From microscopic theory to macroscopic theory: dynamics of the rod-like liquid crystal molecules

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Abstract

Starting from Doi-Onsager equation for the liquid crystal, we first derive the Q-tensor equation by the Bingham closure. Then we derive the Ericksen-Leslie equation from the Q-tensor equation by taking the small Deborah number limit.

1 Introduction

Liquid crystals are a state of matter that have properties between those of a conventional liquid and those of a solid crystal. One of the most common liquid crystal phases is the nematic. The nematic liquid crystals are composed of rod-like molecules with the long axes of neighboring molecules approximately aligned to one another. There are three different kinds of theories to model the nematic liquid crystals.

1.1 Doi-Onsager theory

The state of alignment of the nematic liquid crystal molecules (LCP) is described by the orientational distribution function. A classic model that predicts isotropic-nematic phase transition is the hard-rod model proposed by Onsager [23], in which the rod-rod interaction is modeled by the excluded volume effect. Maier and Saupe [19] following Onsager proposed a slightly modified interaction potential, now known as the Maier-Saupe potential. Doi and Edwards [6] extended Onsager’s theory in order to describe the behavior of liquid crystal polymer flows.

We use $x \in \mathbb{R}^3$ to denote the material point and $f(x, m, t)$ to represent the number density for the number of molecules whose orientation is parallel to $m$ at point $x$ and time $t$. For the spatially homogeneous liquid crystal flow, the Doi-Onsager equation [6] takes

$$\frac{\partial f}{\partial t} = \frac{1}{De} \mathcal{R} \cdot (\nabla f + f\mathcal{R}U) - \mathcal{R} \cdot (m \times \kappa \cdot mf),$$

where $De$ is the Deborah number, $\mathcal{R} = m \times \nabla m$ is the rotational gradient operator, $\kappa$ is a constant velocity gradient, and $U$ is the mean-field interaction potential. This model has a
free energy
\[ A[f] = \int_{S^2} \left( f(m,t) \ln f(m,t) + \frac{1}{2} f(m,t) U(m,t) \right) dm \] (1.2)
as its Lyapunov functional.

The homogeneous Doi-Onsager equation has been very successful in describing the properties of liquid crystal polymers in a solvent. This model takes into account the effects of hydrodynamic flow, Brownian motion, and intermolecular forces on the molecular orientation distribution. However, it does not include effects such as distortional elasticity. Therefore, it is valid only in the limit of spatially homogeneous flows.

Inhomogeneous flows were first studied by Marrucci and Greco [21], and subsequently by many people [11, 27]. Instead of using the distribution as the sole order parameter, they used a combination of the tensorial order parameter and the distribution function, and used the spatial gradients of the tensorial order parameter to describe the spatial variations. This is a departure from the original motivation that led to the kinetic theory. Wang, E, Liu and Zhang [28] set up a formalism in which the interaction between molecules is treated more directly using the position-orientation distribution function via interaction potentials. They extended the free energy (1.2) to include the effects of nonlocal intermolecular interactions through an interaction potential as follows:
\[ A_\varepsilon[f] = \int_{\mathbb{R}^3} \int_{S^2} f(x,m,t)(\ln f(x,m,t) - 1) + \frac{1}{2} U_\varepsilon(x,m,t)f(x,m,t)dm dx, \]
\[ U_\varepsilon(x,m,t) = \int_{\mathbb{R}^3} \int_{S^2} B_\varepsilon(x,x',m,m')f(x',m',t)dm'dx'. \]

Here \( B_\varepsilon(x,x';m,m') \) is the interaction kernel. There are two typical choices:

1. Long range Maier-Saupe interaction potential:
\[ B_\varepsilon(x,x',m,m') = \frac{1}{\varepsilon^3/2} g\left(\frac{x-x'}{\sqrt{\varepsilon}}\right)\alpha|m \times m'|^2, \]
where \( g(x) \in C^\infty(\mathbb{R}^3) \) is a radial function with \( \int_{\mathbb{R}^3} g(x)dx = 1 \), and the small parameter \( \sqrt{\varepsilon} \) represents the typical interaction distance.

2. Hard-core interaction potential:
\[ B_\varepsilon(x,x',m,m') = \begin{cases} 0, & \text{molecule}(x,m) \text{ is disjoint with molecule } (x',m'), \\ 1, & \text{joint with each other}. \end{cases} \]

In this paper, we first focus on the Maier-Saupe case. In the last section, we will discuss the hard-core potential case.

The chemical potential \( \mu_\varepsilon \) is defined as
\[ \mu_\varepsilon = \frac{\delta A_\varepsilon[f]}{\delta f} = \ln f(x,m,t) + U_\varepsilon(x,m,t). \]

We also introduce non-interacting kernel
\[ B_0(x,x',m,m') = \alpha|m \times m'|^2\delta(x-x'). \]
We denote by $U_0$, $\mu_0$, $A_0[f]$ the corresponding non-interacting potential, chemical potential and free energy respectively. Throughout this paper, we use the notation

$$\langle \cdot \rangle_f = \int_{S^2} \cdot (x, m, t) dm.$$  

The non-dimensional Doi-Onsager equation takes the form:

$$\frac{\partial f}{\partial t} + v \cdot \nabla f = \frac{\varepsilon}{De} \nabla \cdot \left\{ \left( \gamma \parallel mm + \gamma \perp (I - mm) \right) \cdot (\nabla f + f \nabla U_\varepsilon) \right\} \quad (1.5)$$

$$\frac{\partial v}{\partial t} + v \cdot \nabla v = -\nabla p + \frac{\gamma}{Re} \Delta v + \frac{1 - \gamma}{2Re} \nabla \cdot (D : \langle mmmm \rangle_f) + \frac{1 - \gamma}{DeRe} (\nabla \cdot \tau^e + F^e) \quad (1.6)$$

where $\kappa = (\nabla v)^T$, $D = \frac{1}{2} (\kappa + \kappa^T)$, while $\tau^e$ and $F^e$ represent the elastic stress and body force respectively defined as

$$\tau^e = -\langle mm \times R\mu_\varepsilon \rangle_f = (3 \langle mm - \frac{1}{3} I \rangle_f - \langle mm \times RU_\varepsilon \rangle_f), \quad F^e = -\langle \nabla \mu_\varepsilon \rangle_f.$$  

The constants $\gamma \parallel$ and $\gamma \perp$ denote the translational diffusion coefficients parallel to and normal to the orientation of the LCP molecule respectively. In the case when $\gamma \parallel = \gamma \perp = 0$, we may assume that $\int_{S^2} f(x, m) dm = 1$, which means that the density of the molecular is constant.

The Doi-Onsager equation (1.5) has the following the energy dissipation relation:

$$-\frac{d}{dt} \left[ \int_{\mathbb{R}^3} \frac{1}{2} |v|^2 dx + \frac{1 - \gamma}{DeRe} A_\varepsilon[f] \right] = \int_{\mathbb{R}^3} \left( \frac{\gamma}{Re} D : D + \frac{1 - \gamma}{2Re} (\langle mm : D \rangle^2)_f + \frac{1 - \gamma}{De^2Re} (\langle R\mu \cdot R\mu \rangle)_f \right. \left. + \frac{\varepsilon}{De^2Re} \langle \nabla \mu \cdot (\gamma \parallel mm + \gamma \perp (I - mm)) \cdot \nabla \mu \rangle_f \right) dx. \quad (1.7)$$

### 1.2 Landau-de Gennes theory (Q-tensor theory)

One of continuum theory for the nematic liquid crystals is the Landau-de Gennes theory [5]. In this theory, the state of the nematic liquid crystals is described by the macroscopic Q-tensor order parameter, which is a symmetric, traceless $3 \times 3$ matrix. Physically, it can be interpreted as the second-order moment of the orientational distribution function $f$, that is, 

$$Q = \int_{S^2} (mm - \frac{1}{3} I) f dm.$$  

When $Q = 0$, the nematic liquid crystal is said to be isotropic. When $Q$ has two equal non-zero eigenvalues, it is said to be uniaxial. In such case, $Q$ can be written as

$$Q = s (nn - \frac{1}{3} I), \quad n \in S^2.$$
When \( Q \) has three distinct eigenvalues, it is said to be biaxial. In such case, \( Q \) can be written as

\[
Q = s(n n' - \frac{1}{3} I) + \lambda(n n' - \frac{1}{3} I), \quad n, n' \in S^2, \quad n \cdot n' = 0.
\]

The Landau-de Gennes energy functional \( E_{LG} \) is given by

\[
E_{LG} = \int_{\mathbb{R}^3} w(Q, \nabla Q) + f_{\text{bulk}}(Q) d\mathbf{x},
\]

where \( w \) is the elastic energy, which in general takes

\[
w(Q, \nabla Q) = L_1 |\nabla Q|^2 + L_2 Q_{ij,k} Q_{ij,k} + L_3 Q_{ij,j} Q_{ik,k} + L_4 Q_{kl} Q_{ij,k} Q_{ij,l},
\]

where \( Q = (Q_{ij}), \quad Q_{ij,k} = \frac{\partial Q_{ij}}{\partial x_k} \) and \( L_1, \ldots, L_4 \) are elastic constants; \( f_{\text{bulk}} \) is the bulk energy which in the simplest form takes

\[
f_{\text{bulk}}(Q) = a \text{tr}(Q^2) + 2b \text{tr}(Q^3) + c \left( \text{tr}(Q^2) \right)^2,
\]

where \( a, b, c \) are temperature dependent constants. We refer to [22] for more details.

