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FRAME HYDRODYNAMICS OF BIAXIAL NEMATICS FROM MOLECULAR-THEORY-BASED TENSOR MODELS*

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Abstract. Starting from a dynamic tensor model about two second-order tensors, we derive the frame hydrodynamics for the biaxial nematic phase using the Hilbert expansion. The coefficients in the frame model are derived from those in the tensor model. The energy dissipation of the tensor model is maintained in the frame model. The model is reduced to the Ericksen–Leslie model if the biaxial bulk energy minimum of the tensor model is reduced to a uniaxial one.

Key words. liquid crystals, biaxial nematic phase, hydrodynamics, Hilbert expansion, closure approximation

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1. Introduction.

Liquid crystals are featured by local orientational order, typically originated from nonuniform orientational distribution of nonspherical rigid molecules. One case that many of us are familiar with is the uniaxial nematic phase formed by rodlike molecules. For the uniaxial nematic phase, the local orientational order can be described by a unit vector $\mathbf{n}$. The hydrodynamics of liquid crystals then involves dynamics of the vector $\mathbf{n}$, for which the well-known Ericksen–Leslie theory is proposed [8, 14]. The Ericksen–Leslie theory, as well as its variants, has been studied extensively in both analysis [17, 34, 32, 18] and simulation [20, 6, 2, 31]. For a detailed survey on modeling, analysis, and computation of liquid crystals, we refer to [33].

Constructed on the assumption of uniaxial local anisotropy, the Ericksen–Leslie theory is opaque to the building blocks of liquid crystals. Although the elastic constants can be related to experimental measurements, several other coefficients in the hydrodynamics are difficult to obtain. This deficiency can be overcome by studying the relation of the Ericksen–Leslie theory to molecular models about the orientation density function [13, 7], or tensor models about a second-order tensor Q [11]. From molecular models or tensor models, one could derive the Ericksen–Leslie theory with its coefficients expressed by those in the molecular models or tensor models. Such derivations are based on the fact that the minimum of the bulk energy must be uniaxial [21, 9]. When the bulk energy dominates, the dynamics can be regarded as constrained in the states such that the bulk energy takes its minimum, so that it reduces to a dynamics of vector field. The whole procedure is done through the Hilbert expansion that has been shown rigorously [35, 16, 15, 36]. The advantage of such a

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procedure lies in the clear reflection of architecture of different *axisymmetric* molecules in the Ericksen–Leslie model. For example, the uniaxial nematics formed by cylinder, spheroid, hourglass, and spindle can be distinguished by the derived coefficients in the Ericksen–Leslie model.

Local orientational orders other than the uniaxial type have also been considered, of which the biaxial nematics is discussed more [30, 24, 1, 4]. Since the mesoscopic symmetry is no longer axisymmetric, the form of elasticity and hydrodynamics of the biaxial nematics are distinct from the uniaxial nematics, which has been discussed earlier: Its orientational elasticity is written down in various forms that turn out to be equivalent [28, 29]; biaxial hydrodynamics are also proposed [28, 22, 5, 27, 10] in different forms. Analysis has been carried out for a few simplified models [19]. These works focus on the form of the model, in which many more coefficients are involved. A couple of previous works attempt to relate the elastic constants to molecular parameters [12, 44], while other coefficients in the hydrodynamics are yet to be considered. In other words, biaxial hydrodynamics describing specific molecules is still not established.

The main goal of this paper is to reveal the connection between the biaxial hydrodynamics and the molecular architecture. Specifically, we shall derive the coefficients in the biaxial hydrodynamics from molecular parameters. In principle, the procedure is analogous to what is done from a Q-tensor model for axisymmetric molecules to the Ericksen–Leslie model for the uniaxial hydrodynamics. Nevertheless, there turns out to be an essential distinction regardless of the starting point or the derivation, which we explain below.

For the molecular architecture, it is necessary to consider nonaxisymmetric molecules, which is based on previous results. Experimentally, it has *not* been reported that rodlike molecules can form biaxial nematics without imposing external forces. Theoretically, as we have mentioned above, it has been shown that the bulk energy of molecular-theory-based one-tensor models so far considered can only exhibit uniaxial nematics [21, 9]. For the phenomenological Landau–de Gennes theories, the quartic bulk energy only exhibits uniaxial nematics as well [25, 36], while higher-order bulk energies do not have clear relations to molecular information. For this reason, we consider the dynamic tensor model for bent-core molecules (and also star-shaped molecules as their variants) established in [45]. The model has multiple tensors as order parameters because the molecule has no axisymmetry, and is derived from molecular theory. Its free energy is constructed on molecular architecture by expanding the pairwise molecular interaction kernel, established in [41], which has the biaxial nematic phase as an energy minimum. The interaction between the molecule and the fluid is also carefully derived from the molecular architecture. As a result, the form of the dynamic tensor model is determined by molecular symmetry, with all the coefficients calculated from molecular parameters. In this sense, the molecular architecture can be distinguished in the tensor model by the derived coefficients.

Rigorous analyses show that under certain coefficients, the stationary points of the bulk energy can only be isotropic, uniaxial, or biaxial [42, 43, 38]. Although further rigorous analysis is still not available, numerical studies indicate that we can indeed find some coefficients such that the biaxial nematic phase is the bulk energy minimum [30, 23, 42, 41, 38]. Therefore, we assume that it holds and use the Hilbert expansion near this bulk energy minimum. The free energy in the tensor model is rotationally invariant, which is an essential ingredient to be utilized in our derivation. In particular, the rotational invariance of the bulk energy implies that its minimum, if not isotropic, can be freely rotated. The biaxial nematic phase has its own symmetry other than axisymmetry. When axisymmetry does not hold, the orientation of the bulk energy minimum shall generally be described by an orthonormal frame, or an element in $SO(3)$. We would like to call it a "frame model" that gives the elasticity and dynamics of the field of orthonormal frame.

Two key ingredients are needed to be dealt with in the Hilbert expansion. When the tensors are constrained at the biaxial minimum, it actually gives a three-dimensional manifold. We shall constrain the equations of tensors on this manifold to obtain the evolution equation for the orthonormal frame field. The tangent space of the manifold given by the bulk energy minimum gives a zero-eigenvalue subspace of the Hessian of the bulk energy. This subspace is utilized to cancel the nonleading terms in the Hilbert expansion, thus closing the system of the leading order. The free energy about tensors can then be reduced to the orientational elasticity for the biaxial nematic phase, with the elastic constants expressed as the coefficients in the tensor model, which is exactly the results in [44].

Although the free energy can be reduced straightforwardly, we still need to handle several high-order tensors, which call for a closure approximation to express them as functions of the order parameter tensors. Intuitively, these high-order tensors shall be consistent with the symmetry of the biaxial nematic phase, from which the form of high-order tensors can be written down. This intuition can be made rigorously by the closure through minimization of the entropy term. The entropy term can have two choices. One is calculated from the density function of the maximum entropy state, which we call the original entropy. The other is the quasi-entropy, an elementary function of tensors, which maintains essential properties and underlying physics of the original entropy [38]. No matter whether we choose the original entropy or the quasi-entropy, their fine properties result in the particular form of high-order tensors consistent with the symmetry of the biaxial nematic phase. From these symmetry arguments, we could further arrive at alternative expressions of these high-order tensors that are convenient for us to deduce the coefficients.

Using these properties, we could derive the frame model for the biaxial nematic phase. Its form is actually determined by the symmetry of the biaxial nematic phase, which is consistent with early works [10]. The coefficients, on the other hand, are expressed as functions of the coefficients in the tensor model. We would like to emphasize again that since the coefficients in the tensor model are derived from physical parameters, the frame model we obtain is connected to rigid molecules with certain architecture. We shall show that the energy dissipation of the tensor model is maintained in the frame model. Furthermore, we will show that the biaxial hydrodynamics can be reduced to the Ericksen–Leslie theory when the bulk energy has a uniaxial minimum. The corresponding coefficients are also derived, which turn out to be distinct from those derived from the Q-tensor hydrodynamics for rodlike molecules. In other words, combining the results in this paper and those in previous works [41, 45], for bent-core molecules (and star-shaped molecules), we arrive at biaxial hydrodynamics and also uniaxial dynamics of certain architecture (bending angle, length, thickness, etc.) and under certain physical conditions (concentration, temperature, etc.).

Below, we begin by introducing some notations for orthonormal frames and tensors in section 2. The tensor model is briefly described in section 3. Here, we also claim essential properties of the entropy term, bulk energy minima, and high-order tensors. The Hilbert expansion is carried out in section 4, from which we derive the biaxial hydrodynamics. The biaxial hydrodynamics can be reduced to Ericksen–Leslie theory if the bulk energy minimum becomes uniaxial, which is shown in section 5. Concluding remarks are given in section 6. We also provide supplementary materials (bif_suppm.pdf [local/web 446KB]), where detailed calculations and discussions on high-order tensors are presented.

2. Preliminary. Let us introduce some notations for orthonormal frames and tensors to be used subsequently. For the rigid molecules forming liquid crystalline states, several essential quantities are defined through the orientational distribution. The orientation of a single rigid molecule is described by an orthonormal, right-handed frame $(\mathbf{m}_1, \mathbf{m}_2, \mathbf{m}_3)$ fixed on the molecule. The axes of the frame are typically coincident with symmetry axes of the molecule. Under a reference frame $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$, the coordinates of the molecular frame can be expressed by

$$\mathfrak{q}_{ij} = \mathbf{e}_i \cdot \mathbf{m}_j,\ \ i,j = 1,2,3,$$

which define a 3×3 rotation matrix $\mathfrak{q} \in SO(3)$.

