jl}\mathbf{I}_{s,\beta j}]-a^s(Q_{s,kl}\mathbf{I}_{s,\alpha i}(Q_{s,ij}+\tfrac{1}{3}\delta_{ij})\mathbf{I}_{s,j\beta})+\theta_1^s\delta_{kl}\mathbf{I}_{s,\alpha\beta},\\
&A_2^s=\tfrac{v_1^s}{2}(p_{s,j}\mathbf{I}_{s,\alpha k}\mathbf{I}_{s,j\beta}+\mathbf{I}_{s,\alpha j}p_{s,j}\mathbf{I}_{s,\beta k})+\theta_2^s p_{s,k}\mathbf{I}_{s,\alpha\beta},\\
&A_2^{s'}=v_1^s p_{s,\beta}\delta_{\alpha k}\delta_{\beta l}+\theta_2^s p_{s,\alpha}\delta_{kl},\\
&A_3^s=\tfrac{v_2^s}{2}(p_{s,j}\mathbf{I}_{s,\alpha k}\mathbf{I}_{s,j\beta}+\mathbf{I}_{s,\alpha j}p_{s,j}\mathbf{I}_{s,\beta k})+\theta_3^s p_{s,k}\mathbf{I}_{s,\alpha\beta},\\
&A_3^{s'}=v_2^s p_{s,\beta}\mathbf{I}_{s,\alpha k}\delta_{\beta l}+\theta_3^s\mathbf{I}_{s,\alpha\beta}p_{s,\beta}\delta_{kl},\\
&A_4^s=\mathbf{I}_{s,\alpha i}(\zeta^s p_{s,i}p_{s,j}+\zeta_0^s Q_{s,ij}+\beta_1^s(\partial_i p_{s,j}+\partial_j p_{s,i})+\beta_2^s\mathbf{p}_s\cdot\nabla_s Q_{s,ij}+\beta_3^s\nabla_s^2 Q_{s,ij}-(\zeta_2^s+\zeta_3^s p_{s,i}p_{s,i})\delta_{ij})\mathbf{I}_{s,j\beta},\\
&A_4^{s'}=A_4^s\delta_{\alpha k}\delta_{\beta l},\\
&A_5^s=\zeta_1^s(\mathbf{p}_s\mathbf{p}_s-\tfrac{\|\mathbf{p}_s\|^2}{3}\mathbf{I})+(\zeta_2^s-\omega_2^s\nabla_s\cdot\mathbf{p}_s-\omega_2^s\mathbf{p}_s\cdot\nabla_s)\mathbf{Q}_s.
\end{aligned}
\tag{74}
$$

Notice that structures of the coefficient matrices in the bulk and on the surface are similar. The resultant transport equations on the boundary are summarized in the following:

$$
\partial_t c_s+\nabla_s\cdot((\mathbf{v}+\omega_0^s\hat\mu_s\mathbf{I}_s\cdot\mathbf{p}_s)c_s)=-\nabla_s\cdot(-\gamma^s\mathbf{I}_s\cdot\nabla_s\mu_s+\chi_2^s\mathbf{I}_s\cdot\mathbf{G_s}\cdot\mathbf{p}_s-
$$
$$
\tfrac{\chi_2^s}{3}tr(\mathbf{G}_s)\mathbf{I}_s\cdot\mathbf{p}_s+\lambda^s\mathbf{I}_s\cdot\mathbf{h_s}+\kappa^s\mathbf{I}_s\cdot\mathbf{p}_s\hat\mu_s+v_2^s\mathbf{I}_s\cdot\mathbf{D}_s\cdot\mathbf{p}_s+\theta_3^s D_{s,\gamma\gamma}\mathbf{I}_s\cdot\mathbf{p}_s)+j_c,
$$

$$
\partial_t\mathbf{p}_s+\nabla_s\cdot((\mathbf{v}+\omega^s\hat\mu_s\mathbf{p}_s)\mathbf{p}_s)-\nabla_s\cdot\mathbf{v}\mathbf{p}_s+\Omega_s\cdot\mathbf{p}_s=\tfrac{1}{\gamma_1^s}\mathbf{h_s}+\chi_1^s\mathbf{G}_s\cdot\mathbf{p}_s-\tfrac{\chi_1^s}{3}tr(\mathbf{G}_s)\mathbf{p}_s-
$$
$$
\lambda^s\nabla_s\mu_s+\lambda_1^s\hat\mu_s\mathbf{p}_s+v_1^s\mathbf{D}_s\cdot\mathbf{p}_s+\theta_2^s D_{s,\gamma\gamma}\mathbf{p}_s,
$$

$$
\tfrac{\partial\mathbf{Q}_s}{\partial t}+\nabla_s\cdot((\mathbf{v}+\omega_2^s\hat\mu_s\mathbf{p}_s)\mathbf{Q}_s)-\nabla_s\cdot\mathbf{v}\mathbf{Q}_s+\Omega_s\cdot\mathbf{Q}_s\cdot\mathbf{I}_s-\mathbf{I}_s\cdot\mathbf{Q}_s\cdot\Omega_s-a^s[\mathbf{I}_s\cdot\mathbf{Q}_s\cdot\mathbf{D}_s\cdot\mathbf{I}_s+\mathbf{I}_s\cdot\mathbf{D}_s\cdot\mathbf{Q}_s\cdot\mathbf{I}_s]
$$
$$
=\tfrac{1}{\gamma_2^s}\mathbf{G}_s+\tfrac{\chi_1^s}{2}(\mathbf{p}_s\mathbf{h}_s+\mathbf{h}_s\mathbf{p}_s)-\tfrac{\chi_2^s}{2}(\mathbf{p}_s\nabla_s\mu_s+\nabla_s\mu_s\mathbf{p}_s)+\zeta_1^s\hat\mu_s\mathbf{p}_s\mathbf{p}_s+v_0^s\mathbf{I}_s\cdot\mathbf{D}_s\cdot\mathbf{I}_s-a^s(\mathbf{Q}_s:\mathbf{D}_s)\mathbf{I}_s\cdot\mathbf{Q}_s\cdot\mathbf{I}_s+
$$
$$
(\theta_1^s D_{s,\gamma\gamma}-\tfrac{a^s\mathbf{Q}_s:\mathbf{D}_s}{3})\mathbf{I}_s+(\tfrac{\chi_2^s\mathbf{p}_s\cdot\nabla_s\mu_s}{3}-\tfrac{\chi_1^s\mathbf{p}_s\cdot\mathbf{h}_s}{3}-\tfrac{\hat\mu_s\zeta_1^s\|\mathbf{p}_s\|^2}{3})\mathbf{I}+\zeta_2^s\hat\mu_s\mathbf{Q}_s,
$$