There are two popular dynamical \( Q \)-tensor models for liquid crystals, which are derived by Beris-Edwards [2] and Qian-Sheng [25] separately. When the total energy in \( Q \)-tensor form is given by \( E(Q, \nabla Q) \), we define

\[
\mu_Q = \frac{\delta E(Q, \nabla Q)}{\delta Q}.
\]

The dynamical \( Q \)-tensor theory could written in the following form in general:

\[
\begin{align*}
\frac{\partial Q}{\partial t} + \mathbf{v} \cdot \nabla Q & = D^{\text{rot}}(\mu_Q) + F(Q, \mathbf{D}) + \mathbf{\Omega} \cdot Q - \mu_Q \cdot \mathbf{\Omega}, \\
\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} & = -\nabla p + \nabla \cdot (\sigma^{\text{dis}} + \sigma^a + \sigma^d),
\end{align*}
\]

where \( D^{\text{rot}}(\mu_Q) \) is the rotational diffusion term, \( F(Q, \mathbf{D}) \) is the velocity-induced term, and \( \sigma^d \) is the distortion stress, \( \sigma^a \) is the anti-symmetric part of orientational-induced stress, \( \sigma^s = \gamma F(Q, \mu_Q) \) is the symmetric stress induced by the orientational, which conjugates to \( F(Q, \mathbf{D}) \) (\( \gamma \) is a constant), \( \sigma^{\text{dis}} \) is the additional dissipation stress.

In Beris-Edwards’s model and Qian-Shen’s model, module some constants, \( \sigma^a \) and \( \sigma^d \) are the same, i.e.,

\[
\sigma^a_{ij} = \frac{\partial E}{\partial (Q_{kl,j})} Q_{kl,i}, \quad \sigma^a = Q \cdot \mu_Q - \mu_Q \cdot Q.
\]

In Beris-Edwards’s model, the other terms are given by

\[
\begin{align*}
D^{\text{rot}}_{BE} & = -\Gamma \mu_Q, \quad \sigma^{\text{dis}}_{BE} = 0, \quad \sigma^a_{BE} = F_{BE}(Q, \mu_Q), \\
F_{BE}(Q, A) & = \xi \left( (Q + \frac{1}{3} \mathbf{I}) \cdot A + A \cdot (Q + \frac{1}{3} \mathbf{I}) - 2(Q + \frac{1}{3} \mathbf{I})(A : Q) \right).
\end{align*}
\]
In Qian-Sheng’s model, they are given by

$$D_{QS}^{\text{rot}} = -\Gamma \mu_Q, \quad \sigma_{QS}^2 = -\frac{1}{2} \mu_2^2 \mu_Q, \quad F_{QS}(Q, D) = -\frac{1}{2} \mu_2 D,$$

$$\sigma_{QS}^{\text{dis}} = \beta_1(Q : A) + \beta_2 D + \beta_3(Q \cdot D + D \cdot Q).$$

There are also other dynamic models by using $Q$ tensor to describe the flow of the nematic liquid crystals, which are obtained by various closure approximations or the variational principle. We refer to [11, 12, 26] and references therein.

1.3 Ericksen-Leslie theory

The Ericksen-Leslie theory [8, 9, 16] is an elastic continuum theory, which is a very powerful tool for modeling liquid crystal devices. This theory treats the liquid crystal material as a continuum and completely ignores molecular details. Moreover, this theory considers perturbations to a presumed oriented sample.

In this theory, the configuration of the liquid crystals is described by a director field $n(x, t)$. The Ericksen-Leslie equation takes the form

$$\begin{cases}
v_t + v \cdot \nabla v = -\nabla p + \frac{\gamma}{Re} \Delta v + \frac{1 - \gamma}{Re} \nabla \cdot \sigma, \\
\nabla \cdot v = 0, \\
n \times (h - \gamma_1 N - \gamma_2 D \cdot n) = 0,
\end{cases}$$

(1.13)

where $v$ is the velocity of the fluid, $p$ is the pressure, $Re$ is the Reynolds number and $\gamma \in (0, 1)$. The stress $\sigma$ is modeled by the phenomenological constitutive relation

$$\sigma = \sigma^L + \sigma^E,$$

where $\sigma^L$ is the viscous (Leslie) stress

$$\sigma^L = \alpha_1(nn : D)nn + \alpha_2nN + \alpha_3Nn + \alpha_4 D + \alpha_5nn \cdot D + \alpha_6D \cdot nn$$

(1.14)

with $D = \frac{1}{2}(\kappa^T + \kappa)$, $\kappa = (\nabla v)^T$, and

$$N = n_t + v \cdot \nabla n + \Omega \cdot n, \quad \Omega = \frac{1}{2}(\kappa^T - \kappa).$$

The six constants $\alpha_1, \cdots, \alpha_6$ are called the Leslie coefficients. While, $\sigma^E$ is the elastic (Ericksen) stress

$$\sigma^E = -\frac{\partial E_F}{\partial (\nabla n)} \cdot (\nabla n)^T,$$

(1.15)

where $E_F = E_F(n, \nabla n)$ is the Oseen-Frank energy with the form

$$E_F = \frac{k_1}{2} (\nabla \cdot n)^2 + \frac{k_2}{2} |n \cdot (\nabla \times n)|^2 + \frac{k_3}{2} |n \times (\nabla \times n)|^2 + \frac{1}{2}(k_2 + k_4)(\text{tr}(\nabla n)^2 - (\nabla \cdot n)^2).$$
Here \( k_1, k_2, k_3, k_4 \) are the elastic constant. Especially, in the case when \( k_1 = k_2 = k_3 = 1 \) and \( k_4 = 0 \), we have \( E_F = \frac{1}{2} |\nabla n|^2 \), and the molecular field \( h \) is given by

\[
\mathbf{h} = -\frac{\delta E_F}{\delta n} = \nabla \cdot \frac{\partial E_F}{\partial (\nabla n)} - \frac{\partial E_F}{\partial n} = -\Delta n,
\]

\[
(\sigma^F)_{ij} = - (\nabla n \odot \nabla n)_{ij} = - \partial_i n_k \partial_j n_k.
\]

The Leslie coefficients and \( \gamma_1, \gamma_2 \) satisfy the following relations

\[
\alpha_2 + \alpha_3 = \alpha_6 - \alpha_5, \quad (1.16)
\]

\[
\gamma_1 = \alpha_3 - \alpha_2, \quad \gamma_2 = \alpha_6 - \alpha_5, \quad (1.17)
\]

where (1.16) is called Parodi’s relation derived from the Onsager reciprocal relation [24].

These two relations ensure that the system has a basic energy dissipation law:

\[
- \frac{d}{dt} \left( \int_{\mathbb{R}^3} \frac{Re}{2(1 - \gamma)} |\mathbf{v}|^2 \mathbf{d}x + E_F \right) = \int_{\mathbb{R}^3} \left( \frac{\gamma}{1 - \gamma} |\nabla \mathbf{v}|^2 + (\alpha_1 + \frac{\gamma^2}{\gamma_1})(\mathbf{D} : n n)^2 + \alpha_4 \mathbf{D} : \mathbf{D} \right.
\]

\[
\left. + (\alpha_5 + \alpha_6 - \frac{\gamma^2}{\gamma_1})|\mathbf{D} \cdot n|^2 + \frac{1}{\gamma_1} |n \times \mathbf{h}|^2 \right) \mathbf{d}x. \quad (1.18)
\]

### 1.4 From the molecular kinetic theory to the continuum theory

Two kinds of theories were put forward to investigate the liquid crystalline polymers from the different points of view. The Q-tensor theory and Ericksen-Leslie theory are phenomenological. Especially, there are some unknown parameters in the continuum theory, which are difficult to determine by using experimental results. In the spirit of Hilbert sixth problem, it is very important to explore the relationship between these two theories.

Our goal is to derive two commonly used continuum theories: Q-tensor theory and Ericksen-Leslie theory starting from Doi-Onsager theory. In [15, 7], Kuzzu-Doi and E-Zhang formally derive the Ericksen-Leslie equation from the Doi-Onsager equations by taking small Deborah number limit. We justify their formal derivation in our recent work [29]. An natural question is whether one can derive the Ericksen-Leslie model from the Q-tensor models and derive the Q-tensor model from the Doi-Onsager equations. In the static case, similar questions have been studied by Ball-Majumdar [1], Majumdar-Zarnescu [20] and the second paper in this series [13].