In this paper, we also deal with fields of the orthonormal frame. To be distinguished from the molecular frame, we use the notation $\mathfrak{p} = (\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3)$ for a frame field that is a function of the position $\mathbf{x}$. The notations for $\mathbf{n}_i$ are similar to those for $\mathbf{m}_i$ above.

Next, let us describe notations for tensors. An nth-order tensor U in $\mathbb{R}^3$ can be expressed as a linear combination of tensors generated by the axes of the reference frame $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$, written as

$$U = U_{i_1\dots i_n}\mathbf{e}_{i_1} \otimes \cdots \otimes \mathbf{e}_{i_n},\ \ i_1,\dots,i_n \in \{1,2,3\}, \tag{2.1}$$

where $U_{i_1\dots i_n}$ are the coordinates of the tensor U. Hereafter, we adopt the Einstein summation convention on repeated indices. For any two nth-order tensors U_1 and U_2, the dot product $U_1 \cdot U_2$ is defined as

$$U_1 \cdot U_2 = (U_1)_{i_1\dots i_n}(U_2)_{i_1\dots i_n}.$$

A tensor can be symmetrized by calculating its permutational average,

$$U_{\text{sym}} = \frac{1}{n!}\sum_{\sigma} U_{i_{\sigma(1)}\dots i_{\sigma(n)}}\mathbf{e}_{i_1} \otimes \cdots \otimes \mathbf{e}_{i_n},$$

where the summation is taken over all the permutations σ of $\{1,\dots,n\}$. If $U = U_{\text{sym}}$, we say that the tensor U is symmetric. For an nth-order symmetric tensor, we define its trace as the contraction of two of its indices, giving an $(n-2)$th-order symmetric tensor,

$$(\text{tr}U)_{i_1\dots i_{n-2}} = U_{i_1\dots i_{n-2}kk}.$$

If a symmetric tensor U satisfies $\text{tr}U = 0$, then U is called a symmetric traceless tensor. For any symmetric tensor U of the order n, there exists a unique symmetric traceless tensor $(U)_0$ of the form

$$(U)_0 = U - (\mathfrak{i} \otimes W)_{\text{sym}}, \tag{2.2}$$

where W is an $(n-2)$th-order tensor (for the proof, see Proposition 3.2 in [37]). We call $(U)_0$ the symmetric traceless tensor generated by U.

It could be convenient to express symmetric traceless tensors by polynomials. The basic monomial notation is defined as

$$\mathbf{m}_1^{k_1}\mathbf{m}_2^{k_2}\mathbf{m}_3^{k_3}\mathfrak{i}^l = \Bigg(\underbrace{\mathbf{m}_1 \otimes \cdots \otimes \mathbf{m}_1}_{k_1} \otimes \underbrace{\mathbf{m}_2 \otimes \cdots \otimes \mathbf{m}_2}_{k_2} \otimes \underbrace{\mathbf{m}_3 \otimes \cdots \otimes \mathbf{m}_3}_{k_3} \otimes \underbrace{\mathfrak{i} \otimes \cdots \otimes \mathfrak{i}}_{l}\Bigg)_{\text{sym}}, \tag{2.3}$$

where $\mathfrak{i}$ is the second-order identity tensor that can be expressed as

$$\mathfrak{i} = \mathbf{m}_1^2 + \mathbf{m}_2^2 + \mathbf{m}_3^2.$$

This equality holds independently of what frame $(\mathbf{m}_1, \mathbf{m}_2, \mathbf{m}_3)$ is chosen. As we have commented, the above definitions are also suitable for $\mathbf{n}_i$. When the symbol $\otimes$ is absent in a product, it means that the resulting tensor is symmetrized.

The orientational distribution of rigid molecules is denoted by $\rho(\mathbf{x}, \mathfrak{q})$. However, it is significant to introduce some simple quantities to classify the local anisotropy given by the density function ρ. Such quantities are defined through the moments of $\mathbf{m}_i$,

(2.4)
$$\langle \mathbf{m}_{i_1} \otimes \cdots \otimes \mathbf{m}_{i_n} \rangle = \int_{SO(3)} \mathbf{m}_{i_1}(\mathfrak{q}) \otimes \cdots \otimes \mathbf{m}_{i_n}(\mathfrak{q}) \rho(\mathbf{x}, \mathfrak{q}) \mathrm{d}\mathfrak{q}, \quad i_1, \ldots, i_n = 1, 2, 3.$$

Hereafter, the notation $\langle \cdot \rangle$ is employed to represent the average of the distribution function $\rho(\mathbf{x}, \mathfrak{q})$ on $SO(3)$, and $\mathrm{d}\mathfrak{q}$ denotes the Haar measure on $SO(3)$. These moments, as well as their components, might be linearly dependent. To ensure that the quantities we choose are linearly independent, it is necessary to use symmetric traceless tensors averaged by ρ [37]. These chosen averaged symmetric traceless tensors are the so-called order parameters.

We will frequently encounter derivatives involving orthonormal frames. Let us first define rotational differential operators. For any frame $\mathfrak{p} = (\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3) \in SO(3)$, its tangent space in $SO(3)$ is spanned by three matrices, given by $(0, \mathbf{n}_3, -\mathbf{n}_2)$, $(-\mathbf{n}_3, 0, \mathbf{n}_1)$, $(\mathbf{n}_2, -\mathbf{n}_1, 0)$. Thus, we define three differential operators $\mathscr{L}_j$ by taking the inner products of the above three matrices and $\partial/\partial\mathfrak{p} = (\partial/\partial\mathbf{n}_1, \partial/\partial\mathbf{n}_2, \partial/\partial\mathbf{n}_3)$, i.e.,

(2.5)
$$\mathscr{L}_1 = \mathbf{n}_3 \cdot \frac{\partial}{\partial \mathbf{n}_2} - \mathbf{n}_2 \cdot \frac{\partial}{\partial \mathbf{n}_3}, \quad \mathscr{L}_2 = \mathbf{n}_1 \cdot \frac{\partial}{\partial \mathbf{n}_3} - \mathbf{n}_3 \cdot \frac{\partial}{\partial \mathbf{n}_1}, \quad \mathscr{L}_3 = \mathbf{n}_2 \cdot \frac{\partial}{\partial \mathbf{n}_1} - \mathbf{n}_1 \cdot \frac{\partial}{\partial \mathbf{n}_2}.$$

The subscript indicates the differential operator is along the infinitesimal rotation about $\mathbf{n}_j (j = 1, 2, 3)$. This can be verified by acting the differential operators on the axes of the frame, resulting in

$$\mathscr{L}_j \mathbf{n}_k = \epsilon^{jkl} \mathbf{n}_l, \tag{2.6}$$

where ϵ^{jkl} denotes the Levi-Civita symbol.

For a frame field $\mathfrak{p}(\mathbf{x})$, its orientational elasticity is characterized by an elastic energy of the spatial derivatives of $\mathfrak{p}(\mathbf{x})$. Let us express these spatial derivatives under the local frame $\mathfrak{p}$. The derivative of $\mathbf{n}_\mu$ along the direction $\mathbf{n}_\lambda$ is given by $\mathbf{n}_\lambda \cdot \nabla \mathbf{n}_\mu$. Its ν-component in the frame $\mathfrak{p}$ can be written as $n_{\lambda i} n_{\nu j} \partial_i n_{\mu j}$. Using the equality $n_{\mu j} n_{\nu j} = \delta_{\mu\nu}$, where we use the Kronecker delta, we obtain the relation $n_{\lambda i} n_{\nu j} \partial_i n_{\mu j} = -n_{\lambda i} n_{\mu j} \partial_i n_{\nu j}$. Consequently, the first-order derivatives of the frame $\mathfrak{p}$ has nine degrees of freedom:

$$\begin{cases} D_{11} = n_{1i} n_{2j} \partial_i n_{3j}, \ D_{12} = n_{1i} n_{3j} \partial_i n_{1j}, \ D_{13} = n_{1i} n_{1j} \partial_i n_{2j}, \\ D_{21} = n_{2i} n_{2j} \partial_i n_{3j}, \ D_{22} = n_{2i} n_{3j} \partial_i n_{1j}, \ D_{23} = n_{2i} n_{1j} \partial_i n_{2j}, \\ D_{31} = n_{3i} n_{2j} \partial_i n_{3j}, \ D_{32} = n_{3i} n_{3j} \partial_i n_{1j}, \ D_{33} = n_{3i} n_{1j} \partial_i n_{2j}. \end{cases} \tag{2.7}$$

3. Tensor model. In tensor models, the local orientational order is described by one or several order parameter tensors. From the structure of nonzero components in the tensors, local anisotropy could be divided into several classes. Each class is recognized as a phase, and phase transitions between them can be described. For example, the transition between the isotropic and uniaxial nematic phases for rodlike molecules can be described by an energy about a second-order symmetric traceless tensor Q. The dynamic tensor models could either be phenomenological, such as the Beris–Edwards model [3] and the Qian–Sheng model [26] based on the Landau–de Gennes theory, or be derived from the molecular theory [11]. In the vicinity of a bulk energy minimum, the tensors possess the nonzero structure of a certain phase, so that the tensor model is reduced to a model with fewer variables. For the uniaxial nematic phase of rodlike molecules, the models of a field of the Q-tensor, which has five degrees of freedom, could be reduced to models of a field of unit vectors, which has two degrees of freedom.

When rigid molecules of more complex architecture are taken into account, such as bent-core and star molecules, the corresponding molecular-theory-based tensor models have also been derived [41, 45]. The most notable feature of this model lies in the fact that its form and coefficients are determined by molecular symmetry and molecular parameters, respectively. Depending on the coefficients, the bulk energy may exhibit isotropic, uniaxial nematic, or biaxial nematic phases. The modulated twist-bend nematic phase can also be described together with elastic energy. Since the biaxial nematic phase is included in this tensor model, we choose this model as our starting point.