$$
\partial_t\rho_s+\nabla_s\cdot(\rho_s\mathbf{v})=0,
$$

$$
\partial_t(\rho_s\mathbf{v})=\nabla_s\cdot(\sigma_s-\rho_s\mathbf{v}\mathbf{v})+\mathbf{F}_s,
\tag{75}
$$

$$
\sigma_s^s=\sigma_s-(g-c_s\mu_s)\mathbf{I}_s-\tfrac{1}{2}\mathbf{I}_s\cdot(\mathbf{p}_s\mathbf{h}_s-\mathbf{h}_s\mathbf{p}_s)-(\mathbf{I}_s\cdot\mathbf{Q}_s\cdot\mathbf{I}_s\cdot\mathbf{G}_s-\mathbf{I}_s\cdot\mathbf{G}_s\cdot\mathbf{I}_s\cdot\mathbf{Q}_s),
$$

$$
\mathbf{F}_s+[[(\sigma-\sigma^e)]]\cdot\mathbf{n}+[[f-\mu c]]\mathbf{n}-K_c\nabla_s c_s(\mathbf{n}\cdot\tfrac{\partial f}{\partial\nabla c})-K_p\nabla_s\mathbf{p}_s\cdot(\mathbf{n}\cdot\tfrac{\partial f}{\partial\nabla\mathbf{p}})-
$$
$$
K_Q\nabla_s\mathbf{Q}_s:(\mathbf{n}\cdot\tfrac{\partial f}{\partial\nabla\mathbf{Q}})-2\kappa\sigma_s\cdot\mathbf{n}=0,
$$

$$
-[[\mu\mathbf{j}]]\cdot\mathbf{n}+j_c\mu_s\le 0,
$$

$$
\sigma_s^s=\mathbf{I}_s\cdot(-\Pi^s\mathbf{I}_s+2\eta^s\mathbf{D}_s+\alpha_1^s(\mathbf{Q}_s\cdot\mathbf{D}_s+\mathbf{D}_s\cdot\mathbf{Q}_s\cdot\mathbf{I}_s)+\alpha_2^s(\mathbf{Q}_s:\mathbf{D}_s)\mathbf{Q}_s\cdot\mathbf{I}_s+\alpha_3^s(\mathbf{p}_s\mathbf{p}_s\cdot\mathbf{D}_s+\mathbf{D}_s\cdot\mathbf{p}_s\mathbf{p}_s\cdot\mathbf{I}_s)+
$$
$$
\alpha_4^s(\mathbf{p}_s\mathbf{p}_s:\mathbf{D}_s)\mathbf{p}_s\mathbf{p}_s\cdot\mathbf{I}_s-a^s(\mathbf{Q}_s\cdot\mathbf{G}_s\cdot\mathbf{I}_s+\mathbf{G}_s\cdot\mathbf{Q}_s\cdot\mathbf{I}_s)-v_0^s\mathbf{G}_s\cdot\mathbf{I}_s+a^s(\mathbf{Q}_s:\mathbf{G}_s)\mathbf{Q}_s\cdot\mathbf{I}_s-\tfrac{v_1^s}{2}(\mathbf{p}_s\mathbf{h}_s\cdot\mathbf{I}_s+\mathbf{h}_s\mathbf{p}_s\cdot\mathbf{I}_s)+
$$
$$
\tfrac{v_2^s}{2}(\mathbf{p}_s\nabla_s\mu_s\cdot\mathbf{I}_s+\nabla_s\mu_s\mathbf{p}_s\cdot\mathbf{I}_s)+\zeta^s\hat\mu_s\mathbf{p}_s\mathbf{p}_s\cdot\mathbf{I}_s+\zeta_0^s\hat\mu_s\mathbf{Q}_s\cdot\mathbf{I}_s+\beta_1^s\hat\mu_s(\nabla_s\mathbf{p}_s+\nabla_s\mathbf{p}_s^T)\cdot\mathbf{I}_s+
$$
$$
\beta_2^s\hat\mu_s\mathbf{p}_s\cdot\nabla_s\mathbf{Q}_s\cdot\mathbf{I}_s+\beta_3^s\hat\mu_s\nabla_s^2\mathbf{Q}_s\cdot\mathbf{I}_s),
$$

where $\Pi^s = -(\bar{\eta}^s - \frac{2}{3}\eta^s)D_{s,\gamma\gamma} - \frac{a^s Q_{s,kl} G_{s,kl}}{3} + \theta_1^s G_{\gamma\gamma} + \theta_2^s p_{s,\gamma} h_{s,\gamma} - \theta_3^s p_{s,\gamma} \partial_{s,\gamma} \mu_s + (\zeta_2^s + \zeta_3^s p_{s,\gamma} p_{s,\gamma})\widehat{\mu}_s$ is the surface-excess pressure.

Let's examine the inequality $-[[\mu\mathbf{j}]] \cdot \mathbf{n} + j_c \mu_s \leq 0$. If we assume $j_c = 0$ and $[[\mathbf{j}]] \cdot \mathbf{n} = 0$, the inequality is satisfied. If on the other hand we assign $[[\mathbf{j}]] \cdot \mathbf{n} = 0$ and $j_c = -\frac{1}{\gamma^s}\mu_s$, the inequality is satisfied. If in addition, we assume the flux $\mathbf{j}_s$ as zero, the transport equation for c_s is given by

$$\partial_t c_s + \nabla_s \cdot (c_s \mathbf{v}) = -\frac{1}{\gamma^s}\mu_s. \tag{76}$$

This is an Allen–Cahn type transport equation for the excessive surface concentration.

We have derived the governing system of equations for the bulk as well as for the free surface. The surface transport equations serve as the dynamic boundary conditions for the bulk transport equations at the free interface. The passive liquid crystal limit is embedded in the model for active liquid crystals. One important point we show in this derivation is that the boundary transport equations together with the bulk transport equations can be derived together through the generalized Onsager principle to ensure consistency in the model. If we impose that the passive limit is dissipative, the corresponding submatrix in the Onsager relation must be nonnegative definite. The model we present can be extended by adding additional higher order terms. The mathematical structure behind the model is persistent, in which variational structure and energy dissipation structure for the passive component are clearly delineated. We next reduce the model to the isotropic viscous fluid model so that one can examine the consistency in a simple fluid limit.

4.3. Static Boundary Conditions

In a simple case, we consider the static boundary conditions on the free surface. If we set $\gamma_1^s, \gamma_2^s, \gamma^s$ as zero, we recover the static boundary conditions given below,

$$\mu_s = 0, \quad \mathbf{h}_s = 0, \quad \mathbf{G}_s = 0. \tag{77}$$

If g depends on the internal variables rather than their spatial gradients, these translate into the following.

$$K_c \frac{\partial f}{\partial \nabla_i c} n_i + \frac{\partial g}{\partial c_s} = 0, \quad K_p \frac{\partial f}{\partial \nabla_i \mathbf{P}} n_i + \frac{\partial g}{\partial \mathbf{p}_s} = 0, \quad K_Q \frac{\partial f}{\partial \nabla_i \mathbf{Q}} n_i + \frac{\partial g}{\partial \mathbf{Q}_s} = 0, \tag{78}$$

where we assume that outside of the active liquid crystal region is an isotropic viscous fluid, thus the jumps $[[\cdot]]$ across the surface are the limits of the variables to the surface in the active liquid crystal domain. These are most likely Robin type boundary conditions.