In this paper, we first derive a new Q-tensor model by the Bingham closure, then we derive the Ericksen-Leslie equation from the derived Q-tensor model (see Fig. 1). The existing Q-tensor models are usually derived by various closure approximations, such as the Doi’s quadratic closure [6], the HL closures [14], the orthotropic closure [3] and the Bingham closure [4]. Feng et al. [12] provided detailed numerical comparisons among five commonly used closures and found that the Bingham closure gives better results than others. Moreover, in these closure methods, the Bingham closure seems to be the only one which persists the energy dissipation law.
2 From Doi-Onsager equation to Q-tensor equation

2.1 Bingham closure and Q-tensor equation

The Bingham closure is a kind of quasi-equilibrium closure approximation. The idea is to calculate $\langle \mathbf{m} \mathbf{m} \mathbf{m} \mathbf{m} \rangle_f$ by using the quasi-equilibrium $f_Q$ given by

$$
    f_Q = \frac{\exp(\mathbf{m} : B_Q)}{\int_{S^2} \exp(\mathbf{m} : B_Q) d\mathbf{m}}, \quad Q = \int_{S^2} (\mathbf{m} - \frac{1}{3} \mathbf{I}) f d\mathbf{m}.
$$

(2.1)

Given a symmetric and trace free matrix $Q$, the symmetric traceless matrix $B_Q$ is determined by the following relation:

$$
    Q = \frac{\int_{S^2} (\mathbf{m} - \frac{1}{3} \mathbf{I}) \exp(\mathbf{m} : B_Q) d\mathbf{m}}{\int_{S^2} \exp(\mathbf{m} : B_Q) d\mathbf{m}}.
$$

(2.2)

Remark 2.1. If the eigenvalues $\lambda_i (i = 1, 2, 3)$ of $Q$ satisfy the constraint:

$$
    -\frac{1}{3} < \lambda_i < \frac{2}{3} \quad i = 1, 2, 3,
$$

then $B_Q$ is uniquely determined by $Q$ (see [7]).

We denote

$$
    Z_Q = \int_{S^2} \exp(\mathbf{m} : B_Q) d\mathbf{m}, \quad M_Q^{(4)} = \int_{S^2} \mathbf{m} \mathbf{m} \mathbf{m} \mathbf{m} f_Q d\mathbf{m},
$$

$$
    M_Q^{(6)} = \int_{S^2} \mathbf{m} \mathbf{m} \mathbf{m} \mathbf{m} \mathbf{m} \mathbf{m} f_Q d\mathbf{m}, \quad Q^\varepsilon = \int_{\mathbb{R}^3} g_\varepsilon(\mathbf{x} - \mathbf{x}') Q(\mathbf{x}') d\mathbf{x}'.
$$
It is easy to compute that
\[ U_\varepsilon f = -\alpha \int_{\mathbb{R}^3} \int_{\mathbb{R}^2} (\mathbf{m} \cdot \mathbf{m}')^2 f(x', \mathbf{m}') g_\varepsilon(x - x') \, dx' \, dm \]
\[ = -\alpha (\mathbf{mm} - \frac{1}{3} \mathbf{I}) : Q^\varepsilon, \]
\[ \mu_\varepsilon f = \mathbf{mm} : B_Q - \ln Z_Q - \alpha (\mathbf{mm} - \frac{1}{3} \mathbf{I}) : Q^\varepsilon, \]
\[ \mathcal{R}_\mu \mu_\varepsilon f = \mathbf{m} \times ((B_Q - \alpha Q^\varepsilon) \cdot \mathbf{m}). \]

Introduce the operator
\[ \mathcal{M}_Q(A) = \frac{1}{3} A + Q \cdot A - A : M_Q^{(4)}, \]
\[ N_Q(A)_{\alpha\beta} = \partial_i \left\{ \frac{1}{2} \left( M_Q(M_{\alpha\beta\kappa\lambda}) \delta_{ij} - \frac{\delta_{\alpha\beta} M_{\kappa\lambda}}{3} \right) + (\gamma - \gamma_1) \left( M_{\alpha\beta\kappa\lambda} - \frac{\delta_{\alpha\beta} M_{\kappa\lambda}}{3} \right) \right\} \partial_j A_{k\ell}. \]

Then the Doi-Onsager equation (1.5) is transformed to a system in terms of \((Q, \mathbf{v})\):
\[ \frac{\partial Q}{\partial t} + \mathbf{v} \cdot \nabla Q = \frac{\varepsilon}{D_\varepsilon} N_Q(B_Q - \alpha Q^\varepsilon) + \frac{1}{D_\varepsilon} \left( -6Q + 2\alpha [\mathcal{M}_Q(Q^\varepsilon) + \mathcal{M}_Q^T(Q^\varepsilon)] \right) \]
\[ + (\mathcal{M}_Q(\kappa^T) + \mathcal{M}_Q^T(\kappa^T)), \]
\[ \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} = -\nabla p + \frac{\gamma}{Re} \Delta \mathbf{v} + \frac{1 - \gamma}{2Re} \nabla \cdot (\mathbf{D} : M_Q^{(4)}) \]
\[ + \frac{1 - \gamma}{D_\varepsilon Re} \left( -\nabla \cdot [ -3Q + 2\alpha M_Q(Q^\varepsilon)] + \alpha Q : \nabla Q^\varepsilon \right). \]

Since the typical interaction distance \(\sqrt{\varepsilon}\) is very small, we make the following Taylor expansion for \(Q^\varepsilon\):
\[ Q^\varepsilon(x) = Q(x) + \frac{\varepsilon}{2} \Delta Q(x) + O(\varepsilon^2), \]
where the constant \(G = \frac{1}{3} \int_{\mathbb{R}^3} g(y) |y|^2 \, dy.\)

Replacing \(Q^\varepsilon\) by \(Q(x) + \varepsilon \frac{G}{2} \Delta Q(x)\) in (2.3)-(2.4), we derive the following Q-tensor equation from the Doi-Onsager equation:
\[ \frac{\partial Q}{\partial t} + \mathbf{v} \cdot \nabla Q = \frac{\varepsilon}{D_\varepsilon} N_Q(B_Q - \alpha Q - \frac{G}{2} \alpha \varepsilon \Delta Q) + (\mathcal{M}_Q(\kappa^T) + \mathcal{M}_Q^T(\kappa^T)) \]
\[ + \frac{1}{D_\varepsilon} \left( -6Q + 2\alpha [\mathcal{M}_Q(Q + \frac{G}{2} \varepsilon \Delta Q) + \mathcal{M}_Q^T(Q + \frac{G}{2} \varepsilon \Delta Q)] \right), \]
\[ \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} = -\nabla p + \frac{\gamma}{Re} \Delta \mathbf{v} + \frac{1 - \gamma}{2Re} \nabla \cdot (\mathbf{D} : M_Q^{(4)}) \]
\[ + \frac{1 - \gamma}{D_\varepsilon Re} \left( -\nabla \cdot [ -3Q + 2\alpha M_Q(Q + \frac{G}{2} \varepsilon \Delta Q)] + \frac{1}{2} G \alpha \varepsilon Q : \nabla Q^\varepsilon \right). \]

### 2.2 Energy dissipation law of Q-tensor equation

In this subsection, we derive the energy dissipation law of Q-tensor equation (2.5)-(2.6). We need the following lemmas.
Lemma 2.1. For any symmetric and trace free matrix $Q$, there hold

$$
\frac{3}{2}Q = \mathcal{M}_Q(B_Q) \equiv B_Q \cdot Q + \frac{1}{3}B_Q - B_Q : M_Q^{(4)};
B_Q \cdot Q = Q \cdot B_Q.
$$

Proof. For any constant matrix $\kappa$, we have

$$
0 = \int \left( \mathbf{m} \times (\kappa \cdot \mathbf{m}) \cdot \mathcal{R} f_Q + \mathcal{R} \cdot (\mathbf{m} \times (\kappa \cdot \mathbf{m})) f_Q \right) d\mathbf{m}
$$

$$
= \int \left\{ 2 \mathbf{m} \times (\kappa \cdot \mathbf{m}) \cdot (\mathbf{m} \times (B_Q \cdot \mathbf{m})) + (I - 3\mathbf{m} \otimes \mathbf{m}) : \kappa f_Q \right\} d\mathbf{m}
$$

$$
= \kappa : (2B_Q \cdot \mathbf{m} - 2B_Q : M_Q^{(4)} - 3Q),
$$

where $M_Q = \int \mathbf{m} \otimes \mathbf{m} f_Q d\mathbf{m} = Q + \frac{1}{3}I$, which implies the first equality. The second equality is a direct consequence of the first equality by noting that $Q, B_Q$ are symmetric. □

Lemma 2.2. For any matrix $E$, there holds

$$
M_Q(E) : E \equiv E : (Q + \frac{1}{3}I) \cdot E - E : M_Q^{(4)} : E = \int_{S^2} \mathbf{m} \times (E \cdot \mathbf{m})^2 f_Q d\mathbf{m} \geq 0.
$$

$$
\int \mathcal{N}(E) : E dx = - \int \left[ \gamma \| \mathbf{m} \|^2 + \gamma_\perp (I - \mathbf{m} \otimes \mathbf{m}) \right]_{ij} f_Q \partial_i \left[ (\mathbf{m} \otimes \mathbf{m}) - \frac{1}{3}I : E \right] \partial_j \left[ (\mathbf{m} \otimes \mathbf{m}) - \frac{1}{3}I : E \right] dx \leq 0.
$$

We define the energy functional

$$
E_1(Q) = \int_{\mathbb{R}^3} \left( - \ln Z_Q + Q : B_Q - \frac{\alpha}{2} Q : Q^\varepsilon \right) dx. \quad (2.7)
$$

The system \((2.3)-(2.4)\) obeys the energy law

$$
\frac{d}{dt} \left\{ \int_{\mathbb{R}^3} \frac{1}{2} |\mathbf{v}|^2 dx + \frac{1 - \gamma}{Re De} E_1(Q) \right\}
$$

$$
= -\int_{\mathbb{R}^3} \left\{ \gamma \frac{Re}{D} |\mathbf{D}|^2 + \frac{1 - \gamma}{2Re} \mathbf{D} : M_Q^{(4)} : \mathbf{D} - (B_Q - \alpha Q^\varepsilon) : \mathcal{N}(B_Q - \alpha Q^\varepsilon)
+ \frac{4(1 - \gamma)}{Re De^2} \left( B_Q - \alpha Q^\varepsilon \right) : \mathcal{M}_Q \left( B_Q - \alpha Q^\varepsilon \right) \right\} dx. \quad (2.8)
$$

An important property is that the energy law \((2.8)\) is dissipated by Lemma 2.2.