Compared with the original form in [45], we have made a couple of simplifications that are clarified below.

- The model in [45] has three order parameter tensors, one first-order and two second-order. In the biaxial nematic phases, the first-order tensor takes the value zero. This is also maintained in the leading order of the Hilbert expansion. As a result, keeping the first-order tensor makes no difference in our derivation. For this reason, we assume that the first-order tensor is zero to discard all the terms about it.
- We ignore the spatial diffusion term. This is also adopted in the derivation from dynamic Q-tensor models to the Ericksen–Leslie model (see [11]), because the spatial diffusion term is actually not considered in the Ericksen–Leslie model. Since we would like to derive an analog of the Ericksen–Leslie model, this shall be a reasonable choice. The role of the spatial diffusion term will be addressed in future works.

The tensor model is then about two second-order symmetric traceless tensors, defined as

$$Q_1 = \langle (\mathbf{m}_1^2)_0 \rangle = \left\langle \mathbf{m}_1^2 - \frac{\mathfrak{i}}{3} \right\rangle, \quad Q_2 = \langle (\mathbf{m}_2^2)_0 \rangle = \left\langle \mathbf{m}_2^2 - \frac{\mathfrak{i}}{3} \right\rangle.$$

Denote $\mathbf{Q} = (Q_1, Q_2)^T$. Let us also define a projection on to symmetric traceless tensors,

$$(\mathscr{P}R)_{ij} = \frac{1}{2}(R_{ij} + R_{ji}) - \frac{1}{3}R_{kk}\delta_{ij}. \tag{3.1}$$

The projection can also be imposed on an array of second-order tensors:

$$\mathscr{P}(R_1, \ldots, R_k) = (\mathscr{P}R_1, \ldots, \mathscr{P}R_k).$$

3.1. Free energy. Assume that the concentration c of rigid molecules is constant in space. The free energy contains two parts, the bulk energy and elastic energy,

$$\frac{\mathcal{F}[\mathbf{Q},\nabla\mathbf{Q}]}{k_BT}=\int \mathrm{d}\mathbf{x}\left(\frac{1}{\varepsilon}F_b(\mathbf{Q})+F_e(\nabla\mathbf{Q})\right), \tag{3.2}$$

which is measured by the product of the Boltzmann constant k_B and the absolute temperature T. The bulk energy density, which can describe transitions between homogeneous phases, consists of an entropy term and pairwise interaction terms,

$$F_b=cF_{\text{entropy}}+\frac{c^2}{2}\left(c_{02}|Q_1|^2+c_{03}|Q_2|^2+2c_{04}Q_1\cdot Q_2\right). \tag{3.3}$$

The elastic energy density penalizing spatial inhomogeneity contains a few quadratic terms of $\nabla\mathbf{Q}$:

$$\begin{aligned}F_e=\frac{c^2}{2}\Big(&c_{22}|\nabla Q_1|^2+c_{23}|\nabla Q_2|^2+2c_{24}\partial_iQ_{1jk}\partial_iQ_{2jk}\\&+c_{28}\partial_iQ_{1ik}\partial_jQ_{1jk}+c_{29}\partial_iQ_{2ik}\partial_jQ_{2jk}+2c_{2,10}\partial_iQ_{1ik}\partial_jQ_{2jk}\Big).\end{aligned} \tag{3.4}$$

The free energy (3.2)–(3.4) can be derived from the molecular model [41]. We have introduced a small parameter ε in the free energy (3.2). It can be regarded as the reciprocal of squared relative scale $\tilde{L}$ between the domain of observation and the rigid molecule by a change of variable $\tilde{\mathbf{x}}=\mathbf{x}/\tilde{L}$. We shall revisit the rescaling later in the dynamic model to clarify it.

The entropy term acts as a stabilizing term that guarantees the lower-boundedness of the bulk energy. There can be different choices, but it is always independent of molecule architecture. Moreover, the entropy term is related to expressing the tensors of higher order by Q_1 and Q_2. For this reason, we shall specify the entropy term afterwards.

On the other hand, the coefficients c_{ij} of the quadratic terms can be calculated as functions of molecular parameters. For instance, if the hardcore molecular interaction is adopted, we are able to compute these coefficients from molecular shape parameters [41]. This is also the case for the dynamic tensor model, which we introduce below.

3.2. Dynamic model. Based on the free energy functional (3.2), (3.3), and (3.4), let us write down the molecular-theory-based dynamic tensor model derived in [45]. We define the variational derivative of (3.2) as

$$\begin{aligned}\mu_{\mathbf{Q}}&=\frac{1}{ck_BT}\frac{\delta\mathcal{F}(\mathbf{Q},\nabla\mathbf{Q})}{\delta\mathbf{Q}}=\frac{1}{ck_BT}\mathscr{P}\left(\frac{1}{\varepsilon}\frac{\partial F_b(\mathbf{Q})}{\partial\mathbf{Q}}-\partial_i\left(\frac{\partial F_e(\nabla\mathbf{Q})}{\partial(\partial_i\mathbf{Q})}\right)\right)\\&\overset{\text{def}}{=}\frac{1}{\varepsilon}\mathcal{J}(\mathbf{Q})+\mathcal{G}(\mathbf{Q}),\end{aligned} \tag{3.5}$$

where $\mu_{\mathbf{Q}}=(\mu_{Q_1},\mu_{Q_2})^T$, $\mathcal{J}(\mathbf{Q})=(\mathcal{J}_1(\mathbf{Q}),\mathcal{J}_2(\mathbf{Q}))^T$, and $\mathcal{G}(\mathbf{Q})=(\mathcal{G}_1(\mathbf{Q}),\mathcal{G}_2(\mathbf{Q}))^T$ are calculated as

$$\begin{aligned}\mu_{Q_1}&=\frac{1}{\varepsilon}\mathcal{J}_1(\mathbf{Q})+\mathcal{G}_1(\mathbf{Q})\\&=\frac{1}{\varepsilon}\left(\mathscr{P}\frac{\partial F_{entropy}}{\partial Q_1}+cc_{02}Q_1+cc_{04}Q_2\right)\\&\quad-cc_{22}\Delta Q_{1jk}-cc_{24}\Delta Q_{2jk}-\mathscr{P}(cc_{28}\partial_j\partial_iQ_{1ik}+cc_{2,10}\partial_j\partial_iQ_{2ik}),\end{aligned} \tag{3.6}$$

$$\mu_{Q_2} = \frac{1}{\varepsilon}\mathcal{J}_2(\mathbf{Q}) + \mathcal{G}_2(\mathbf{Q})$$
$$= \frac{1}{\varepsilon}\left(\mathscr{P}\frac{\partial F_{entropy}}{\partial Q_2} + cc_{04}Q_1 + cc_{03}Q_2\right)$$
$$- cc_{24}\Delta Q_{1jk} - cc_{23}\Delta Q_{2jk} - \mathscr{P}(cc_{2,10}\partial_j\partial_i Q_{1ik} + cc_{29}\partial_j\partial_i Q_{2ik}). \tag{3.7}$$

Recall the rescaling $\tilde{\mathbf{x}} = \mathbf{x}/\tilde{L}$. We rescale the time $\tilde{t} = t/\tilde{T}$, so that other variables are rescaled accordingly, such as the velocity $\mathbf{v} = \tilde{L}\tilde{\mathbf{v}}/\tilde{T}$. By taking $\tilde{T} = \tilde{L}^2 = 1/\varepsilon$ and some staightforward calculations, the dynamic tensor model can be expressed as

$$\frac{\partial \mathbf{Q}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{Q} = \mathcal{K}_{\mathbf{Q}} + \mathcal{W}_{\mathbf{Q}}, \tag{3.8}$$

$$\rho_s\left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{v}\right) = -\nabla p + \nabla\cdot\sigma + \mathbf{F}^e, \tag{3.9}$$

$$\nabla\cdot\mathbf{v} = 0, \tag{3.10}$$

where ρ_s is the density of the fluid (assumed to be constant), $\mathbf{v}$ the fluid velocity, and p is the pressure to maintain the incompressibility. Let us denote by $\kappa_{ij} = \partial_j v_i$ the velocity gradient. The terms $\mathcal{K}_{\mathbf{Q}} = (\mathcal{K}_{Q_1}, \mathcal{K}_{Q_2})$ and $\mathcal{W}_{\mathbf{Q}} = (\mathcal{W}_{Q_1}, \mathcal{W}_{Q_2})$ on the right-hand side of (3.8) characterize the rotational diffusions and rotational convections, respectively. They are given by