The kinematic boundary condition is given by the following

$$(\partial_t + \mathbf{v} \cdot \nabla)\Phi = 0. \tag{79}$$

The kinetic boundary condition is

$$\nabla_s \cdot \sigma_s^s + \nabla_s g + 2\kappa g \mathbf{n} + \mathbf{F}_s = 0,$$

$$\mathbf{F}_s = -[[\sigma - \sigma^e]] \cdot \mathbf{n} - [[f - \mu c]]\mathbf{n} - \nabla_s c_s \frac{\partial g}{\partial c_s} - \nabla_s \mathbf{p}_s \cdot \frac{\partial g}{\partial \mathbf{p}_s} - \nabla_s \mathbf{Q}_s : \frac{\partial g}{\partial \mathbf{Q}_s}, \tag{80}$$

where σ_s^s is defined in the above subsection, and we have used the boundary conditions (78) and $\sigma_s \cdot \mathbf{n} = 0$.

Next, we consider the specific apolar active liquid crystal system, whose model is given in Section 3. The bulk and surface free energy of the system are given by

$$f = f(c, \nabla c, \mathbf{Q}, \nabla \mathbf{Q}),$$

$$g = g_0(c_s) + g_1 \mathbf{Q}_s : \mathbf{nn}. \tag{81}$$

Then

$$\mu_s = \frac{\partial g_0}{\partial c_s} + K_c \frac{\partial f}{\partial (\nabla c)} \cdot \mathbf{n},$$

$$\mathbf{G}_s = g_1(\mathbf{nn}) + K_Q \frac{\partial f}{\partial (\nabla \mathbf{Q})} \cdot \mathbf{n}. \tag{82}$$

Thus the boundary conditions for $c_s, \mathbf{Q}_s$ on the free surface are $\mu_s = 0, \mathbf{G}_s = 0$. The kinetic boundary condition is

$$\nabla_s \cdot \sigma_s^s + \nabla_s g + 2\kappa g \mathbf{n} + \mathbf{F}_s = 0,$$

$$\mathbf{F}_s = -[[\sigma - \sigma^e]] \cdot \mathbf{n} - [[f - \mu c]]\mathbf{n} - \nabla_s c_s \frac{\partial g}{\partial c_s} - \nabla_s \mathbf{Q}_s : \frac{\partial g}{\partial \mathbf{Q}_s},$$

$$\sigma_s^s = \mathbf{I}_s \cdot (-\Pi^s \mathbf{I}_s + 2\eta^s \mathbf{D}_s + \alpha_1^s(\mathbf{Q}_s \cdot \mathbf{D}_s + \mathbf{D}_s \cdot \mathbf{Q}_s \cdot \mathbf{I}_s) + \alpha_2^s(\mathbf{Q}_s : \mathbf{D}_s)\mathbf{Q}_s \cdot \mathbf{I}_s + \zeta_0^s \widehat{\mu}_s \mathbf{Q}_s \cdot \mathbf{I}_s + \beta_3^s \widehat{\mu}_s \nabla_s^2 \mathbf{Q}_s \cdot \mathbf{I}_s). \tag{83}$$

The model we derived include many liquid crystal models and the viscous fluid model. For an isotropic viscous fluid, the surface stress tensor and elastic force are given by,

$$\sigma_s = g\mathbf{I}_s, \mathbf{F}_s = -[[\sigma]] \cdot \mathbf{n}. \tag{84}$$

The surface excessive momentum transport equation is given by

$$\partial_t(\rho_s \mathbf{v}) = \nabla_s \cdot (\sigma_s - \rho_s \mathbf{vv}) - [[\sigma]] \cdot \mathbf{n}. \tag{85}$$

In the inertialess limit, the kinetic boundary condition reduces to

$$\nabla_s \cdot \sigma_s - [[\sigma]] \cdot \mathbf{n} = 0. \tag{86}$$

This is the kinetic boundary condition commonly used in studies of fluid dynamics of viscous fluids with free surface boundaries.

5. Conclusions

We have derived systematically the transport equations together with the boundary conditions for an active liquid crystal in a confined fixed domain and in free surface domains using the generalized Onsager principle. The model reduces to a general hydrodynamic model for passive liquid crystals when the activity is absent, where energy dissipation is guarranteed. Likewise, the boundary conditions reduce to static boundary conditions. The resulting model equations incorporate many momentum-conserving models for liquid crystals with which to study complex interfacial phenomena involving active as well as passive liquid crystals. Detailed analyses of the model together with their applications to active matter systems and development of numerical schemes will be pursued in subsequent studies.

Appendix A: Translational and Rotational Invariance of the Free Energy

In this appendix, we identify the Ericksen stress σ^e from the translational invariance of the free energy and the antisymmetric stress σ^a from the rotational invariance of the free energy. In addition, we use the angular momentum conservational law to prove symmetry of stress σ^s.

A.1. Ericksen Stress σ^e

Our goal is to drive the Ericksen stress σ^e of this system. The free energy density $f = f(c, \partial_\alpha c, p_\alpha, \partial_\beta p_\alpha, Q_{\alpha\beta}, \partial_\gamma Q_{\alpha\beta})$. The total free energy is $F = \int_V d\mathbf{x} f$. If the volume V (with surface $S = \partial V$) of the system is changed by an amount δV to volume $V + \delta V$, the change of the free energy is