Now let us prove \((2.8)\). It is easy to see that

$$
\mathcal{M}_Q(A) : B = \mathcal{M}_Q(B) : A, \quad (2.9)
$$

if $A$ or $B$ is symmetric. A direct computation tells us that

$$
\frac{\partial}{\partial Q} \left( - \ln Z_Q + Q : B_Q \right) = B_Q. \quad (2.10)
$$
Then by using (2.3)-(2.4), we obtain
\[
\frac{d}{dt} E_1(Q) = \int_{\mathbb{R}^3} (B_Q - \alpha Q_\varepsilon) : \partial_t Q \, dx
\]
\[
= \int_{\mathbb{R}^3} \frac{1}{De} (B_Q - \alpha Q_\varepsilon) : \left( -6Q + 2\alpha \left[ M_Q(Q_\varepsilon) + M_Q^T(Q_\varepsilon) \right] \right) + \frac{\varepsilon}{De} (B_Q - \alpha Q_\varepsilon) : N(B_Q - \alpha Q_\varepsilon)
\]
\[
+ (B_Q - \alpha Q_\varepsilon) : \left( M_Q(\kappa^T) + M_Q^T(\kappa^T) - \nu \cdot \nabla Q \right) \, dx,
\]
\[
\frac{d}{dt} \int_{\mathbb{R}^3} \frac{1}{2} |v|^2 \, dx = \int_{\mathbb{R}^3} \left\{ -\gamma \frac{\varepsilon}{Re} |\mathbf{D}|^2 - \frac{1-\gamma}{2Re} \mathbf{D} : M_Q^{(4)} : \mathbf{D}
\right.
\]
\[
+ \frac{1}{DeRe} \left[ -3Q + 2\alpha M_Q(Q_\varepsilon) \right] : \nabla v + \alpha Q : (v \cdot \nabla Q_\varepsilon) \right\} \, dx,
\]
from which, Lemma 2.1 and (2.9), we infer that
\[
\frac{d}{dt} \left( \frac{1}{ReDe} E_1(Q) + \int_{\mathbb{R}^3} \frac{1}{2(1-\gamma)} |v|^2 \, dx \right)
\]
\[
= \int_{\mathbb{R}^3} \left\{ -\frac{\varepsilon}{ReDe} (B_Q - \alpha Q_\varepsilon) : N(B_Q - \alpha Q_\varepsilon) - \frac{4}{ReDe^2} (B_Q - \alpha Q_\varepsilon) : M_Q(B_Q - \alpha Q_\varepsilon)
\right.
\]
\[
+ \frac{1}{ReDe} (B_Q - \alpha Q_\varepsilon) : \left( 2M_Q(\kappa^T) - \nu \cdot \nabla Q \right) - \frac{\gamma}{Re(1-\gamma)} |\mathbf{D}|^2 - \frac{1}{2Re} \mathbf{D} : M_Q^{(4)} : \mathbf{D}
\]
\[
+ \frac{1}{DeRe} \left[ -2M_Q(B_Q - \alpha Q_\varepsilon) : \nabla v + \alpha Q : (v \cdot \nabla Q_\varepsilon) \right\} \, dx
\]
\[
= - \int_{\mathbb{R}^3} \left\{ -\frac{\varepsilon}{ReDe} (B_Q - \alpha Q_\varepsilon) : N(B_Q - \alpha Q_\varepsilon) + \frac{4}{ReDe^2} (B_Q - \alpha Q_\varepsilon) : M_Q(B_Q - \alpha Q_\varepsilon)
\right.
\]
\[
+ \frac{\gamma}{Re(1-\gamma)} |\mathbf{D}|^2 + \frac{1}{2Re} \mathbf{D} : M_Q^{(4)} : \mathbf{D} \right\} \, dx.
\]
Define the energy functional
\[
E_2(Q) = \int_{\mathbb{R}^3} -\ln Z_Q + Q : B_Q + \frac{\alpha}{2} \left( -|Q|^2 + \frac{G}{2\varepsilon} |\nabla Q|^2 \right) \, dx. \tag{2.11}
\]
Then the system (2.5)-(2.6) obeys the following energy dissipation law
\[
\frac{d}{dt} \left\{ \int_{\mathbb{R}^3} \frac{1}{2} |v|^2 \, dx + \frac{1-\gamma}{2Re} E_2(Q) \right\} = -\int_{\mathbb{R}^3} \left\{ \frac{\gamma}{Re} |\mathbf{D}|^2 + \frac{1-\gamma}{2Re} \mathbf{D} : M_Q^{(4)} : \mathbf{D}
\right.
\]
\[
- \frac{\varepsilon}{ReDe^2} (B_Q - \alpha Q - \frac{G}{2\alpha\varepsilon} \Delta Q) : N(B_Q - \alpha Q - \frac{G}{2\alpha\varepsilon} \Delta Q)
\]
\[
+ \frac{4(1-\gamma)}{ReDe^2} (B_Q - \alpha Q - \frac{G}{2\alpha\varepsilon} \Delta Q) : M_Q(B_Q - \alpha Q - \frac{G}{2\alpha\varepsilon} \Delta Q) \right\} \, dx. \tag{2.12}
\]

2.3 Some remarks on new Q-tensor equation

New tensor equation (2.5)-(2.6) derived from the Doi-Onsager equation by the Bingham closure keeps many important physical properties:

- Two kinds of physical diffusions (translational and rotational diffusion) are preserved;
• The parameters are not phenomenological but have definite physical meaning;
• The eigenvalues of $Q$ satisfy the physical constrain: $-\frac{1}{3} \leq \lambda_i \leq \frac{2}{3}$ if they are satisfied initially;
• The Ericksen-Leslie equation can be deduced from the Q-tensor equation by taking the small Deborah number limit.

Furthermore, we want to comment that Q-tensor equation can be viewed as some kind of regularization of the Ericksen-Leslie equation, since it removes the constrain $|n| = 1$, and allows the liquid crystal to be biaxial. Motivated by the work of the harmonic heat flow, the classical regularization of the Ericksen-Leslie equation is to add a penalty term $\frac{1}{\varepsilon}(|n|^2 - 1)^2$ in $E_F$ to remove some higher-order nonlinearities due to the constrain $|n| = 1$ [17]. That is so called the Ginzburg-Landau approximation. However, whether the Ericksen-Leslie equation can be recovered from the approximated equation by taking $\varepsilon \to 0$ is still a challenging question. Moreover, the physical meaning of Ginzburg-Landau approximation is also unclear.

3 The critical points of the bulk free energy

Let $F_B(Q)$ be the bulk energy of $E_2(Q)$, that is,

$$F_B(Q) = \int_{\mathbb{R}^3} -\ln Z_Q + Q : B_Q - \frac{\alpha}{2} |Q|^2 dx.$$  \hspace{1cm} (3.1)

Due to (2.10), it is easy to see that its critical point satisfies the equation

$$B_Q = \alpha Q.$$  

The solution of this equation is related to the critical points of the Maier-Saupe energy functional. More precisely, the following proposition has been proven by [10] [18] [31].