$$-(\mathcal{K}_{Q_1})_{kl} = 4\Gamma_2(\mu_{Q_1})_{ij}\left\langle \mathbf{m}_1\mathbf{m}_3\otimes\mathbf{m}_1\mathbf{m}_3\right\rangle_{ijkl} + 4\Gamma_3(\mu_{Q_1}-\mu_{Q_2})_{ij}\left\langle \mathbf{m}_1\mathbf{m}_2\otimes\mathbf{m}_1\mathbf{m}_2\right\rangle_{ijkl},$$
$$-(\mathcal{K}_{Q_2})_{kl} = 4\Gamma_1(\mu_{Q_2})_{ij}\left\langle \mathbf{m}_2\mathbf{m}_3\otimes\mathbf{m}_2\mathbf{m}_3\right\rangle_{ijkl} - 4\Gamma_3(\mu_{Q_1}-\mu_{Q_2})_{ij}\left\langle \mathbf{m}_1\mathbf{m}_2\otimes\mathbf{m}_1\mathbf{m}_2\right\rangle_{ijkl},$$
$$(\mathcal{W}_{Q_1})_{kl} = 2\kappa_{ij}\big(\langle(\mathbf{m}_1\otimes\mathbf{m}_3)\otimes\mathbf{m}_1\mathbf{m}_3\rangle + e_1\langle(\mathbf{m}_1\otimes\mathbf{m}_2)\otimes\mathbf{m}_1\mathbf{m}_2\rangle$$
$$-e_2\langle(\mathbf{m}_2\otimes\mathbf{m}_1)\otimes\mathbf{m}_1\mathbf{m}_2\rangle\big)_{ijkl},$$
$$(\mathcal{W}_{Q_2})_{kl} = 2\kappa_{ij}\big(\langle(\mathbf{m}_2\otimes\mathbf{m}_3)\otimes\mathbf{m}_2\mathbf{m}_3\rangle - e_1\langle(\mathbf{m}_1\otimes\mathbf{m}_2)\otimes\mathbf{m}_1\mathbf{m}_2\rangle$$
$$+e_2\langle(\mathbf{m}_2\otimes\mathbf{m}_1)\otimes\mathbf{m}_1\mathbf{m}_2\rangle\big)_{ijkl},$$

where $\Gamma_i = \frac{m_0}{\zeta I_{ii}}(i=1,2,3)$ are the diffusion coefficients, m_0 is the mass of a rigid molecule, ζ is the friction constant, $e_i\,(i=1,2)$ are defined as $e_1 = 1 - e_2 = \frac{I_{22}}{I_{11}+I_{22}}$, and $I_{ii}(i=1,2,3)$ are diagonal elements of the moment of inertia for a molecule.

In (3.9), the stress tensor σ consists of the viscous stress σ_v and the elastic stress σ_e. The viscous stress σ_v includes the contribution of the fluid itself with a viscous coefficient η, and the fluid-molecule friction,

$$\sigma_v = \eta(\kappa + \kappa^T) + \sigma_{vf}. \tag{3.11}$$

The second term σ_{vf} is determined by the following equation:

$$(\sigma_{vf})_{ij} = c\zeta\kappa_{kl}\left(I_{22}\langle\mathbf{m}_1^4\rangle + I_{11}\langle\mathbf{m}_2^4\rangle + \frac{4I_{11}I_{22}}{I_{11}+I_{22}}\langle\mathbf{m}_1\mathbf{m}_2\otimes\mathbf{m}_1\mathbf{m}_2\rangle\right)_{ijkl}.$$

The elastic stress σ_e can be written as

$$(\sigma_e)_{kl} = 2ck_BT\Big[(\mu_{Q_2})_{ij}\left\langle\mathbf{m}_2\mathbf{m}_3\otimes(\mathbf{m}_2\otimes\mathbf{m}_3)\right\rangle_{ijkl} + (\mu_{Q_1})_{ij}\left\langle\mathbf{m}_1\mathbf{m}_3\otimes(\mathbf{m}_1\otimes\mathbf{m}_3)\right\rangle_{ijkl}$$
$$+ \frac{1}{I_{11}+I_{22}}\left((\mu_{Q_1}-\mu_{Q_2})_{ij}\left\langle\mathbf{m}_1\mathbf{m}_2\otimes(I_{22}\mathbf{m}_1\otimes\mathbf{m}_2 - I_{11}\mathbf{m}_2\otimes\mathbf{m}_1)\right\rangle_{ijkl}\right)\Big].$$

The body force $\mathbf{F}^e$ is given by

$$\mathbf{F}^e_i = ck_BT\mu_{\mathbf{Q}} \cdot \partial_i\mathbf{Q} \stackrel{\text{def}}{=} ck_BT(\mu_{Q_1} \cdot \partial_i Q_1 + \mu_{Q_2} \cdot \partial_i Q_2). \tag{3.12}$$

The system (3.8)–(3.10) obeys the following energy dissipation law (see [45]):

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t}\left(\int \mathrm{d}\mathbf{x}\frac{\rho_s|\mathbf{v}|^2}{2} + \mathcal{F}[\mathbf{Q},\nabla\mathbf{Q}]\right)\\
&\quad = \int \mathrm{d}\mathbf{x}\Bigg\{ - ck_BT\Big[\Gamma_1\left\langle(2\mu_{Q_2}\cdot\mathbf{m}_2\mathbf{m}_3)^2\right\rangle + \Gamma_2\left\langle(2\mu_{Q_1}\cdot\mathbf{m}_1\mathbf{m}_3)^2\right\rangle\\
&\qquad + \Gamma_3\left\langle\left(2(\mu_{Q_1}-\mu_{Q_2})\cdot\mathbf{m}_1\mathbf{m}_2\right)^2\right\rangle\Big] - 2\eta\frac{\kappa+\kappa^T}{2}\cdot\frac{\kappa+\kappa^T}{2}\\
&\qquad - c\zeta\left[I_{22}\left\langle(\kappa\cdot\mathbf{m}_1^2)^2\right\rangle + I_{11}\left\langle(\kappa\cdot\mathbf{m}_2^2)^2\right\rangle + \frac{I_{11}I_{22}}{I_{11}+I_{22}}\left\langle(2\kappa\cdot\mathbf{m}_1\mathbf{m}_2)^2\right\rangle\right]\Bigg\}.
\end{aligned} \tag{3.13}$$

Note that several fourth-order tensors appear in the dynamic model. In order to close the system, it is necessary to find a certain way to express them by Q_1 and Q_2. The closure approximation can be done by the entropy term, which will be introduced below. Although there might be other ways of closure, one advantage of closure by the entropy term is that it guarantees the nonpositiveness of the terms on the right-hand side of (3.13).

3.3. Original entropy and quasi-entropy. We have mentioned that the entropy term plays a significant role in both free energy and closure approximation. A general approach is to deduce the entropy term by minimizing $\int_{SO(3)}\rho\ln\rho\mathrm{d}\mathfrak{q}$ with the values of the tensors fixed, or finding the maximum entropy state. When the two tensors Q_1 and Q_2 are involved, the maximum entropy state is given by

$$\rho(\mathfrak{q}) = \frac{1}{Z}\exp(B_1\cdot\mathbf{m}_1^2 + B_2\cdot\mathbf{m}_2^2), \tag{3.14}$$

where the normalizing constant Z and two second-order symmetric traceless tensors B_1 and B_2 are Lagrange multipliers for the constraints,

$$\begin{aligned}
Z &= \int_{SO(3)}\exp(B_1\cdot\mathbf{m}_1^2 + B_2\cdot\mathbf{m}_2^2)\mathrm{d}\mathfrak{q},\\
Q_i &= \frac{1}{Z}\int_{SO(3)}\left(\mathbf{m}_i^2 - \frac{1}{3}\mathfrak{i}\right)\exp(B_1\cdot\mathbf{m}_1^2 + B_2\cdot\mathbf{m}_2^2)\mathrm{d}\mathfrak{q}.
\end{aligned} \tag{3.15}$$

Taking (3.14) into $\int_{SO(3)}\rho\ln\rho\mathrm{d}\mathfrak{q}$, we obtain that the entropy term F_{entropy} is given by

$$F_{\text{orig}} = B_1\cdot Q_1 + B_2\cdot Q_2 - \ln Z, \tag{3.16}$$

where we use the notation F_{orig} to stand for the "original entropy." The maximum entropy state (3.14) is uniquely determined by Q_1 and Q_2 [41]. Therefore, F_{orig} can be viewed as a function around Q_1 and Q_2. It is observed that F_{orig} is invariant under rotations on Q_1 and Q_2. Generally, a rotation of a tensor U can be understood as follows: The coordinates $U_{i_1\dots i_n}$ in (2.1) are kept, while the basis $(\mathbf{e}_i)$ is replaced with another right-handed orthonormal frame $(\mathbf{e}_i{}')$. Specifically, a rotation on Q_1 and Q_2 is done by choosing a particular $\mathfrak{t}\in SO(3)$ and transforming Q_i into $\mathfrak{t}Q_i\mathfrak{t}^{-1}$. It is easy to verify that (3.16) is rotationally invariant under this transformation (see section SM2 of the supplementary materials).

The closure approximation can be done with the maximum entropy state, as the high-order tensors can be calculated using the density function (3.14). An equivalent viewpoint is that when Q_1 and Q_2 are given, the high-order tensors obtained in this way minimize $\int_{SO(3)} \rho \ln \rho \mathrm{d}\mathfrak{q}$.

The entropy term defined from the maximum entropy state that involves integrals on $SO(3)$, is given implicitly, which could bring difficulties in both analyses and numerical studies. An alternative approach is proposed [38], where the original entropy is substituted by the quasi-entropy. The quasi-entropy is defined by a log-determinant covariance matrix, which is an elementary function of the order parameter tensors. To write down the expression of the quasi-entropy, it is necessary to specify the highest tensor order (that shall be even) to be involved. When only second-order tensors are involved, the quasi-entropy for Q_1 and Q_2 is given by [38] (see also section SM2 of the supplementary materials),

(3.17)
$$\Xi_2(Q_1, Q_2) = \nu\left(-\ln\det\left(Q_1 + \frac{\mathfrak{i}}{3}\right) - \ln\det\left(Q_2 + \frac{\mathfrak{i}}{3}\right) - \ln\det\left(\frac{\mathfrak{i}}{3} - Q_1 - Q_2\right)\right).$$

Let us briefly explain how Ξ_2 is obtained (see [38] or section SM2 in the supplementary materials for details). Notice that three log-determinants appear in Ξ_2. This is because the covariance matrix can be reduced to a block diagonal one, with the blocks given by the three matrices in log-determinants. Apparently, Ξ_2 does not have a finite value if any of the three matrices is singular. We restrain its domain in those (Q_1, Q_2) such that the three matrices are positive definite:

$$\mathrm{dom}(\Xi_2) = \left\{\mathbf{Q} : Q_1 + \frac{\mathfrak{i}}{3},\ Q_2 + \frac{\mathfrak{i}}{3},\ \frac{\mathfrak{i}}{3} - Q_1 - Q_2 \text{ positive definite}\right\}.$$

Actually, in this domain Ξ_2 gives a barrier function: Consider a sequence $\mathrm{dom}(\Xi_2) \ni \mathbf{Q}_k \to \mathbf{Q}_0$ such that $\mathbf{Q}_0$ makes any of the three matrices singular, then $\lim \Xi_2(\mathbf{Q}_k) \to +\infty$.