$$
\begin{aligned}
\delta F &= \int_{V+\delta V} d\mathbf{x} f(c + \delta c, \partial_\alpha c + \delta \partial_\alpha c, p_\alpha + \delta p_\alpha, \partial_\beta p_\alpha + \delta \partial_\beta p_\alpha, Q_{\alpha\beta} + \delta Q_{\alpha\beta}, \partial_\gamma Q_{\alpha\beta} + \delta \partial_\gamma Q_{\alpha\beta}) \\
&\quad - \int_V d\mathbf{x} f(c, \partial_\alpha c, p_\alpha, \partial_\beta p_\alpha, Q_{\alpha\beta}, \partial_\gamma Q_{\alpha\beta}) \\[2mm]
&= \int_{\delta V} d\mathbf{x} f(c, \partial_\alpha c, p_\alpha, \partial_\beta p_\alpha, Q_{\alpha\beta}, \partial_\gamma Q_{\alpha\beta}) \\
&\quad + \int_V d\mathbf{x} [\frac{\partial f}{\partial c} \delta c + \frac{\partial f}{\partial (\partial_\alpha c)} \delta \partial_\alpha c + \frac{\partial f}{\partial p_\alpha} \delta p_\alpha + \frac{\partial f}{\partial (\partial_\beta p_\alpha)} \delta \partial_\beta p_\alpha + \frac{\partial f}{\partial Q_{\alpha\beta}} \delta Q_{\alpha\beta} + \frac{\partial f}{\partial (\partial_\gamma Q_{\alpha\beta})} \delta \partial_\gamma Q_{\alpha\beta}] \\[2mm]
&= \int_S dS_\alpha [f u_\alpha] + \int_V d\mathbf{x} [\mu \delta c - h_\alpha \delta p_\alpha - G_{\alpha\beta} \delta Q_{\alpha\beta}] \\
&\quad + \int_V d\mathbf{x} [\partial_\alpha (\frac{\partial f}{\partial (\partial_\alpha c)} \delta c) + \partial_\beta (\frac{\partial f}{\partial (\partial_\beta p_\alpha)} \delta p_\alpha) + \partial_\gamma (\frac{\partial f}{\partial (\partial_\gamma Q_{\alpha\beta})} \delta Q_{\alpha\beta})] \quad (d\mathbf{x} = u_\alpha dS_\alpha \text{ in } \delta V) \\[2mm]
&= \int_S dS_\alpha [f u_\alpha] + \int_V d\mathbf{x} [\mu \delta c - h_\alpha \delta p_\alpha - G_{\alpha\beta} \delta Q_{\alpha\beta}] \\
&\quad + \int_S dS_\alpha [\frac{\partial f}{\partial (\partial_\alpha c)} \delta c] + \int_S dS_\beta [\frac{\partial f}{\partial (\partial_\beta p_\alpha)} \delta p_\alpha] + \int_S dS_\gamma [\frac{\partial f}{\partial (\partial_\gamma Q_{\alpha\beta})} \delta Q_{\alpha\beta}] \\[2mm]
&= \int_S dS_\alpha [(f - \mu c) u_\alpha] + \int_V d\mathbf{x} [c \partial_\alpha (\mu u_\alpha) + h_\alpha (\partial_\beta p_\alpha) u_\beta + G_{\alpha\beta} (\partial_\gamma Q_{\alpha\beta}) u_\gamma] \\
&\quad - \int_S dS_\alpha [\frac{\partial f}{\partial (\partial_\alpha c)} (\partial_\beta c) u_\beta] - \int_S dS_\beta [\frac{\partial f}{\partial (\partial_\beta p_\alpha)} (\partial_\gamma p_\alpha) u_\gamma] - \int_S dS_\gamma [\frac{\partial f}{\partial (\partial_\gamma Q_{\alpha\beta})} (\partial_\theta Q_{\alpha\beta}) u_\theta],
\end{aligned}
\tag{A1}
$$

where $\mu = \frac{\delta F}{\delta c} = \frac{\partial f}{\partial c} - \partial_\alpha (\frac{\partial f}{\partial (\partial_\alpha c)})$ is the chemical potential, $h_\alpha = -\frac{\delta F}{\delta p_\alpha} = -\frac{\partial f}{\partial p_\alpha} + \partial_\beta (\frac{\partial f}{\partial (\partial_\beta p_\alpha)})$ is the molecule field, $G_{\alpha\beta} = -\frac{\delta F}{\delta G_{\alpha\beta}} = -\frac{\partial f}{\partial Q_{\alpha\beta}} + \partial_\gamma (\frac{\partial f}{\partial (\partial_\gamma Q_{\alpha\beta})})$ is the conjugation field of $\mathbf{Q}$.

Here, we have made use of $\delta c = -(\partial_\alpha c) u_\alpha$ and $\delta p_\alpha = -(\partial_\beta p_\alpha) u_\beta$ and $\delta Q_{\alpha\beta} = -(\partial_\gamma Q_{\alpha\beta}) u_\gamma$, that means the movement of the matter volume is linear and there is no rotation, where $\mathbf{u}(\mathbf{r})$ is the change from V to $V + \delta V$ in the direction normal to the original boundary ∂V. We obtain the expression of the Ericksen stress tensor σ^e:

$$
\sigma_{\alpha\beta}^e = (f - c\mu) \delta_{\alpha\beta} - \frac{\partial f}{\partial (\partial_\beta c)} \partial_\alpha c - \frac{\partial f}{\partial (\partial_\beta p_\gamma)} \partial_\alpha p_\gamma - \frac{\partial f}{\partial (\partial_\beta Q_{\gamma\theta})} \partial_\alpha Q_{\gamma\theta}.
\tag{A2}
$$

In order to derive the corresponding Gibbs–Duhem relation, we first calculate the total differential of the free energy

$$df = \frac{\partial f}{\partial c}dc + \frac{\partial f}{\partial(\partial_\alpha c)}d(\partial_\alpha c) + \frac{\partial f}{\partial p_\alpha}dp_\alpha + \frac{\partial f}{\partial(\partial_\beta p_\alpha)}d(\partial_\beta p_\alpha) + \frac{\partial f}{\partial Q_{\alpha\beta}}dp_{\alpha\beta} + \frac{\partial f}{\partial(\partial_\beta Q_{\alpha\gamma})}d(\partial_\beta Q_{\alpha\gamma})$$

$$= \mu dc - h_\alpha dp_\alpha - G_{\alpha\beta}dQ_{\alpha\beta} + \partial_\alpha(\frac{\partial f}{\partial(\partial_\alpha c)}dc) + \partial_\beta(\frac{\partial f}{\partial(\partial_\beta p_\alpha)}dp_\alpha) + \partial_\gamma(\frac{\partial f}{\partial(\partial_\gamma Q_{\alpha\beta})}dQ_{\alpha\beta}).$$

(A3)

Then, we have

$$d\sigma^e_{\alpha\beta} = (df - d(c\mu))\delta_{\alpha\beta} - d(\frac{\partial f}{\partial(\partial_\beta c)}\partial_\alpha c + \frac{\partial f}{\partial(\partial_\beta p_\gamma)}\partial_\alpha p_\gamma + \frac{\partial f}{\partial(\partial_\beta Q_{\gamma\theta})}\partial_\alpha Q_{\gamma\theta})$$

$$= [-cd\mu - h_\gamma dp_\gamma - G_{\gamma\theta}dQ_{\gamma\theta}]\delta_{\alpha\beta} + \partial_\gamma(\frac{\partial f}{\partial(\partial_\gamma c)}dc)\delta_{\alpha\beta} + \partial_\gamma(\frac{\partial f}{\partial(\partial_\gamma p_\delta)}dp_\delta)\delta_{\alpha\beta}$$

$$+\partial_\gamma(\frac{\partial f}{\partial(\partial_\gamma Q_{\theta\delta})}dQ_{\theta\delta})\delta_{\alpha\beta} - d(\frac{\partial f}{\partial(\partial_\beta c)}\partial_\alpha c + \frac{\partial f}{\partial(\partial_\beta p_\gamma)}\partial_\alpha p_\gamma + \frac{\partial f}{\partial(\partial_\beta Q_{\gamma\theta})}\partial_\alpha Q_{\gamma\theta}).$$