**Proposition 3.1.** Let $\eta$ be a solution of the equation

$$\frac{3e^\eta}{\int_0^1 e^{\eta z^2} dz} = 3 + 2\eta + \frac{\eta^2}{\alpha}. \hspace{1cm} (3.2)$$

Then

$$B_Q - \alpha Q = 0 \iff B_Q = \eta(\eta - \frac{1}{3}I), \quad n \in S^2.$$  \hspace{1cm} (3.3)

There exists a critical number $\alpha^* > 0$ such that

1. When $\alpha < \alpha^*$, $\eta = 0$ is the only solution of (3.2);
2. When $\alpha = \alpha^*$, except $\eta = 0$, there is another solution $\eta = \eta^*$ of (3.2);
3. When $\alpha > \alpha^*$, except $\eta = 0$, there are other two solutions $\eta_1 > \eta^* > \eta_2$ of (3.2).
In the sequel, we always take \( \eta = \eta_1 \). Let \( A_k = \int_0^1 x^k e^{\eta x^2} dx \). The following facts have been proved in \([29]\): for \( \eta > \eta^* \)

\[
3A_2^2 + 2A_0 A_2 - 5A_0 A_4 > 0, \quad 6A_2 - 5A_4 - A_0 > 0.
\]  

(3.4)

We also define

\[
S_2 = \frac{3A_2 - A_0}{2A_0}, \quad S_4 = \frac{1}{8A_0} (35A_4 - 30A_2 + 3A_0).
\]  

(3.5)

If \( B_{Q_0} = \alpha Q_0 \), then we have

\[
Q_0 = S_2 (nn - \frac{1}{3} I), \quad B_0 \equiv B_{Q_0} = \eta (nn - \frac{1}{3} I).
\]  

(3.6)

In such case, we have

\[
f_0 \equiv f_{Q_0} = \frac{e^{\eta (nn)^2}}{\int_{S^2} e^{\eta (nn)^2} d\mathbf{n}},
\]

\[
M_{Q_0,ijkl}^{(4)} = S_4 n_in_j n_k n_l + \frac{S_2 - S_4}{7} \left( n_i n_j \delta_{kl} + n_i n_k \delta_{jl} + n_i n_l \delta_{jk} + n_j n_k \delta_{il} + n_j n_l \delta_{ik} + n_k n_l \delta_{ij} \right) + \left( \frac{S_4}{35} - \frac{2S_2}{21} + \frac{1}{15} \right) (\delta_{ij} \delta_{kl} + \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}).
\]

Now we introduce some linear operators associated to the critical point \( Q_0 \), which will play an important role in the derivation of the Ericksen-Leslie equation from the Q-tensor equation. We first introduce the space

\[ \mathcal{S} = \{ B \in M^{3 \times 3} : B \text{ is symmetric and trace free} \} \]

endowed with the inner product

\[ (B_1, B_2)_{\mathcal{S}} \equiv B_1 : B_2 = \sum_{i,j=1,2,3} B_{1ij} B_{2ij}. \]

Given \( n \in S^2 \), the linear operators \( Q_n, J_n, K_n, L_n : \mathcal{S} \to \mathcal{S} \) defined as

\[
Q_n(B) = M_{Q_0}^{(4)} : B - \frac{1}{3} I (Q_0 : B) - Q_0 (Q_0 : B),
\]

\[
J_n(B) = \frac{1}{3} B + \frac{1}{2} (B \cdot Q_0 + Q_0 \cdot B) - B : M_{Q_0}^{(4)},
\]

\[
K_n(B) = B - \alpha Q_n(B),
\]

\[
L_n(B) = -2J_n(K_n(B)),
\]

where the operator \( L_n \) can be written as

\[
L_n(B) = \frac{1}{3} (B - \alpha Q_n(B)) + \frac{1}{2} ((B - \alpha Q_n(B)) \cdot Q_0 + Q_0 \cdot (B - \alpha Q_n(B))) - (B - \alpha Q_n(B)) : M_{Q_0}^{(4)}.
\]

\[ \text{Proposition 3.2.} \quad \text{We have the following properties:} \]

1. \( Q_n, J_n, K_n, L_n \) are self-adjoint.
2. $J_n$ is positive, and $\mathcal{K}_n$ is non-negative;

3. $\ker \mathcal{K}_n = \ker L_n = \{ \mathbf{n} \perp + \mathbf{n} \perp : \mathbf{n} \perp \in \mathbb{R}^3, \mathbf{n} \cdot \mathbf{n} \perp = 0 \}$.

Proof. It is easy to see that $Q_n$, $J_n$, $\mathcal{K}_n$ are self-adjoint. In the following, we prove that $L_n$ is self-adjoint. We have

$$Q_0 \cdot Q_n(B_1) = Q_0 \cdot \left( S_4 \mathbf{mn} : B_1 + \frac{S_2 - S_4}{7} (2(\mathbf{n} \cdot B_1 + B_1 \cdot \mathbf{n}) + \mathbf{nn} : B_1) + \frac{S_4}{35} - \frac{2S_2}{21} + \frac{1}{15} \right) 2B_1 - \frac{1}{3} Q_0 \cdot (\mathbf{n} : B_1)$$

$$= S_2 S_4 \frac{2}{3} \mathbf{nn} : B_1 + \frac{S_2 (S_2 - S_4)}{7} \left( \frac{4}{3} \mathbf{n} \cdot B_1 + 3 \mathbf{nn} \cdot B_1 \right) - \frac{2}{3} B_1 \cdot \mathbf{n} - \frac{1}{3} \mathbf{I} (\mathbf{n} : B_1)$$

$$+ \left( \frac{S_4}{35} - \frac{2S_2}{21} + \frac{1}{15} \right) 2S_2 (\mathbf{n} \cdot B_1 - \frac{1}{3} B_1) - \frac{S_2^2}{3} (\mathbf{n} - \frac{1}{3} \mathbf{I}) (\mathbf{n} : B_1).$$

Hence,

$$\langle Q_0 \cdot Q_n(B_1), B_2 \rangle = \langle Q_0 \cdot Q_n(B_2), B_1 \rangle.$$

Similarly, we have

$$\langle Q_n(B_1) \cdot Q_0, B_2 \rangle = \langle Q_n(B_2) \cdot Q_0, B_1 \rangle.$$

On the other hand, we have

$$\langle Q_n(B_1) : M_{Q_0}^{(4)}, B_2 \rangle = \langle Q_n(B_1), M_{Q_0}^{(4)} : B_2 \rangle$$

$$= \langle M_{Q_0}^{(4)} : B_1 + \frac{S_2}{3} \mathbf{I} (\mathbf{n} : B_1) + S_2^2 (\mathbf{n} \cdot B_1 - \frac{1}{3} \mathbf{I}) (\mathbf{n} : B_1), M_{Q_0}^{(4)} : B_2 \rangle$$

$$= \langle M_{Q_0}^{(4)} : B_1, M_{Q_0}^{(4)} : B_2 \rangle + S_2^2 \left( \mathbf{n} : B_1 \right) \left[ \mathbf{nn} : M_{Q_0}^{(4)} : B_2 \right]$$

$$= \langle M_{Q_0}^{(4)} : B_1, M_{Q_0}^{(4)} : B_2 \rangle + S_2^2 (\mathbf{n} : B_1) (\mathbf{nn} : B_2) \left( \frac{12S_4}{35} + \frac{11S_2}{21} + \frac{1}{15} \right)$$

$$= \langle Q_n(B_2) : M_{Q_0}^{(4)}, B_1 \rangle.$$

Thus, the operator $L_n$ is self adjoint.

It follows from Lemma 2.2 that the operator $J_n$ is positive. Now we prove that the operator $\mathcal{K}_n$ is non-negative. By the definition, we have

$$\langle \mathcal{K}_n(B), B \rangle = |B|^2 - \alpha M_{Q_0}^{(4)} : BB + \alpha (Q_0 : B)^2$$

$$= |B|^2 + \alpha \left( (S_2^2 - S_4) (\mathbf{n} : B)^2 - \frac{S_2 - S_4}{7} 4 |\mathbf{n} \cdot B|^2 - \left( \frac{S_4}{35} - \frac{2S_2}{21} + \frac{1}{15} \right) 2 |B|^2 \right).$$

Thanks to the definition of $S_2$ and $S_4$, we know that

$$\frac{S_2 - S_4}{7} = \frac{1}{8A_0} (-5A_4 + 6A_2 - A_0),$$

$$\frac{S_4}{35} - \frac{2S_2}{21} + \frac{1}{15} = \frac{1}{8A_0} (A_4 - 2A_2 + A_0).$$
Choose an orthogonal matrix $P = (n_1, n_2, n_3)^T$ such that $n_3 = n$, hence $P \cdot n = e_3 = (0, 0, 1)^T$. Let $\hat{B} = PBTP^T$. We have

\[
|B|^2 = |\hat{B}|^2, \\
|B \cdot n|^2 = |PB \cdot n|^2 = |\hat{B} \cdot e_3|^2 = \hat{B}_{13}^2 + \hat{B}_{23}^2 + \hat{B}_{33}^2, \\
nn \cdot B = n^T B n = e_3^T PBP^T e_3 = \hat{B}_{33}.
\]

Then we get

\[
\langle K_n(B), B \rangle = \hat{B}_{12}^2 + \alpha \left( (S_2^2 - S_4) \hat{B}_{33}^2 - \frac{S_2 - S_4}{7} (\hat{B}_{13}^2 + \hat{B}_{23}^2 + \hat{B}_{33}^2) - \left( \frac{S_4}{35} - \frac{2S_2}{21} + \frac{1}{15} \right) 2\hat{B}_{ij}^2 \right) = 2 \left( 1 - 2\alpha \left( \frac{S_4}{35} - \frac{2S_2}{21} + \frac{1}{15} \right) \right) \hat{B}_{12}^2 + 2 \left( 1 - 2\alpha \left( \frac{S_4}{35} - \frac{2S_2}{21} + \frac{1}{15} \right) \right) (\hat{B}_{11}^2 + \hat{B}_{22}^2) + \left( 1 - 2\alpha \left( \frac{S_4}{35} - \frac{2S_2}{21} + \frac{1}{15} \right) \right) (\hat{B}_{11} + \hat{B}_{22})^2.
\]