A free parameter ν is introduced above. It can be estimated as $\nu = 5/9$ from special cases (see section 6 in [38]), which we adopt in the current work. Moreover, analyses show that the quasi-entropy possesses similar properties to the original entropy. In particular, the results from the quasi-entropy (3.17) are very similar to those from the original entropy (3.16), provided that other terms in the free energy are identical. These results have all been reported in [38].

The quasi-entropy is also suitable for closure approximation. To deduce high-order tensors in the dynamic model, we shall use the log-determinant covariance matrix up to fourth order, denoted by Ξ_4 which is provided in (SM2.5) of the supplementary materials. Similarly to Ξ_2, the domain of Ξ_4 is specified by those tensors (including Q_1, Q_2, and some tensors up to fourth-order) such that the covariance matrix is positive definite. To carry out the closure approximation, the fourth-order tensors shall minimize Ξ_4 with the given values of Q_1 and Q_2, so that they can be solved as functions of $\mathbf{Q}$. Thus, we can see that the closure approximation by the original entropy and the quasi-entropy share the rationale, with the only difference lying in the function to be minimized. In what follows, we shall see that these two approaches of closure approximation lead to high-order tensors of the same form due to the same symmetry arguments.

The properties of the quasi-entropy have been discussed previously [38]. Here, let us state those to be utilized in this paper. The proof is also provided in section SM2 of the supplementary materials.

PROPOSITION 3.1. *The two functions* Ξ_2 *(see* (3.17)*) and* Ξ_4 *(see* (B.5)*) have the following properties:*

- *They are invariant under rotations on the tensors.*
- *They act as barrier functions on the corresponding domains that have been discussed above.*
- *They are strictly convex with respect to the tensors.*

As an example, it is straightfoward to see the rotational invariance for Ξ_2 by taking the rotation $Q_i \to \mathfrak{t} Q_i \mathfrak{t}^{-1}$ into (3.17).

The properties stated above are all crucial in our derivation below. The rotational invariance is a foundation for the frame model to be established. The positive-definiteness of covariance matrices is essential for energy dissipation to hold. The strict convexity guarantees that the closure approximation by minimization results in a unique solution.

Remark 3.2. A problem of interest is whether the domains of F_{orig} and Ξ_2 are identical. Unfortunately, in general cases this problem is still open. However, if we further require that Q_1 and Q_2 share an eigenframe, the two domains are indeed identical, as we will discuss right away. This turns out to be sufficient for the current work.

3.4. Stationary points of bulk energy. There are analyses on the stationary points of the bulk energy F_b (given by (3.3)), but they are far from well-understood. We summarize the main results up to date in the following proposition [38, 43]. To simplify the presentation, the conditions on the coefficients are stricter than they need to be.

PROPOSITION 3.3. *Assume that the matrix* $\begin{pmatrix} c_{02} & c_{04} \\ c_{04} & c_{03} \end{pmatrix}$ *is not negative definite, or is negative but* $c_{04}^2/c_{03} - c_{02} \le 2$*. Consider the two cases of the entropy term:*

1. F_{entropy} *takes* F_{orig} *(see* (3.16)*);*
2. F_{entropy} *takes* Ξ_2 *(see* (3.17)*) with* $\nu = 5/9$*.*

For both cases, at the stationary points, Q_1 *and* Q_2 *have a shared eigenframe.*

When Q_1 and Q_2 has the same eigenframe, they can be written as

$$Q_i = s_i \left(\mathbf{n}_1^2 - \frac{\mathfrak{i}}{3} \right) + b_i (\mathbf{n}_2^2 - \mathbf{n}_3^2), \quad i = 1, 2. \tag{3.18}$$

Numerical studies indicate that the global energy minimum could be either uniaxial (where $b_i = 0$) or biaxial (where at least one $b_i \neq 0$). For the original entropy, the results can be found in [23, 30, 41, 42]; for the quasi-entropy Ξ_2, the results can be found in section 6.3 in [38]. Here, we assume that under certain coefficients c_{02}, c_{03}, and c_{04}, we have a biaxial global minimum $\mathbf{Q}^{(0)} = (Q_1^{(0)}, Q_2^{(0)})$ of the form (3.18).

It shall be noticed that the bulk energy F_b is rotationally invariant, i.e. invariant of $\mathfrak{p} = (\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3)$. This can be observed by combining Proposition 3.3 and the fact that the three c_{0i} terms are rotationally invariant. Thus, a rotation of an energy minimum also results in an energy minimum.

At any energy minimum, we have $\mathcal{J}(\mathbf{Q}^{(0)}) = 0$. Let us fix s_i and b_i and let $\mathfrak{p} = (\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3)$ vary, so that $\mathbf{Q}^{(0)} = \mathbf{Q}^{(0)}(\mathfrak{p})$ becomes a function of $\mathfrak{p}$. Since $\mathbf{Q}^{(0)}$ is an energy minimum whatever $\mathfrak{p}$ is, it implies that $\mathcal{J}(\mathbf{Q}^{(0)}(\mathfrak{p})) = 0$. We then impose the operators $\mathscr{L}_i$ on it. By the chain rule, we obtain

$$\mathscr{L}_m \mathcal{J}(\mathbf{Q}^{(0)})_{ij} = \mathcal{J}'(\mathbf{Q}^{(0)})_{ijkl}(\mathscr{L}_m \mathbf{Q}^{(0)})_{kl} = 0, \ m = 1,2,3. \tag{3.19}$$

This implies that the kernel of the Hessian $\mathcal{J}'(\mathbf{Q}^{(0)})$ contains the space spanned by $\mathscr{L}_m \mathbf{Q}^{(0)}$.

With the form (3.18), the scalars s_i and b_i shall satisfy

$$\frac{2}{3}s_i + \frac{1}{3} > 0, \quad \frac{1}{3} - \frac{1}{3}s_i \pm b_i > 0, \qquad i = 1,2,3, \tag{3.20}$$

where we define $s_3 = -s_1 - s_2$ and $b_3 = -b_1 - b_2$. If we only consider the cases where Q_1 and Q_2 share an eigenframe, this is exactly the range such that both F_{orig} and Ξ_2 are well-defined: For the original entropy, the derivation can be found in [41]; for the quasi-entropy Ξ_2, the condition (3.20) is equivalent to the requirement that $Q_1 + \mathfrak{i}/3$, $Q_2 + \mathfrak{i}/3$, and $-Q_1 - Q_2 + \mathfrak{i}/3$ are positive definite. Furthermore, when we fix Q_1 and Q_2 that share an eigenframe with the scalars satisfying (3.20), the domain of Ξ_4 is nonempty so that the closure approximation is indeed well-posed (see section SM2 in the supplementary materials for details).

3.5. High-order tensors and their symmetry. We have mentioned that the high-order tensors in the dynamic model are determined from closure approximation. However, there are many linear relations between these high-order tensors. It is necessary to specify their linearly independent components, which can be done with the help of symmetric traceless tensors. The use of symmetric traceless tensors turn out to be crucial to figuring out symmetry arguments for these high-order tensors.

For the high-order tensors appearing in the dynamic tensor model, it turns out that only the tensors below are involved other than Q_1 and Q_2:

$$\langle \mathbf{m}_1\mathbf{m}_2\mathbf{m}_3 \rangle, \ \langle (\mathbf{m}_1^4)_0 \rangle, \ \langle (\mathbf{m}_2^4)_0 \rangle, \ \langle (\mathbf{m}_1^2\mathbf{m}_2^2)_0 \rangle. \tag{3.21}$$

Here, we recall the notation $(U)_0$ in (2.2) for the symmetric traceless tensor generated by U. The explicit expressions of these tensors, as well as the expressions of the fourth-order tensors in the dynamic model by these tensors, are given in section SM1 of the supplementary materials.

Therefore, in a closure approximation, our task is to determine the third-order and fourth-order tensors in (3.21). In particular, when Q_1 and Q_2 have the form (3.18), the tensors in (3.21) have the form indicated by the following theorem.

THEOREM 3.4. *If Q_1 and Q_2 are biaxial of the form* (3.18)*, then the third- and fourth-order symmetric traceless tensors, solved from closure approximation by the original entropy or the quasi-entropy, take the form*

$$\begin{aligned}
\langle \mathbf{m}_1\mathbf{m}_2\mathbf{m}_3 \rangle &= z\mathbf{n}_1\mathbf{n}_2\mathbf{n}_3, \\
\langle (\mathbf{m}_1^4)_0 \rangle &= a_1(\mathbf{n}_1^4)_0 + a_2(\mathbf{n}_2^4)_0 + a_3(\mathbf{n}_1^2\mathbf{n}_2^2)_0, \\
\langle (\mathbf{m}_2^4)_0 \rangle &= \tilde{a}_1(\mathbf{n}_1^4)_0 + \tilde{a}_2(\mathbf{n}_2^4)_0 + \tilde{a}_3(\mathbf{n}_1^2\mathbf{n}_2^2)_0, \\
\langle (\mathbf{m}_1^2\mathbf{m}_2^2)_0 \rangle &= \bar{a}_1(\mathbf{n}_1^4)_0 + \bar{a}_2(\mathbf{n}_2^4)_0 + \bar{a}_3(\mathbf{n}_1^2\mathbf{n}_2^2)_0.
\end{aligned} \tag{3.22}$$

The scalars z, a_i, $\tilde{a}_i$, $\bar{a}_i$ are solved as functions of s_i and b_i. Furthermore, if s_i and b_i satisfy (3.20)*, these scalars can be uniquely solved.*

Theorem 3.4 is actually a special case of Theorem 4.8 in [38]. The proof can be also found in section SM2 of the supplementary materials. This result actually determines the form of high-order tensors in the Hilbert expansion, which in turn makes a great difference in determining the form of the frame hydrodynamics for the biaxial nematic phase.