(A4)

It follows that

$$\partial_\beta\sigma^e_{\alpha\beta} = [-c\partial_\beta\mu - h_\gamma\partial_\beta p_\gamma - G_{\gamma\theta}\partial_\beta Q_{\gamma\theta}]\delta_{\alpha\beta} + \partial_\gamma(\frac{\partial f}{\partial(\partial_\gamma c)}\partial_\beta c)\delta_{\alpha\beta} + \partial_\gamma(\frac{\partial f}{\partial(\partial_\gamma p_\delta)}\partial_\beta p_\delta)\delta_{\alpha\beta}$$

$$+\partial_\gamma(\frac{\partial f}{\partial(\partial_\gamma Q_{\theta\delta})}\partial_\beta Q_{\theta\delta})\delta_{\alpha\beta} - \partial_\beta(\frac{\partial f}{\partial(\partial_\beta c)}\partial_\alpha c + \frac{\partial f}{\partial(\partial_\beta p_\gamma)}\partial_\alpha p_\gamma + \frac{\partial f}{\partial(\partial_\beta Q_{\gamma\theta})}\partial_\alpha Q_{\gamma\theta})$$

$$= -c\partial_\alpha\mu - h_\gamma\partial_\alpha p_\gamma - G_{\gamma\theta}\partial_\alpha Q_{\gamma\theta}.$$

(A5)

This is the Gibbs–Duhem relation. Finally, the change of the free energy is given by

$$\delta F = \int_V d\mathbf{x}[c\partial_\alpha(\mu u_\alpha) + h_\alpha(\partial_\beta p_\alpha)u_\beta + G_{\alpha\beta}(\partial_\gamma Q_{\alpha\beta})u_\gamma] + \int_S dS_\beta[\sigma^e_{\alpha\beta}u_\alpha]$$

$$= \int_V d\mathbf{x}[c\partial_\alpha(\mu u_\alpha) + h_\alpha(\partial_\beta p_\alpha)u_\beta + G_{\alpha\beta}(\partial_\gamma Q_{\alpha\beta})u_\gamma + \partial_\beta(\sigma^e_{\alpha\beta}u_\alpha)].$$

(A6)

If the displacement $\mathbf{u}(\mathbf{r})$ is constant, that means the change is a pure linear translation, $\partial_\beta u_\alpha = 0$, then

$$\delta F = \int_V d\mathbf{x}[c\partial_\alpha\mu + h_\gamma(\partial_\alpha p_\gamma) + G_{\beta\gamma}(\partial_\alpha Q_{\beta\gamma}) + \partial_\beta\sigma^e_{\alpha\beta}]u_\alpha = 0.$$

(A7)

This is the translational invariance of the free energy.

A.2. Antisymmetric Stress σ^a

The free energy is also invariant under a pure uniform rotation around the original point with respect to an angle θ. The displacement $\mathbf{u} = \theta \times \mathbf{r}$, that is $u_\alpha = \epsilon_{\alpha\beta\gamma}\theta_\beta r_\gamma$. The changes of the variables are $\delta c = -u_\beta\partial_\beta c, \delta p_\alpha = -(u_\beta\partial_\beta p_\alpha + \epsilon_{\alpha\beta\gamma}\theta_\beta p_\gamma), \delta Q_{\alpha\beta} = -(u_\gamma\partial_\gamma Q_{\alpha\beta} + \epsilon_{\alpha\delta\gamma}\theta_\delta Q_{\gamma\beta} + \epsilon_{\beta\delta\gamma}\theta_\delta Q_{\gamma\alpha})$. Under the pure uniform rotation, the convected co-rotational derivatives of a scale, a vector and a tensor are all zero. For the scalar, that is $\partial_t c + \mathbf{v} \cdot \nabla c = 0$, then

$$\delta c = \frac{\partial c}{\partial t}\delta t = -v_\beta\partial_\beta c\delta t = -u_\beta\partial_\beta c,$$

(A8)

where the velocity is defined as $v_\beta = u_\beta/\delta t$, that means that after a period of time δt the displacement is u_β. For a vector, we have $\partial_t\mathbf{p} + \mathbf{v} \cdot \nabla\mathbf{p} + \Omega \cdot \mathbf{p} = 0$, then

$$\delta p_\alpha = \frac{\partial p_\alpha}{\partial t}\delta t = -(v_\beta\partial_\beta p_\alpha + \Omega_{\alpha\beta}p_\beta)\delta t = -u_\beta\partial_\beta p_\alpha + \epsilon_{\alpha\beta\gamma}\theta_\beta p_\gamma,$$

(A9)

where $\Omega_{\alpha\beta}\delta t = -\epsilon_{\alpha\gamma\beta}\theta_\gamma$. For a tensor, the convected co-rotational derivative $\partial_t \mathbf{Q} + \mathbf{v} \cdot \nabla \mathbf{Q} + \Omega \cdot \mathbf{Q} - \mathbf{Q} \cdot \Omega = 0$, then

$$\delta Q_{\alpha\beta} = \frac{\partial Q_{\alpha\beta}}{\partial t}\delta t = -(v_\gamma \partial_\gamma Q_{\alpha\beta} + \Omega_{\alpha\gamma}Q_{\gamma\beta} - Q_{\alpha\gamma}\Omega_{\gamma\beta})\delta t = \\ -u_\gamma \partial_\gamma Q_{\alpha\beta} + \epsilon_{\alpha\delta\gamma}\theta_\delta Q_{\gamma\beta} + \epsilon_{\beta\delta\gamma}\theta_\delta Q_{\gamma\alpha}. \tag{A10}$$

We list some useful formulas as follows:

$$\epsilon_{\alpha\beta\gamma} = -\epsilon_{\gamma\beta\alpha}, \quad \epsilon_{\alpha\alpha\gamma} = 0,$$

$$\partial_\beta(u_\beta) = \epsilon_{\alpha\beta\gamma}\theta_\beta \partial_\beta(r_\gamma) = \epsilon_{\alpha\beta\gamma}\theta_\beta\delta_{\beta\gamma} = \epsilon_{\alpha\beta\beta}\theta_\beta = 0, \tag{A11}$$

$$\partial_\delta(u_\alpha) = \epsilon_{\alpha\beta\gamma}\theta_\beta \partial_\delta(r_\gamma) = \epsilon_{\alpha\beta\gamma}\theta_\beta\delta_{\delta\gamma} = \epsilon_{\alpha\beta\delta}\theta_\beta.$$