Furthermore, we know by (3.4) that

\[
4\alpha(S_2^2 - S_4) = \frac{6A_2 - 5A_4 - A_0}{2(A_2 - A_4)} - \frac{6A_2 - 5A_4 - A_0}{2(A_2 - A_4)} = \frac{A_2 - A_4}{A_2 - A_4} \cdot \frac{2(3A_2 - A_0)^2 - 2A_0(15A_4 - 12A_2 + A_0)}{A_2 - A_4} > 0,
\]

and $6A_2 - 5A_4 - A_0 > 0$. This proves

\[
\langle K_n(B), B \rangle \geq 0.
\]

Moreover, the equality holds if and only if $\hat{B}_{ij} = 0$ for $\{i, j\} \neq \{1, 3\}, \{2, 3\}$, which means that

\[
B = P^T \hat{B} P = \hat{B}_{13} n_1 \otimes n_1^T + \hat{B}_{23} n_2 \otimes n_2^T + \hat{B}_{13} n_1 \otimes n^T + \hat{B}_{23} n_2 \otimes n^T = n^\perp \cdot n = 0.\]

This proves the second point and third point of the proposition. \qed
Proposition 3.3. We have

\[ B_0 : [M_{Q_0}^{(6)} : B - M_{Q_0}^{(4)}(Q_0 : B)] = B_0 \cdot Q_n(B) + B \cdot Q_0 + \frac{1}{3}B - B : M_{Q_0}^{(4)} - \frac{3}{2}Q_n(B). \]

Proof. Proposition follows from the following two equalities:

\[ \int_{S^2} ((\mathbf{m} \cdot \mathbf{v})(\mathbf{m} \times \mathbf{u}) \cdot \mathcal{R}(f_0 \mathbf{mm} : B) + \mathcal{R} \cdot (\mathbf{m} \times \mathbf{um} \cdot \mathbf{v})f_0 \mathbf{mm} : B) \mathbf{dm} = 0, \]
\[ \int_{S^2} ((\mathbf{m} \cdot \mathbf{v})(\mathbf{m} \times \mathbf{u}) \cdot \mathcal{R}f_0 + \mathcal{R} \cdot (\mathbf{m} \times \mathbf{um} \cdot \mathbf{v})f_0) \mathbf{dm} = 0, \]

for any \( \mathbf{u}, \mathbf{v} \in \mathbb{R}^3 \).

\[ Q \]  

Remark 3.1. A direct consequence of Proposition 3.3 is that

\[ B_0 \cdot Q_n(B) + B \cdot Q_0 = Q_n(B) \cdot B_0 + Q_0 \cdot B, \]

or equivalently (recalling \( B_0 = \alpha Q_0 \))

\[ (B - \alpha Q_n(B)) \cdot Q_0 = Q_0 \cdot (B - \alpha Q_n(B)). \] (3.7)

4 From Q-tensor equation to Ericksen-Leslie equation

In this section, we will derive the Ericksen-Leslie equation (1.13) from the Q-tensor equation (2.5)-(2.6) by taking small Deborah number limit. For this end, we take \( De = \varepsilon \).

4.1 Formal expansion

We make a formal Taylor expansion in \( \varepsilon \) for \((Q, \mathbf{v}, BQ)\):

\[ Q = Q_0 + \varepsilon Q_1 + \varepsilon^2 Q_2 + \cdots, \]
\[ \mathbf{v} = \mathbf{v}_0 + \varepsilon \mathbf{v}_1 + \varepsilon^2 \mathbf{v}_2 + \cdots, \]
\[ BQ = B_0 + \varepsilon B_1 + \varepsilon^2 B_2 + \cdots. \]

Hence,

\[ Z_Q = \int_{S^2} e^{\mathbf{mm}\cdot\{B_0 + \varepsilon B_1 + \varepsilon^2 B_2 + \cdots\}} \mathbf{dm} = Z_{Q_0}(1 + \varepsilon Q_0 : B_1 + O(\varepsilon^2)), \]
\[ Q_0 + \varepsilon Q_1 + \cdots = \int_{S^2} (\mathbf{mm} - \frac{1}{3}I)e^{\mathbf{mm} : B_0}\left(1 + \varepsilon \mathbf{mm} : B_1 + O(\varepsilon^2)\right) \mathbf{dm} \]
\[ = Q_0 + \varepsilon ((M_{Q_0}^{(4)} - \frac{1}{3}I)Q_0 : B_1 - Q_0(Q_0 : B_1)) + O(\varepsilon^2). \]

This implies that

\[ Q_1 = (M_{Q_0}^{(4)} - \frac{1}{3}IQ_0) : B_1 - Q_0(Q_0 : B_1). \]
We also have
\[
M^{(4)}_Q = \frac{\int_{\Omega} m \, dm : B_0 (1 + \varepsilon m : B_1 + \cdots) \, dm}{Z_{Q_0} \left( 1 + \varepsilon Q_0 : B_1 + O(\varepsilon^2) \right)}
\]
\[
= M^{(4)}_{Q_0} + \varepsilon \left( M^{(6)}_{Q_0} : B_1 - M^{(4)}_{Q_0} (Q_0 : B_1) \right) + O(\varepsilon^2).
\]
Plugging them into \((2.5)-(2.6)\), we find that the terms of \(O(\varepsilon^{-1})\) satisfy
\[
-3Q_0 + 2\alpha \left( \frac{1}{3}Q_0 + Q_0 : Q_0 - Q_0 : M^{(4)}_{Q_0} \right) = 0. \tag{4.1}
\]
While the terms of \(O(1)\) satisfy
\[
\partial Q_0 \partial t + \nu_0 \cdot \nabla Q_0 = \left\{ -6Q_1 + 2\alpha \left[ 2J_n(Q_1) - 2Q_0 : \{ M^{(6)}_{Q_0} : B_1 - M^{(4)}_{Q_0} (Q_0 : B_1) \} \right] \right. \\
+ 2GQ_1 + (M^{(6)}_{Q_0} (Q_0 : B_1) + 2GQ_1)
\]
\[
+ G M_{Q_0} (\Delta Q_0) - Q_0 : \{ M^{(6)}_{Q_0} : B_1 - M^{(4)}_{Q_0} (Q_0 : B_1) \} \right\} + \alpha G M_{Q_0} (\Delta Q_0) \right\}.
\tag{4.2}
\]
By Lemma 2.1 \((4.1)\) implies that
\[
M_{Q_0}(B_0) - \alpha M_{Q_0}(Q_0) = 0,
\]
which means that
\[
M_{Q_0}(B_0 - \alpha Q_0) = 0,
\]
or
\[
\langle M_{Q_0}(B_0 - \alpha Q_0), B_0 - \alpha Q_0 \rangle = 0,
\]
from which and Lemma 2.2 it follows that
\[
B_0 - \alpha Q_0 = 0.
\]
Hence, we get by Proposition 3.1 that
\[
B_0 = \eta (n \cdot \frac{1}{3} I), \quad Q_0 = S_2 (n \cdot \frac{1}{3} I). \tag{4.4}
\]
It follows from Proposition 3.3 that
\[
-6Q_1 + 2\alpha \left[ 2J_n(Q_1) - 2Q_0 : \{ M^{(6)}_{Q_0} : B_1 - M^{(4)}_{Q_0} (Q_0 : B_1) \} \right] \]
\[
= -6Q_1 + 4\alpha J_n(Q_1) - 4 \left( B_0 \cdot Q_1 + B_1 \cdot Q_0 + \frac{1}{3} B_1 - B_1 : M^{(4)}_{Q_0} - \frac{3}{2} Q_1 \right) \]
\[
= -4 \left( \frac{1}{3} (B_1 - \alpha Q_1) + (B_1 - \alpha Q_1) \cdot Q_0 - (B_1 - \alpha Q_1) : M^{(4)}_{Q_0} \right) \]
\[
= 2L_n(B_1)
\]
where in the last equality we used the fact that \((B_1 - \alpha Q_1) \cdot Q_0 = Q_0 \cdot (B_1 - \alpha Q_1)\), which follows from (3.7) and \(Q_1 = Q_n(B_1)\). Thus, the system (4.2)-(4.3) can be written as

\[
\frac{\partial Q_0}{\partial t} + v_0 \cdot \nabla Q_0 = 2\mathcal{L}_n(B_1) + 2G\alpha J_n(\Delta Q_0) + (M_{Q_0}(\kappa^T) + M_{Q_0}^T(\kappa^T)),
\]

\[
\frac{\partial v_0}{\partial t} + v_0 \cdot \nabla v_0 = -\nabla p_0 + \frac{\gamma}{Re} \Delta v_0 + \frac{1 - \gamma}{2Re} \nabla \cdot (D_0 : M_{Q_0}^{(4)}) + \frac{1}{Re} \left\{ -\nabla \cdot \left[ \mathcal{L}_n(B_1) + G\alpha M_{Q_0}(\Delta Q_0) \right] + \alpha \frac{G}{2} Q_0 : \nabla \Delta Q_0 \right\}.
\]