4. From tensor model to orthonormal frame model. We make the Hilbert expansion (also called the Chapman–Enskog expansion) of solutions with respect to the small parameter ε. The $O(1)$ system results in the orthonormal frame model for the biaxial nematic phase, with the energy dissipation maintained. The coefficients in the frame model are derived from those in the tensor model. Since the coefficients in the tensor model are derived from physical parameters, we finally build the relation between the frame model and the physical parameters. We also point out that the derivations afterwards are suitable for both the original entropy and the quasi-entropy.

For convenience, we denote seven fourth-order tensor moments as follows:

$$\begin{cases} \mathcal{R}_1 = \langle (\mathbf{m}_1^2 - \frac{\mathfrak{i}}{3}) \otimes (\mathbf{m}_1^2 - \frac{\mathfrak{i}}{3}) \rangle, \quad \mathcal{R}_2 = \langle (\mathbf{m}_2^2 - \frac{\mathfrak{i}}{3}) \otimes (\mathbf{m}_2^2 - \frac{\mathfrak{i}}{3}) \rangle, \\ \mathcal{R}_3 = 4\langle \mathbf{m}_1\mathbf{m}_2 \otimes \mathbf{m}_1\mathbf{m}_2 \rangle, \quad \mathcal{R}_4 = 4\langle \mathbf{m}_1\mathbf{m}_3 \otimes \mathbf{m}_1\mathbf{m}_3 \rangle, \quad \mathcal{R}_5 = 4\langle \mathbf{m}_2\mathbf{m}_3 \otimes \mathbf{m}_2\mathbf{m}_3 \rangle, \\ \mathcal{V}_{Q_1} = 2\left(\langle \mathbf{m}_1\mathbf{m}_3 \otimes (\mathbf{m}_1 \otimes \mathbf{m}_3) \rangle + e_1 \langle \mathbf{m}_1\mathbf{m}_2 \otimes (\mathbf{m}_1 \otimes \mathbf{m}_2) \rangle - e_2 \langle \mathbf{m}_1\mathbf{m}_2 \otimes (\mathbf{m}_2 \otimes \mathbf{m}_1) \rangle \right), \\ \mathcal{V}_{Q_2} = 2\left(\langle \mathbf{m}_2\mathbf{m}_3 \otimes (\mathbf{m}_2 \otimes \mathbf{m}_3) \rangle - e_1 \langle \mathbf{m}_1\mathbf{m}_2 \otimes (\mathbf{m}_1 \otimes \mathbf{m}_2) \rangle + e_2 \langle \mathbf{m}_1\mathbf{m}_2 \otimes (\mathbf{m}_2 \otimes \mathbf{m}_1) \rangle \right). \end{cases} \tag{4.1}$$

We frequently deal with contractions between fourth-order tensors and second-order tensors. We could regard a fourth-order tensor as a matrix, and a second-order tensor as a vector, so that the contractions can be formulated as matrix-matrix and matrix-vector multiplications, as we explain below. When a fourth-order tensor is contracted with a second-order tensor, we could write it in short as a matrix-vector product, say

$$(\mathcal{V}_{Q_1})_{ijkl}\kappa_{kl} = (\mathcal{V}_{Q_1}\kappa)_{ij}. \tag{4.2}$$

When using this short notation, we always assume that the second to last index of the fourth-order tensor is contracted with the first of the second-order tensor, and the last of the fourth-order tensor is contracted with the last of the second-order tensor. By the convention (4.2), we could define the transpose of a fourth-order tensor, such as

$$(\mathcal{V}_{Q_1}^T)_{ijkl} = (\mathcal{V}_{Q_1})_{klij}.$$

Let us define

$$\mathcal{M} = \begin{pmatrix} \mathcal{M}_{11} & \mathcal{M}_{12} \\ \mathcal{M}_{12} & \mathcal{M}_{22} \end{pmatrix} \overset{\text{def}}{=} \begin{pmatrix} \Gamma_2\mathcal{R}_4 + \Gamma_3\mathcal{R}_3 & -\Gamma_3\mathcal{R}_3 \\ -\Gamma_3\mathcal{R}_3 & \Gamma_1\mathcal{R}_5 + \Gamma_3\mathcal{R}_3 \end{pmatrix}, \tag{4.3}$$

$$\mathcal{V} \overset{\text{def}}{=} \begin{pmatrix} \mathcal{V}_{Q_1} \\ \mathcal{V}_{Q_2} \end{pmatrix}, \quad \mathcal{N} \overset{\text{def}}{=} (\mathcal{N}_{Q_1}, \mathcal{N}_{Q_2}) = (\mathcal{V}_{Q_1}^T, \mathcal{V}_{Q_2}^T), \tag{4.4}$$

$$\mathcal{P} \overset{\text{def}}{=} c\zeta \left(I_{22}\mathcal{R}_1 + I_{11}\mathcal{R}_2 + e_1 I_{11}\mathcal{R}_3 \right). \tag{4.5}$$

The system (3.8)–(3.10) can then be rewritten as

$$\frac{\partial \mathbf{Q}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{Q} = -\mathcal{M}\mu_{\mathbf{Q}} + \mathcal{V}\kappa, \tag{4.6}$$

$$\rho_s \left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{v} \right)_i = -\partial_i p + \eta\Delta v_i + \partial_j(\mathcal{P}\kappa)_{ij} + ck_BT\partial_j(\mathcal{N}\mu_{\mathbf{Q}})_{ij} + ck_BT\mu_{\mathbf{Q}}\cdot\partial_i\mathbf{Q}, \tag{4.7}$$

$$\nabla\cdot\mathbf{v} = 0, \tag{4.8}$$

where $\mathcal{M}\mu_{\mathbf{Q}}$ is carried out by matrix-vector multiplication,

$$\mathcal{M}\mu_{\mathbf{Q}} = \begin{pmatrix} \mathcal{M}_{11}\mu_{Q_1} + \mathcal{M}_{12}\mu_{Q_2} \\ \mathcal{M}_{12}\mu_{Q_1} + \mathcal{M}_{22}\mu_{Q_2} \end{pmatrix}.$$

The terms involving $\mathcal{V}$ and $\mathcal{N}$ are interpreted similarly. In the above, we have incorporated some simple calculations for the viscous stress, such as

$$\langle \mathbf{m}_1^4 \rangle \kappa = (\mathcal{R}_1 + Q_1 \otimes \mathfrak{i} + \mathfrak{i} \otimes Q_1 + \mathfrak{i} \otimes \mathfrak{i})\,\kappa = \mathcal{R}_1 \kappa + (Q_1 \cdot \kappa)\mathfrak{i}, \tag{4.9}$$

because the incompressibility can also be written as $\mathfrak{i} \cdot \kappa = 0$. Furthermore, the second term in (4.9) can be merged into the pressure p, so that only the term $\mathcal{R}_1 \kappa$ remains in the operator $\mathcal{P}$.

The fourth-order tensors $\mathcal{R}_i (i = 1, \ldots, 5)$ are positive definite in the sense that for any second-order symmetric traceless tensor Y, we have $Y \cdot \mathcal{R}_i Y \geq 0$ and the equality implies $Y = 0$. This result comes from the property of the entropy term, which is shown in section SM2 of the supplementary materials. Consequently, we deduce that for arbitrary second-order symmetric traceless tensors Y_1 and Y_2, it holds that

$$Y_1 \cdot \mathcal{P} Y_1 = c\zeta\,(I_{22} Y_1 \cdot \mathcal{R}_1 Y_1 + I_{11} Y_1 \cdot \mathcal{R}_2 Y_1 + e_1 I_{11} Y_1 \cdot \mathcal{R}_3 Y_1) \geq 0, \tag{4.10}$$

$$(Y_1, Y_2)\mathcal{M}\begin{pmatrix} Y_1 \\ Y_2 \end{pmatrix} = \Gamma_1 Y_2 \cdot \mathcal{R}_3 Y_2 + \Gamma_2 Y_1 \cdot \mathcal{R}_4 Y_1 + \Gamma_1 (Y_1 - Y_2) \cdot \mathcal{R}_3 (Y_1 - Y_2) \geq 0. \tag{4.11}$$

The equality in (4.11) leads to $Y_1 = Y_2 = 0$, so that $\mathcal{M}(Y_1, Y_2)^T = 0$ implies $Y_1 = Y_2 = 0$.