Then, we calculate the change of the free energy,

$$dF = \int_S dS_\alpha [fu_\alpha] + \int_V d\mathbf{x}[\mu\delta c - h_\alpha\delta p_\alpha - G_{\alpha\beta}\delta Q_{\alpha\beta}] \\ + \int_V d\mathbf{x}[\partial_\alpha(\frac{\partial f}{\partial(\partial_\alpha c)}\delta c) + \partial_\beta(\frac{\partial f}{\partial(\partial_\beta p_\alpha)}\delta p_\alpha) + \partial_\gamma(\frac{\partial f}{\partial(\partial_\gamma Q_{\alpha\beta})}\delta Q_{\alpha\beta})]$$

$$= \int_S dS_\alpha[f - c\mu]u_\alpha - \int_V d\mathbf{x}[\partial_\beta(\sigma^e_{\alpha\beta})u_\alpha] - \int_V d\mathbf{x}[h_\alpha\epsilon_{\alpha\beta\gamma}\theta_\beta p_\gamma + G_{\alpha\beta}(\epsilon_{\alpha\delta\gamma}\theta_\delta Q_{\gamma\beta} + \epsilon_{\beta\delta\gamma}\theta_\delta Q_{\gamma\alpha})] \\ + \int_S dS_\beta[-\frac{\partial f}{\partial(\partial_\beta c)}\partial_\alpha c - \frac{\partial f}{\partial(\partial_\beta p_\gamma)}\partial_\alpha p_\gamma - \frac{\partial f}{\partial(\partial_\beta Q_{\gamma\theta})}\partial_\alpha Q_{\gamma\theta}]u_\alpha + \int_S dS_\delta[\frac{\partial f}{\partial(\partial_\delta p_\alpha)}\epsilon_{\alpha\beta\gamma}\theta_\beta p_\gamma] \\ + \int_S dS_\delta[\frac{\partial f}{\partial(\partial_\delta Q_{\alpha\beta})}(\epsilon_{\alpha\delta\gamma}\theta_\delta Q_{\gamma\beta} + \epsilon_{\beta\delta\gamma}\theta_\delta Q_{\gamma\alpha})]$$

$$= \int_S dS_\beta[\sigma^e_{\alpha\beta}u_\alpha] - \int_V d\mathbf{x}[\partial_\beta(\sigma^e_{\alpha\beta})u_\alpha] - \int_V d\mathbf{x}[h_\alpha\epsilon_{\alpha\beta\gamma}\theta_\beta p_\gamma + G_{\alpha\beta}(\epsilon_{\alpha\delta\gamma}\theta_\delta Q_{\gamma\beta} + \epsilon_{\beta\delta\gamma}\theta_\delta Q_{\gamma\alpha})] \tag{A12} \\ + \int_S dS_\delta[\frac{\partial f}{\partial(\partial_\delta p_\alpha)}\epsilon_{\alpha\beta\gamma}\theta_\beta p_\gamma] + \int_S dS_\theta[\frac{\partial f}{\partial(\partial_\theta Q_{\alpha\beta})}(\epsilon_{\alpha\delta\gamma}\theta_\delta Q_{\gamma\beta} + \epsilon_{\beta\delta\gamma}\theta_\delta Q_{\gamma\alpha})]$$

$$= \int_V d\mathbf{x}[\sigma^e_{\alpha\beta}\epsilon_{\alpha\gamma\beta}\theta_\gamma] - \int_V d\mathbf{x}[\frac{1}{2}(h_\alpha p_\gamma - p_\alpha h_\gamma) + (G_{\alpha\delta}Q_{\delta\gamma} - Q_{\alpha\delta}G_{\delta\gamma})]\epsilon_{\alpha\beta\gamma}\theta_\beta \\ + \int_S dS_\delta[\frac{\partial f}{\partial(\partial_\delta p_\alpha)}p_\gamma + \frac{\partial f}{\partial(\partial_\delta Q_{\alpha\theta})}Q_{\gamma\theta} + \frac{\partial f}{\partial(\partial_\delta Q_{\theta\alpha})}Q_{\gamma\theta}]\epsilon_{\alpha\beta\gamma}\theta_\beta$$

$$= \int_V \epsilon_{\alpha\beta\gamma}\theta_\beta[\sigma^e_{\alpha\gamma} + \sigma^a_{\alpha\gamma}]d\mathbf{x} + \int_S \epsilon_{\alpha\beta\gamma}\theta_\beta p_\gamma(\sigma^p \cdot d\mathbf{S})_\alpha + 2\int_S \epsilon_{\alpha\beta\gamma}\theta_\beta[(\mathbf{Q} \cdot \mathbf{M}^Q \cdot d\mathbf{S})_{\gamma\alpha}]$$

$$= 0,$$

where we define $\sigma^a_{\alpha\beta} = \frac{1}{2}(p_\alpha h_\beta - h_\alpha p_\beta) + (Q_{\alpha\delta}G_{\delta\gamma} - G_{\alpha\delta}Q_{\delta\gamma})$, $\sigma^p_{\alpha\beta} = \frac{\partial f}{\partial(\partial_\beta p_\alpha)}$, $M^Q_{\alpha\beta\gamma} = \frac{\partial f}{\partial(\partial_\gamma Q_{\alpha\beta})}$. $M^Q_{\alpha\beta\gamma}$ is symmetric about α, β. Because the rotation angle is arbitrary, we get the relationship of the angular momentum.

$$\int_V \epsilon_{\alpha\beta\gamma}[\sigma^e_{\alpha\gamma} + \sigma^a_{\alpha\gamma}]d\mathbf{x} + \int_S \epsilon_{\alpha\beta\gamma}p_\gamma(\sigma^p \cdot d\mathbf{S})_\alpha + 2\int_S \epsilon_{\alpha\beta\gamma}[(\mathbf{Q} \cdot \mathbf{M}^Q \cdot d\mathbf{S})_{\gamma\alpha}] = 0. \tag{A13}$$

We show the *z*-component clearly,

$$\int_V d\mathbf{x}\{[\sigma^e_{yx} - \sigma^e_{xy}] + [\sigma^a_{yx} - \sigma^a_{xy}]\} + \int_S [\mathbf{p} \times (\sigma^p \cdot d\mathbf{S})]_z + \\ 2\int_S \epsilon_{\gamma z\alpha}[(\mathbf{Q} \cdot \mathbf{M}^Q \cdot d\mathbf{S})_{\gamma\alpha}] = 0. \tag{A14}$$

The second term on the right-hand side is the torque on the surface due to polar order **p**, and the last term is the torque on the surface due to nematic order tensor **Q**.