4.2 The derivation of Ericksen-Leslie equation

We show that the system (4.5)-(4.6) is equivalent to the Ericksen-Leslie equation (we replace \(v_0\) by \(v\) for convenience)

\[
\begin{cases}
\v_t + v \cdot \nabla v = -\nabla p + \frac{\gamma}{Re} \Delta v + \frac{1 - \gamma}{Re} \nabla \cdot (\sigma^L + \sigma^E), \\
\n \times (h - \gamma_1 N - \gamma_2 D \cdot n) = 0,
\end{cases}
\]

where the Leslie stress \(\sigma^L\) is given by

\[
\sigma^L = \alpha_1 (nn : D)nn + \alpha_2 nN + \alpha_3 Nn + \alpha_4 D + \alpha_5 nn \cdot D + \alpha_6 D \cdot nn,
\]

with the Leslie coefficients taking the values

\[
\begin{align*}
\alpha_1 &= -\frac{S_4}{2}, \\
\alpha_2 &= -\frac{S_2}{2} \left( 1 + \frac{1}{\lambda} \right), \\
\alpha_3 &= -\frac{S_2}{2} \left( 1 - \frac{1}{\lambda} \right), \\
\alpha_4 &= \frac{4}{15} - \frac{5}{21} S_2 - \frac{1}{35} S_4, \\
\alpha_5 &= \frac{1}{7} S_4 + \frac{6}{7} S_2, \\
\alpha_6 &= \frac{1}{7} S_4 - \frac{1}{7} S_2,
\end{align*}
\]

and

\[
\begin{align*}
\gamma_1 &= \frac{1}{S_2^2} \left( \frac{2 S_2^2}{S_2^2} - \frac{2}{S_2^2 \alpha} \right), \\
\gamma_2 &= -S_2, \\
\lambda &= \frac{\gamma_2}{\gamma_1} = \frac{1}{3} + \frac{\frac{2}{3 S_2^2} - \frac{2}{S_2^2 \alpha}}{\lambda}.
\end{align*}
\]

The Ericksen stress \(\sigma^E\) is given by

\[
\sigma^E = -\frac{\partial E_F}{\partial (\nabla n)} \cdot (\nabla n)^T,
\]

with \(E_F = \frac{1}{2} \alpha G S_2^2 |\nabla n|^2\).

First of all, for any \(nn^\perp + n^\perp n \in \text{Ker} \mathcal{L}_n\) where \(n \cdot n^\perp = 0\), we have

\[
\left\langle \frac{\partial Q_0}{\partial t} + v_0 \cdot \nabla Q_0 - 2G\alpha J_n(\Delta Q_0) - (M_{Q_0}(\kappa^T) + M_{Q_0}^T(\kappa^T)), nn^\perp + n^\perp n \right\rangle = 0.
\]
By direct computations, we obtain

\[
\begin{align*}
\langle \frac{\partial Q_0}{\partial t} + v_0 \cdot \nabla Q_0, nn^\perp + n^\perp n \rangle &= 2S_2(\frac{\partial n}{\partial t} + v_0 \cdot \nabla n) \cdot n^\perp, \\
\langle \Delta Q_0, nn^\perp + n^\perp n \rangle &= 2S_2 n^\perp \cdot \Delta n, \\
\langle (\Delta Q_0 \cdot Q_0 + Q_0 \cdot \Delta Q_0), nn^\perp + n^\perp n \rangle &= \frac{2}{3}S_2^2 \Delta n \cdot n^\perp, \\
\langle \Delta Q_0 : M_Q^{(4)}(n), nn^\perp + n^\perp n \rangle &= \frac{1}{\alpha} \langle \Delta Q_0, (nn^\perp + n^\perp n) \rangle = \frac{2S_2}{\alpha} n^\perp \cdot \Delta n, \\
\langle (\kappa_0 \cdot Q_0 + Q_0 \cdot \kappa_0^T + \frac{2}{3}D_0 - 2\kappa_0 : M_Q^{(4)}), nn^\perp + n^\perp n \rangle &= \langle (D_0 - \Omega_0) \cdot Q_0 + Q_0 \cdot (D_0 + \Omega_0) + \frac{2}{3}D_0 - 2D_0 : M_Q^{(4)}), nn^\perp + n^\perp n \rangle \\
&= -2S_2 n^\perp \cdot (\Omega_0 \cdot n) + \frac{2}{3}S_2 n^\perp \cdot (D_0 \cdot n) + \frac{4}{3}n^\perp \cdot (D_0 \cdot n) - \frac{4}{\alpha} n^\perp \cdot (D_0 \cdot n),
\end{align*}
\]

which along with (4.10) gives

\[
\begin{align*}
2S_2\left(\frac{\partial n}{\partial t} + v_0 \cdot \nabla n\right) \cdot n^\perp &= \frac{4}{3} \alpha G S_2 n^\perp \cdot \Delta n - \frac{2}{3} \alpha G S_2^2 \Delta n \cdot n^\perp + 4G S_2 n^\perp \cdot \Delta n \\
+ 2S_2 n^\perp \cdot (\Omega_0 \cdot n) - \frac{2}{3}S_2 n^\perp \cdot (D_0 \cdot n) - \frac{4}{3}n^\perp \cdot (D_0 \cdot n) + \frac{4}{\alpha} n^\perp \cdot (D_0 \cdot n) &= 0,
\end{align*}
\]

or

\[
\begin{align*}
\left(\frac{\partial n}{\partial t} + v_0 \cdot \nabla n + \Omega_0 \cdot n\right) \cdot n^\perp + \alpha G S_2 \left(\frac{2}{3S_2} - \frac{1}{3} + \frac{2}{\alpha S_2}\right)n^\perp \cdot \Delta n \\
- \left(\frac{1}{3} + \frac{2}{3S_2} - \frac{2}{S_2 \alpha}\right)n^\perp \cdot (D_0 \cdot n) &= 0.
\end{align*}
\]

Thus we derive the equation of \( n \):

\[
n \times \left( h - \gamma_1 \left(\frac{\partial n}{\partial t} + v_0 \cdot \nabla n + \Omega_0 \cdot n\right) - \gamma_2 D_0 \cdot n \right) = 0. \tag{4.11}
\]
In order to derive the equation of $v_0$, let us compute that

\[
\begin{align*}
\frac{1}{2} \mathbf{D}_0 & : M^{(4)}_{Q_0} - \mathcal{L}_n(B_1) - G\alpha M_{Q_0}(\Delta Q_0) \\
&= \frac{1}{2} \mathbf{D}_0 : M^{(4)}_{Q_0} - \mathcal{L}_n(B_1) - \alpha \left( \frac{1}{3} G \Delta Q_0 + G Q_0 \cdot \Delta Q_0 - G \Delta Q_0 : M^{(4)}_{Q_0} \right) \\
&= \frac{1}{2} \mathbf{D}_0 : M^{(4)}_{Q_0} - \mathcal{L}_n(B_1) - \alpha \left( \frac{1}{3} G \Delta Q_0 + \frac{G}{2} (Q_0 \cdot \Delta Q_0 + \Delta Q_0 \cdot Q_0) - G \Delta Q_0 : M^{(4)}_{Q_0} \right) \\
& \quad - \alpha \frac{G}{2} (Q_0 \cdot \Delta Q_0 - \Delta Q_0 \cdot Q_0) \\
&= \frac{1}{2} \mathbf{D}_0 : M^{(4)}_{Q_0} - \frac{1}{2} \left( \frac{\partial Q_0}{\partial t} + v_0 \cdot \nabla Q_0 - (\kappa_0 \cdot Q_0 + Q_0 \cdot \kappa_0^T + \frac{2}{3} \mathbf{D}_0 - 2\kappa_0 : M^{(4)}_{Q_0}) \right) \\
& \quad - \alpha \frac{G}{2} (Q_0 \cdot \Delta Q_0 - \Delta Q_0 \cdot Q_0) \\
&= \frac{1}{2} \left( S_2 (\mathbf{nn} + \kappa \mathbf{nN}) - S_2 (\mathbf{D} \cdot \mathbf{nN} + \mathbf{nn} \cdot \mathbf{D}) + \frac{2(S_2 - 1)}{3} \mathbf{D} \right) \\
& \quad + \left( \frac{2S_4}{7} - \frac{4S_2}{21} + \frac{2}{15} \right) (\mathbf{nn} : \mathbf{D}) I + 2(\mathbf{nD} \cdot \mathbf{n} + \mathbf{D} \cdot \mathbf{nn}) \\
& \quad + \left( \frac{4S_4}{15} - \frac{5S_2}{21} - \frac{1}{35} S_4 \right) \mathbf{D} + \left( \frac{1}{7} S_4 + \frac{6}{7} S_2 \right) \mathbf{nn} \cdot \mathbf{D} + \left( \frac{1}{7} S_4 - \frac{1}{7} S_2 \right) \mathbf{D} \cdot \mathbf{nn} \\
&= \frac{1}{2} \left( \mathbf{D} : \mathbf{nn} \right) I + \sigma_L,
\end{align*}
\]