4.1. The Hilbert expansion.

Assume that $(\mathbf{Q}(t, \mathbf{x}), \mathbf{v}(t, \mathbf{x}))$ is a solution to the molecular-theory-based two-tensor system (4.6)–(4.8). We perform the following Hilbert expansion with respect to ε:

$$\mathbf{Q}(t, \mathbf{x}) = \mathbf{Q}^{(0)}(t, \mathbf{x}) + \varepsilon \mathbf{Q}^{(1)}(t, \mathbf{x}) + \varepsilon^2 \mathbf{Q}^{(2)}(t, \mathbf{x}) + \cdots, \tag{4.12}$$

$$\mathbf{v}(t, \mathbf{x}) = \mathbf{v}^{(0)}(t, \mathbf{x}) + \varepsilon \mathbf{v}^{(1)}(t, \mathbf{x}) + \varepsilon^2 \mathbf{v}^{(2)}(t, \mathbf{x}) + \cdots, \tag{4.13}$$

where $\mathbf{Q}^{(i)} = (Q_1^{(i)}, Q_2^{(i)})^T$, and $(\mathbf{Q}^{(i)}, \mathbf{v}^{(i)})(i = 0, 1, 2, \ldots)$ are independent of the small parameter ε.

Based on the expansion (4.12)–(4.13), we could write down the expansion of other terms in (4.6)–(4.8), frequently by Taylor expansion. Since we focus on the $O(1)$ system, we only write down the terms up to $O(1)$. In $\mu_{\mathbf{Q}}$, the term $\mathcal{J}(\mathbf{Q}) = \mathscr{P} \frac{\partial F_b(\mathbf{Q})}{\partial \mathbf{Q}}$ is multiplied by ε^{-1}, so we need to expand it to $O(\varepsilon)$,

$$\mathcal{J}(\mathbf{Q}) = \mathcal{J}(\mathbf{Q}^{(0)}) + \varepsilon \mathcal{J}'\left(\mathbf{Q}^{(0)}\right)\mathbf{Q}^{(1)} + O(\varepsilon^2),$$

where $\mathcal{J}'(\mathbf{Q}^{(0)}) \stackrel{\text{def}}{=} \mathcal{H}^{(0)}$ is a fourth-order tensor. By (3.5), we deduce that

$$\mu_{\mathbf{Q}} = \varepsilon^{-1}\mathcal{J}(\mathbf{Q}) + \mathcal{G}(\mathbf{Q}) = \varepsilon^{-1}\mathcal{J}(\mathbf{Q}^{(0)}) + \mathcal{H}^{(0)}\mathbf{Q}^{(1)} + \mathcal{G}(\mathbf{Q}^{(0)}) + O(\varepsilon). \tag{4.14}$$

Since the tensors in (4.1) are solved from closure approximation, they are functions of $\mathbf{Q}$. Thus, $\mathcal{M}$, $\mathcal{V}$, $\mathcal{N}$, and $\mathcal{P}$ are functions of $\mathbf{Q}$. Let us use the notation $\mathcal{M}^{(0)}$ for the $\mathcal{M}$ when $\mathbf{Q}$ takes $\mathbf{Q}^{(0)}$. Then we have

$$\mathcal{M} = \mathcal{M}^{(0)} + O(\varepsilon), \quad \mathcal{V} = \mathcal{V}^{(0)} + O(\varepsilon),$$
$$\mathcal{N} = \mathcal{N}^{(0)} + O(\varepsilon) = \mathcal{V}^{(0)T} + O(\varepsilon), \quad \mathcal{P} = \mathcal{P}^{(0)} + O(\varepsilon),$$

where $\mathcal{M}^{(0)}$, $\mathcal{V}^{(0)}$, $\mathcal{N}^{(0)}$, and $\mathcal{P}^{(0)}$ are given by adding superscripts (0) to the elements in (4.3)–(4.5).

Substituting the above expansions (4.12) and (4.13) into the system (4.6)–(4.8) and collecting the terms with the same order of ε, we can obtain a series of equations. The $O(\varepsilon^{-1})$ system requires that

$$\mathcal{M}^{(0)}\mathcal{J}(\mathbf{Q}^{(0)}) = 0. \tag{4.15}$$

Recalling the positive-definiteness of $\mathcal{M}^{(0)}$ given by (4.11), (4.15) implies that

$$\mathcal{J}(\mathbf{Q}^{(0)}) = 0.$$

It means that $\mathbf{Q}^{(0)}$ is just the stationary point of $F_b(\mathbf{Q})$. We shall consider the case that $\mathbf{Q}^{(0)}$ is the biaxial global minimum, which takes the form (3.18).

The terms of order $O(1)$ give

(4.16)
$$\frac{\partial \mathbf{Q}^{(0)}}{\partial t} + \mathbf{v}^{(0)}\cdot\nabla\mathbf{Q}^{(0)} = -\mathcal{M}^{(0)}\left(\mathcal{H}^{(0)}\mathbf{Q}^{(1)} + \mathcal{G}(\mathbf{Q}^{(0)})\right) + \mathcal{V}^{(0)}\kappa^{(0)},$$

$$\rho_s\left(\frac{\partial \mathbf{v}^{(0)}}{\partial t} + \mathbf{v}^{(0)}\cdot\nabla\mathbf{v}^{(0)}\right)_i = -\partial_i p^{(0)} + \eta\Delta v_i^{(0)} + \partial_j(\mathcal{P}^{(0)}\kappa^{(0)})_{ij}$$

(4.17)
$$+ ck_BT\partial_j\left(\mathcal{N}^{(0)}(\mathcal{H}^{(0)}\mathbf{Q}^{(1)} + \mathcal{G}(\mathbf{Q}^{(0)}))_{ij}\right) + ck_BT\left(\mathcal{H}^{(0)}\mathbf{Q}^{(1)} + \mathcal{G}(\mathbf{Q}^{(0)})\right)\cdot\partial_i\mathbf{Q}^{(0)},$$

(4.18)
$$\nabla\cdot\mathbf{v}^{(0)} = 0.$$

In the $O(1)$ system (4.16)–(4.18), $\mathbf{Q}^{(0)}$ is a function of $\mathfrak{p} = (\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3)$ and $\kappa^{(0)} = \nabla\mathbf{v}^{(0)}$. The high-order tensors with the superscript (0) are functions of $\mathbf{Q}^{(0)}$, thus are functions of $\mathfrak{p}$. Therefore, if we could eliminate $\mathbf{Q}^{(1)}$ in the $O(1)$ system, we would arrive at a system of only $\mathfrak{p}$ and $\mathbf{v}^{(0)}$. Indeed, this can be done by examining the kernel of $\mathcal{H}^{(0)}$.

Our task becomes expressing terms with the superscript (0) in terms of $\mathbf{n}_1$, $\mathbf{n}_2$, $\mathbf{n}_3$. It turns out that the form (3.18) of $\mathbf{Q}^{(0)}$ results in specific form of the following terms.

- The derivatives of $\mathbf{Q}^{(0)}$, which are related to the kernel of $\mathcal{H}^{(0)}$.
- The variational derivative of the elastic energy, $\mathcal{G}(\mathbf{Q}^{(0)})$.
- The high-order tensors $\mathcal{M}^{(0)}$, $\mathcal{V}^{(0)}$, $\mathcal{N}^{(0)}$, and $\mathcal{P}^{(0)}$.

Up to now, all the equations are expressed by the components in the basis generated by the reference frame $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$. In order to facilitate the specific form of the above terms, we shall first rewrite the $O(1)$ system in the basis generated by $\mathfrak{p} = (\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3)$.

4.2. Change to the local basis. In what follows, we denote by $\mathbf{A}_0$ and $\mathbf{\Omega}_0$ the symmetric and skew-symmetric parts of the velocity gradient $\kappa_{ij}^{(0)} = \partial_j v_i^{(0)}$, respectively, i.e., $\mathbf{A}_0 = (\kappa^{(0)} + \kappa^{(0)T})/2, \mathbf{\Omega}_0 = (\kappa^{(0)} - \kappa^{(0)T})/2$.

We consider the basis for second-order tensors given by $\mathfrak{i}$, five symmetric traceless tensors,

$$\mathbf{s}_1 = \mathbf{n}_1^2 - \frac{1}{3}\mathfrak{i}, \quad \mathbf{s}_2 = \mathbf{n}_2^2 - \mathbf{n}_3^2, \quad \mathbf{s}_3 = \mathbf{n}_1\mathbf{n}_2, \quad \mathbf{s}_4 = \mathbf{n}_1\mathbf{n}_3, \quad \mathbf{s}_5 = \mathbf{n}_2\mathbf{n}_3, \tag{4.19}$$

and three asymmetric traceless tensors,

$$\mathbf{a}_1 = \mathbf{n}_1\otimes\mathbf{n}_2 - \mathbf{n}_2\otimes\mathbf{n}_1, \quad \mathbf{a}_2 = \mathbf{n}_3\otimes\mathbf{n}_1 - \mathbf{n}_1\otimes\mathbf{n}_3, \quad \mathbf{a}_3 = \mathbf{n}_2\otimes\mathbf{n}_3 - \mathbf{n}_3\otimes\mathbf{n}_2. \tag{4.20}$$

Let us look into the fourth-order tensors $\mathcal{M}_{11}^{(0)}, \mathcal{M}_{12}^{(0)}, \mathcal{M}_{22}^{(0)}$. The first two components of $\mathcal{M}_{11}^{(0)}$ are symmetric, and the contraction of the first two components gives a zero second-order tensor. So is the contraction of its last two components. Thus, it can be expressed as

$$\mathcal{M}_{11}^{(0)} = (M_{11})_{ij}\mathbf{s}_i \otimes \mathbf{s}_j. \tag{4.21}$$

Similarly, M_{12} and M_{22} are also defined.