A.3. Angular Momentum Conservation Law

We have calculated that the dissipation of the total energy

$$\frac{dE^{totol}}{dt} = -\int_V d\mathbf{x} \left\{ (\partial_\beta v_\alpha)\sigma^s_{\alpha\beta} + j_\alpha(-\partial_\alpha \bar{\mu}) + P_\alpha h_\alpha + G_{\alpha\beta} \overset{\square}{Q}_{\alpha\beta} + r\widehat{\mu} \right\}, \tag{A15}$$

where $\sigma^s_{\alpha\beta} = \sigma_{\alpha\beta} - \sigma^e_{\alpha\beta} - \sigma^a_{\alpha\beta}$. We need to prove that σ^s is symmetry using the angular momentum conservation. The angular momentum conservation law is given by

$$\frac{\partial}{\partial t}\left(\int_V d\mathbf{x}(\mathbf{r} \times \rho\mathbf{v})\right) = \int_S \mathbf{r} \times ((\sigma - \rho\mathbf{v}\mathbf{v}) \cdot \mathbf{dS}) + \int_S \mathbf{p} \times (\sigma^p \cdot \mathbf{dS})$$
$$+2\int_S \epsilon_{\alpha\beta\gamma}[(\mathbf{Q} \cdot \mathbf{M}^Q \cdot d\mathbf{S})_{\gamma\alpha}], \tag{A16}$$

where $\sigma^p_{\alpha\beta} = \frac{\partial f}{\partial(\partial_\beta p_\alpha)}$ and $M^Q_{\alpha\beta\gamma} = \frac{\partial f}{\partial(\partial_\gamma Q_{\alpha\beta})}$ are defined above. The term on the left-hand side is the derivative of the total angular momentum in the volume. The terms on the right-hand side are the total torque acting on the surface. There are three contributions: the first one is the torque of the stress $(\sigma - \rho\mathbf{v}\mathbf{v})$ acting on the surface; the second one is the torque of the polarity vector (**p**) acting on the surface and the last one is the torque of the nematic order tensor (**Q**) acting on the surface. We use the linear momentum conservation law to transform the left-hand side of Equation (A16) and use the Equation (A14) to arrive at:

$$\int_V d\mathbf{x}[\sigma_{xy} - \sigma_{yx}] = -\int_V d\mathbf{x}\{[\sigma^e_{yx} - \sigma^e_{xy}] + [\sigma^a_{yx} - \sigma^a_{xy}]\}, \tag{A17}$$

where we only show the z-component. Analogously, we can get the x, y-components. Because σ^a is antisymmetric, then we get the antisymmetric part

$$\tfrac{1}{2}[(\sigma - \sigma^e)_{\alpha\beta} - (\sigma - \sigma^e)_{\beta\alpha}] = \sigma^a_{\alpha\beta}. \tag{A18}$$

So, the stress $\sigma^s_{\alpha\beta} = \sigma_{\alpha\beta} - \sigma^a_{\alpha\beta} - \sigma^e_{\alpha\beta}$ is symmetric, *i.e.*, $\partial_\beta v_\alpha \sigma^s_{\alpha\beta} = \mathbf{D} : \sigma^s$.

A.4. The Convected Co-Rotational Derivatives:

The convected co-rotational derivatives of the polarization and nematic order are defined by

$$\dot{\mathbf{p}} = \frac{\partial \mathbf{p}}{\partial t} + \mathbf{v} \cdot \nabla\mathbf{p} + \Omega \cdot \mathbf{p},$$
$$\overset{\square}{\mathbf{Q}} = \frac{\partial \mathbf{Q}}{\partial t} + \mathbf{v} \cdot \nabla\mathbf{Q} + [\Omega \cdot \mathbf{Q} - \mathbf{Q} \cdot \Omega], \tag{A19}$$

where **v** is the velocity of the background fluid, $\Omega_{\alpha\beta} = \frac{1}{2}(\partial_\alpha v_\beta - \partial_\beta v_\alpha)$ is the vorticity tensor. The vector $\dot{\mathbf{p}}$ and tensor $\overset{\square}{\mathbf{Q}}$ represent the rate of change of the field **p** and **Q** with respect to the background fluid, which are translational and rotational invariant.

A.4.1. Translational Invariance

If both the background fluid and the director $\mathbf{p}$ move with a constant velocity $\mathbf{v} = \mathbf{v}_0$, then $\Omega = 0, \Omega \cdot \mathbf{p} = 0$. At time t, the director at the location $\mathbf{r}$ is $\mathbf{p}(\mathbf{r}, t)$. After a small time Δt, at time $t + \Delta t$, the director at the location $\mathbf{r} + \mathbf{v}_0 \Delta t$ is $\mathbf{p}(\mathbf{r} + \mathbf{v}_0 \Delta t, t + \Delta t) = \mathbf{p}(\mathbf{r}, t)$.

$$
\begin{aligned}
\frac{\partial \mathbf{p}}{\partial t} &= \lim_{\Delta t \to 0} \frac{\mathbf{p}(r, t + \Delta t) - \mathbf{p}(\mathbf{r}, t)}{\Delta t} \\[2mm]
&= \lim_{\Delta t \to 0} \frac{\mathbf{p}(\mathbf{r}, t + \Delta t) - \mathbf{p}(\mathbf{r} + \mathbf{v}_0 \Delta t, t + \Delta t) + \mathbf{p}(\mathbf{r} + \mathbf{v}_0 \Delta t, t + \Delta t) - \mathbf{p}(\mathbf{r}, t)}{\Delta t} \\[2mm]
&= \lim_{\Delta t \to 0} \frac{-\mathbf{v}_0 \cdot \nabla \mathbf{p}(\mathbf{r} + a\mathbf{v}_0 \Delta t, t + \Delta t)\Delta t}{\Delta t} \quad = -\mathbf{v} \cdot \nabla \mathbf{p},
\end{aligned}
\tag{A20}
$$

where a is some constant, $0 < a < 1$. So, $\dot{\mathbf{p}} = \frac{\partial \mathbf{p}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{p} + \Omega \cdot \mathbf{p} = 0$ under a pure linear translation. Similarly, we can show $\overset{\square}{\mathbf{Q}} = \frac{\partial \mathbf{Q}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{Q} + [\Omega \cdot \mathbf{Q} - \mathbf{Q} \cdot \Omega] = 0$.