where $\sigma^L$ is the Leslie stress, and

\[
\begin{align*}
\frac{1}{2} \alpha G Q_0 : \nabla \Delta Q_0 &= \frac{1}{2} \nabla (\alpha G Q_0 : \Delta Q_0) - \frac{1}{2} \alpha G S_2^2 \partial_i (n_i n_j) \partial_k^2 (n_i n_j) \\
&= \frac{1}{2} \nabla (\alpha G Q_0 : \Delta Q_0 - \alpha G S_2^2 \partial_i n_i \partial_k^2 n_i \\
&= \frac{1}{2} \nabla (\alpha G Q_0 : \Delta Q_0 + G S_2^2 \partial_i n_i \partial_k n_i - \alpha G S_2^2 \partial_k (\partial_k n_i \partial_i n_i) \\
&= \frac{1}{2} \nabla \left( \alpha G Q_0 : \Delta Q_0 + \alpha G S_2^2 (\nabla n)^2 \right) - \alpha G S_2^2 \nabla \cdot (\nabla n \otimes \nabla n) \\
&= -\nabla p_1 + \nabla \cdot \sigma^E,
\end{align*}
\]

where $\sigma^E = -\alpha G S_2^2 (\nabla n \otimes \nabla n)$ is the Ericksen stress. We denote

\[
\sigma = \sigma^L + \sigma^E, \quad p = p_0 + p_1 + \frac{S_2 - S_4}{14} (\mathbf{D} : \mathbf{nn}).
\]

Thus we derive the equation of $v_0$: \begin{equation} \frac{\partial v_0}{\partial t} + v_0 \cdot \nabla v_0 = -\nabla p + \frac{\gamma}{Re} \Delta v_0 + \nabla \cdot \sigma. \tag{4.12} \end{equation}

This completes the derivation of the Ericksen-Leslie equation. Note that the constraints (1.16) and (1.17) are naturally satisfied.
Remark 4.1. Comparing with the Ericksen-Leslie system directly derived from the Doi-Onsager theory, the only difference is that the value of $\gamma_1$ (and hence $\lambda, \alpha_2, \alpha_3$) has been changed. This change comes from the Bingham closure, which approximates a general probability distribution function by a specific distribution function.

5 The hard-core potential case

In [13], the general Oseen-Frank energy is derived from the Onsager theory with hard-core potential. Here we present a sketch of derivation of the Ericksen-Leslie equation with general Oseen-Frank energy

$$E_{OF}(n, \nabla n) = \frac{1}{2} K_1 (\text{div} n)^2 + \frac{1}{2} K_2 (n \cdot \nabla \times n)^2 + \frac{1}{2} K_3 (n \times \nabla n)^2.$$  

We introduce the fourth order traceless tensor $Q_4 = Q_4(Q)$ defined by

$$Q_{4\alpha\beta\gamma\delta} = \int_{S^2} (m_\alpha m_\beta m_\gamma m_\mu - \frac{1}{7} [m_\alpha m_\beta \delta_{\gamma\mu} + m_\gamma m_\mu \delta_{\alpha\beta} + m_\alpha m_\mu \delta_{\beta\gamma} + m_\beta m_\mu \delta_{\alpha\gamma} + m_\alpha m_\mu \delta_{\gamma\beta} + m_\beta m_\gamma \delta_{\alpha\mu}] + \frac{1}{35} [\delta_{\alpha\beta} \delta_{\gamma\mu} + \delta_{\alpha\gamma} \delta_{\beta\mu} + \delta_{\alpha\mu} \delta_{\beta\gamma}]) f_Q \, d \mu,$$

and the energy $E$ defined by

$$E(Q, \nabla Q) = E_b(Q) + E_e(Q, \nabla Q),$$

where

$$E_b(Q) = \int_{\mathbb{R}^3} \left( - \ln Z_Q + Q : B_Q - \frac{\alpha}{2} |Q|^2 \right) \, dx,$$

$$E_e(Q, \nabla Q) = \frac{\varepsilon}{2} \int_{\mathbb{R}^3} \left\{ J_1 |\nabla Q|^2 + J_2 |\nabla Q_4|^2 + J_3 \left( \partial_i(Q_{ik}) \partial_j(Q_{jk}) + \partial_i(Q_{jk}) \partial_j(Q_{ik}) \right) + J_4 \left( \partial_i(Q_{4iklm}) \partial_j(Q_{4jklm}) + \partial_i(Q_{4jklm}) \partial_j(Q_{4iklm}) \right) + J_5 \partial_i(Q_{4ijkl}) \partial_j(Q_{ijkl}) \right\} \, dx.$$

The coefficients $J_i (i = 1, \cdots, 5)$ are explicitly calculated in terms of the molecular parameters in [13]. Here we set them to be general. Let

$$\mu_Q = \frac{\delta E(Q, \nabla Q)}{\delta Q} = B_Q - \alpha Q + \frac{\delta E_e}{\delta Q}.$$

In such case, the $Q$-tensor equation becomes

$$\frac{\partial Q}{\partial t} + v \cdot \nabla Q = \frac{\varepsilon}{D_e} N(\mu_Q) + M_Q(\kappa_T) + M_Q^T(\kappa_T) + \frac{2}{D_e} \left( M_Q(\mu_Q) + M_Q^T(\mu_Q) \right),$$  \hspace{1cm} (5.1)

$$\frac{\partial v}{\partial t} + v \cdot \nabla v = -\nabla p + \frac{\gamma}{Re} \Delta v + \frac{1}{2Re} \nabla \cdot (D : M_Q^{(4)}) + \frac{1 - \gamma}{DeRe} \left( 2 \nabla \cdot M_Q(\mu_Q) + \mu_Q : \nabla Q \right).$$  \hspace{1cm} (5.2)

Then we can derive the Ericksen-Leslie equation from [5.1] and [5.2] by taking small Deborah number limit, where the Leslie coefficients and $\gamma_1, \gamma_2$ keep the same, but the Ericksen
energy $E_F$ is replaced by the general Oseen-Frank energy $E_{OF}$ with the elastic coefficients $K_1, K_2, K_3$ given by

$$K_1 = 2S_2^2(J_1 + J_3) + S_4^2\left(\frac{16}{7}J_2 + \frac{92}{49}J_4\right) - \frac{6}{7}J_5S_2S_4,$$

$$K_2 = 2S_2^2J_1 + S_4^2\left(\frac{16}{7}J_2 + \frac{12}{49}J_4\right) - \frac{2}{7}J_5S_2S_4,$$

$$K_3 = 2S_2^2(J_1 + J_3) + S_4^2\left(\frac{16}{7}J_2 + \frac{120}{49}J_4\right) + \frac{8}{7}J_5S_2S_4,$$

where $S_2, S_4$ are defined by (3.5). We omit the detailed derivation here.

Let us conclude this section by some comparisons with two dynamical Q-tensor models mentioned in the introduction (see also Remarks in section 2.3). Our dynamical $Q$-tensor theory could written in the following form similar to (1.11):

$$\frac{\partial Q}{\partial t} + \mathbf{v} \cdot \nabla Q = D^{\text{trans}}(\mu Q) + D^{\text{rot}}(\mu Q) + F(Q, D) + \mathbf{\Omega} \cdot \mu Q - \mu Q \cdot \mathbf{\Omega},$$

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} = -\nabla p + \nabla \cdot \left(\sigma^{\text{dis}} + \sigma^s + \sigma^a + \sigma^d\right),$$

$$\nabla \cdot \mathbf{v} = 0.$$

Here the additional term

$$D^{\text{trans}} = \frac{\varepsilon}{De} N(\mu Q)$$

accounts for the translational diffusion, which is not considered in Beris-Edwards’s and Qian-Sheng’s models. The terms $\sigma^a$ and $\sigma^d$, module some constants, are all the same as those in Beris-Edwards’s and Qian-Sheng’s models:

$$\sigma^d_{ij} = \frac{\partial E}{\partial (Q_{kl,j})} Q_{kl,i}, \quad \sigma^a = Q \cdot \mu Q - \mu Q \cdot Q.$$

Here it should be noticed that $\mu Q : \nabla Q$ is actually the same as $\partial_j\left(\frac{\partial E}{\partial (Q_{kl,j})} Q_{kl,i}\right)$ module a pressure term, and

$$(\mathcal{M} - \mathcal{M}^T)(\mu Q) = Q \cdot \mu Q - \mu Q \cdot Q.$$

Our rotational diffusion term is derived from Doi’s kinetic theory, which takes the form:

$$D^{\text{rot}} = \frac{2}{De} (\mathcal{M}_Q + \mathcal{M}_Q^T)(\mu Q).$$

The two conjugated terms $F(Q, D)$ and $\sigma^s = -\frac{1}{Re De} F(Q, \mu Q)$ are given by

$$F(Q, A) = (\mathcal{M}_Q + \mathcal{M}_Q^T)(A).$$

The additional dissipation stress is given by

$$\sigma^{\text{dis}} = \frac{2\gamma}{Re} D + \frac{1 - \gamma}{2Re} D : M_Q^{(4)}.$$

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