A.4.2. Rotational Invariance

If both the background fluid and the director $\mathbf{p}$ rotate around a certain axis at the same angular velocity θ, velocity $\mathbf{v} = \theta \times \mathbf{r}$, and $\Omega \cdot \mathbf{p} = -\theta \times \mathbf{p}$. At time t, the director at the location $\mathbf{r}$ is $\mathbf{p}(\mathbf{r}, t)$. After a small time Δt, at time $t + \Delta t$, the director at the location $\mathbf{r} + \theta \times \mathbf{r}\Delta t$ is $\mathbf{p}(\mathbf{r} + \theta \times \mathbf{r}\Delta t, t + \Delta t) = \mathbf{p}(\mathbf{r}, t) + \theta \times \mathbf{p}(\mathbf{r}, t)\Delta t$.

$$
\begin{aligned}
\frac{\partial \mathbf{p}}{\partial t} &= \lim_{\Delta t \to 0} \frac{\mathbf{p}(\mathbf{r}, t + \Delta t) - \mathbf{p}(\mathbf{r}, t)}{\Delta t} \\[2mm]
&= \lim_{\Delta t \to 0} \frac{\mathbf{p}(\mathbf{r}, t + \Delta t) - \mathbf{p}(\mathbf{r} + \theta \times \mathbf{r}\Delta t, t + \Delta t) + \mathbf{p}(\mathbf{r} + \theta \times \mathbf{r}\Delta t, t + \Delta t) - \mathbf{p}(\mathbf{r}, t)}{\Delta t} \\[2mm]
&= \lim_{\Delta t \to 0} \frac{-(\theta \times \mathbf{r}) \cdot \nabla \mathbf{p}(\mathbf{r} + (\theta \times \mathbf{r})a\Delta t, t + \Delta t)\Delta t + \theta \times \mathbf{p}(\mathbf{r}, t)\Delta t}{\Delta t} \\[2mm]
&= -(\theta \times \mathbf{r}) \cdot \nabla \mathbf{p}(\mathbf{r}, t) + \theta \times \mathbf{p}(\mathbf{r}, t) \quad = -\mathbf{v} \cdot \nabla \mathbf{p} - \Omega \cdot \mathbf{p},
\end{aligned}
\tag{A21}
$$

where a is some constant, $0 < a < 1$. So, $\dot{\mathbf{p}} = \frac{\partial \mathbf{p}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{p} + \Omega \cdot \mathbf{p} = 0$ under a pure rotation. For tensor $\mathbf{Q}$, we recall from its definition $\mathbf{Q} = \int_V (\hat{v}\hat{v} - \frac{\mathbf{I}}{d}) f_d(\mathbf{r}, \hat{v}, t) d\hat{v} = \mathbf{M} - c\frac{\mathbf{I}}{d}$. Using the result of $\mathbf{p}$,

$$
\mathbf{M}(\mathbf{r} + \theta \times \mathbf{r}\Delta t, t + \Delta t) = \int_V (\hat{v} + \theta \times \hat{v})(\hat{v} + \theta \times \hat{v}\Delta t) f_d(\mathbf{r}, \hat{v}, t) d\hat{v}
$$

$$
= \mathbf{M}(\mathbf{r}, t) + \int_V (\hat{v}\theta \times \hat{v} + \theta \times \hat{v}\hat{v}) f_d(\mathbf{r}, \hat{v}, t) d\hat{v}\Delta t + O(\Delta^2 t)
$$

$$
= \mathbf{M}(\mathbf{r}, t) - \int_V (\hat{v}[\Omega \cdot \hat{v}] + [\Omega \cdot \hat{v}]\hat{v}) f_d(\mathbf{r}, \hat{v}, t) d\hat{v}\Delta t + O(\Delta^2 t).
$$

The time derivative is

$$
\frac{\partial \mathbf{M}}{\partial t} = \lim_{\Delta t \to 0} \frac{\mathbf{M}(\mathbf{r}, t + \Delta t) - \mathbf{M}(\mathbf{r}, t)}{\Delta t}
$$

$$
= \lim_{\Delta t \to 0} \frac{\mathbf{M}(\mathbf{r}, t + \Delta t) - \mathbf{M}(\mathbf{r} + \theta \times \mathbf{r}\Delta t, t + \Delta t) + \mathbf{M}(\mathbf{r} + \theta \times \mathbf{r}\Delta t, t + \Delta t) - \mathbf{M}(\mathbf{r}, t)}{\Delta t}
$$

$$
= \lim_{\Delta t \to 0} \frac{-(\theta \times \mathbf{r}) \cdot \nabla \mathbf{M}(\mathbf{r} + (\theta \times \mathbf{r})a\Delta t, t + \Delta t)\Delta t - \int_V (\hat{v}[\Omega \cdot \hat{v}] + [\Omega \cdot \hat{v}]\hat{v}) f_d(\mathbf{r}, \hat{v}, t) d\hat{v}\Delta t + O(\Delta^2 t)}{\Delta t} \tag{A22}
$$

$$
= -(\theta \times \mathbf{r}) \cdot \nabla \mathbf{M}(\mathbf{r}, t) - \int_V (\hat{v}[\Omega \cdot \hat{v}] + [\Omega \cdot \hat{v}]\hat{v}) f_d(\mathbf{r}, \hat{v}, t) d\hat{v}
$$

$$
= -\mathbf{v} \cdot \nabla \mathbf{M} + \mathbf{M} \cdot \Omega - \Omega \cdot \mathbf{M}.
$$

Notice $\mathbf{Q} = \mathbf{M} - c\frac{\mathbf{I}}{d}$, we have the rotational invariance on $\mathbf{Q}$: $\overset{\square}{\mathbf{Q}} = \frac{\partial \mathbf{Q}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{Q} + [\Omega \cdot \mathbf{Q} - \mathbf{Q} \cdot \Omega] = 0$.

Appendix B: Surface Divergence Theorem

The surface divergence theorem is [53]:

$$
\int_{\partial \Gamma} d\mathbf{l}_i \mathcal{R}_{jkl,\dots} = \int_\Gamma [\nabla_{s,i} \mathcal{R}_{jkl,\dots} + 2\kappa \mathbf{n}_i \mathcal{R}_{jkl,\dots}] ds = \int_\Gamma \nabla_{s,\alpha} \cdot (\mathbf{I}_{s,\alpha i} \mathcal{R}_{jkl,\dots}) ds. \tag{B1}
$$

This leads to the integration by parts formula,

$$
\int_\Gamma [\nabla_{s,i}(\mathcal{R}_{jkl,\dots}) \mathcal{S}_{\alpha\beta,\gamma,\dots}] ds = - \int_\Gamma \mathcal{R}_{jkl,\dots} \nabla_{s,i} \mathcal{S}_{\alpha\beta,\gamma,\dots} ds +
$$
$$
\int_{\partial \Gamma} d\mathbf{l}_i \mathcal{R}_{jkl,\dots} \mathcal{S}_{\alpha\beta,\gamma,\dots} - \int_\Gamma 2\kappa \mathbf{n}_i \mathcal{R}_{jkl,\dots} \mathcal{S}_{\alpha\beta,\gamma,\dots} ds, \tag{B2}
$$

where $\kappa = \frac{1}{2}(\kappa_1 + \kappa_2)$ is the mean surface curvature, κ_1, κ_2 are the principal curvatures of the surface.

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