When the last two indices of $\mathcal{M}_{11}^{(0)}$ are contracted with a second-order symmetric traceless tensor $Y = y_i\mathbf{s}_i$, it gives

$$\mathcal{M}_{11}^{(0)}Y = ((M_{11})_{ij}y_k)\,(\mathbf{s}_i \otimes \mathbf{s}_j)\mathbf{s}_k. \tag{4.22}$$

By the convention of the a fourth-order tensor times a second-order tensor (4.2), the product $(\mathbf{s}_i \otimes \mathbf{s}_j)\mathbf{s}_k$ gives a second-order tensor $(\mathbf{s}_j \cdot \mathbf{s}_k)\mathbf{s}_i$. Let us define a matrix Λ by

$$\Lambda_{ij} = \mathbf{s}_i \cdot \mathbf{s}_j = \mathrm{diag}\left(\frac{2}{3}, 2, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right). \tag{4.23}$$

So, $\mathcal{M}_{11}^{(0)}Y$ is written as

$$\mathcal{M}_{11}^{(0)}Y = ((M_{11})_{ij}\Lambda_{jk}y_k)\,\mathbf{s}_i = (M_{11}\Lambda y)_i\mathbf{s}_i. \tag{4.24}$$

In other words, the coordinates of $\mathcal{M}_{11}^{(0)}Y$ under the basis $\mathbf{s}_i$ are given by $M_{11}\Lambda y$.

For a product involving $\mathcal{M}^{(0)}$, we just combine the coordinates into a single vector. For instance, for the term $\mathcal{M}^{(0)}\mathcal{G}(\mathbf{Q}^{(0)})$, let us denote

$$M = \begin{pmatrix} M_{11} & M_{12} \\ M_{12} & M_{22} \end{pmatrix}, \quad g = \begin{pmatrix} g_1 \\ g_2 \end{pmatrix}, \quad \widetilde{\Lambda} = \begin{pmatrix} \Lambda & \\ & \Lambda \end{pmatrix}, \tag{4.25}$$

where g_1 is the vector of the coordinates of $\mathcal{G}_1(\mathbf{Q}^{(0)})$, and g_2 that of $\mathcal{G}_2(\mathbf{Q}^{(0)})$, i.e., $\mathcal{G}_1(\mathbf{Q}^{(0)}) = (g_1)_i\mathbf{s}_i$, $\mathcal{G}_2(\mathbf{Q}^{(0)}) = (g_2)_i\mathbf{s}_i$. Then, the term $\mathcal{M}^{(0)}\mathcal{G}(\mathbf{Q}^{(0)})$ has the coordinates

$$M\widetilde{\Lambda}g = \begin{pmatrix} M_{11}\Lambda g_1 + M_{12}\Lambda g_2 \\ M_{12}\Lambda g_1 + M_{22}\Lambda g_2 \end{pmatrix}.$$

We turn to the tensors $\mathcal{N}_{Q_1}^{(0)}, \mathcal{N}_{Q_2}^{(0)}$. For $\mathcal{N}_{Q_1}^{(0)}$, its first two components are no longer symmetric, so that we can express it as

$$\mathcal{N}_{Q_1}^{(0)} = (N_1^u)_{ij}\mathbf{s}_i \otimes \mathbf{s}_j + (N_1^l)_{ij}\mathbf{a}_i \otimes \mathbf{s}_j. \tag{4.26}$$

The matrices N_2^u and N_2^l are defined in the same way. By $\mathcal{V}^{(0)} = \mathcal{N}^{(0)T}$, we can further write

$$\mathcal{V}_{Q_1}^{(0)} = (N_1^u)_{ij}\mathbf{s}_j \otimes \mathbf{s}_i + (N_1^l)_{ij}\mathbf{s}_j \otimes \mathbf{a}_i. \tag{4.27}$$

Denote

$$N = \begin{pmatrix} N_1^u & N_2^u \\ N_1^l & N_2^l \end{pmatrix}, \quad V = N^T, \tag{4.28}$$

where the matrix N has the size 8×10, so that V is 10×8. We have

$$\mathcal{V}^{(0)}\kappa^{(0)} = \begin{pmatrix} \left((N_1^u)_{ij}\mathbf{s}_j \otimes \mathbf{s}_i + (N_1^l)_{ij}\mathbf{s}_j \otimes \mathbf{a}_i\right)\kappa^{(0)} \\ \left((N_2^u)_{ij}\mathbf{s}_j \otimes \mathbf{s}_i + (N_2^l)_{ij}\mathbf{s}_j \otimes \mathbf{a}_i\right)\kappa^{(0)} \end{pmatrix}. \tag{4.29}$$

We define an 8×1 vector ω by the contraction of $\kappa^{(0)}$ and the vector $\mathbf{u} = (\mathbf{s}_1, \ldots, \mathbf{s}_5, \mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)^T$ formed by eight tensors, which is given by $\omega = (\omega_s^T, \omega_a^T)^T$, where ω_s and ω_a are defined as

$$\omega_s = (\mathbf{A}_0 \cdot \mathbf{s}_1, \ldots, \mathbf{A}_0 \cdot \mathbf{s}_5)^T, \quad \omega_a = (\mathbf{\Omega}_0 \cdot \mathbf{a}_1, \mathbf{\Omega}_0 \cdot \mathbf{a}_2, \mathbf{\Omega}_0 \cdot \mathbf{a}_3)^T.$$

Then, the 10×1 vector $V\omega$ gives the coordinates of $\mathcal{V}^{(0)}\kappa^{(0)}$.

Similarly to the vector g, we denote by $\bar{q}$ the coordinates of $\partial_t \mathbf{Q}^{(0)}$, by $\tilde{q}_i$ the coordinates of $\partial_i \mathbf{Q}^{(0)}$, and by h the coordinates of $\mathcal{H}^{(0)}\mathbf{Q}^{(1)}$. Then, the coordinates of the material derivative $\dot{\mathbf{Q}}^{(0)} = \partial_t \mathbf{Q}^{(0)} + \mathbf{v}^{(0)} \cdot \nabla \mathbf{Q}^{(0)}$ are given by $q = \bar{q} + v_1^{(0)}\tilde{q}_1 + v_2^{(0)}\tilde{q}_2 + v_3^{(0)}\tilde{q}_3$. Therefore, we could write (4.16) in the coordinates

$$q - V\omega = -M\widetilde{\Lambda}(h+g). \tag{4.30}$$

For (4.17), the term $\mathcal{N}^{(0)}(\mathcal{H}^{(0)}\mathbf{Q}^{(1)} + \mathcal{G}(\mathbf{Q}^{(0)}))$ can be expressed under the basis $\mathbf{s}_i$ together with $\mathbf{a}_i$,

$$\sigma_e^{(0)} = ck_BT\mathcal{N}^{(0)}\left(\mathcal{H}^{(0)}\mathbf{Q}^{(1)} + \mathcal{G}(\mathbf{Q}^{(0)})\right) = ck_BT(\mathbf{s}_1, \ldots, \mathbf{s}_5, \mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)N\widetilde{\Lambda}(h+g). \tag{4.31}$$

The term $\mathcal{P}^{(0)}\kappa^{(0)}$ is symmetric traceless, so that it can be written as

$$\mathcal{P}^{(0)}\kappa^{(0)} = (\mathbf{s}_1, \ldots, \mathbf{s}_5)P\omega_s. \tag{4.32}$$

The dot product $(\mathcal{H}^{(0)}(\mathbf{Q}^{(1)}) + \mathcal{G}(\mathbf{Q}^{(0)})) \cdot \partial_i \mathbf{Q}^{(0)}$ is given by $\tilde{q}_i^T\widetilde{\Lambda}(h+g)$. Thus, (4.17) can be rewritten as

$$\begin{aligned} \rho_s\left(\frac{\partial \mathbf{v}^{(0)}}{\partial t} + \mathbf{v}^{(0)} \cdot \nabla \mathbf{v}^{(0)}\right)_i &= -\partial_i p^{(0)} + \eta\Delta v_i^{(0)} + \partial_j\left((\mathbf{s}_1, \ldots, \mathbf{s}_5)P\omega_s\right)_{ij} \\ &\quad + ck_BT\partial_j\left((\mathbf{s}_1, \ldots, \mathbf{s}_5, \mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)N\widetilde{\Lambda}(h+g)\right)_{ij} \\ &\quad + ck_BT\tilde{q}_i^T\widetilde{\Lambda}(h+g). \end{aligned} \tag{4.33}$$

4.3. Expressions of matrices and vectors under the local basis. We begin to write down the matrices and vectors in (4.30) and (4.33). Let us first discuss the derivatives of $\mathbf{Q}^{(0)}$, i.e., $\bar{q}$ and $\tilde{q}_i$. Since $\mathbf{Q}^{(0)}$ is a function of $\mathfrak{p}$, any derivative of $\mathbf{Q}^{(0)}$ can be expressed linearly by $\mathscr{L}_i\mathbf{Q}^{(0)}$. For this reason, let us first look into the coordinates of $\mathscr{L}_i\mathbf{Q}^{(0)}$.

For any differential operator $\mathcal{D}$, we have

$$\mathcal{D}Q_1^{(0)} = 2(s_1 - b_1)(\mathcal{D}\mathbf{n}_1 \cdot \mathbf{n}_2)\mathbf{s}_3 - 2(s_1 + b_1)(\mathcal{D}\mathbf{n}_3 \cdot \mathbf{n}_1)\mathbf{s}_4 + 4b_1(\mathcal{D}\mathbf{n}_2 \cdot \mathbf{n}_3)\mathbf{s}_5.$$

$\mathcal{D}Q_2^{(0)}$ is calculated similarly. We denote by L the coordinates of $(\mathscr{L}_3\mathbf{Q}^{(0)}, \mathscr{L}_2\mathbf{Q}^{(0)}, \mathscr{L}_1\mathbf{Q}^{(0)})$, which is a 10×3 matrix. The calculation above gives

$$L = \left(0_{2\times 3},\ \mathrm{diag}\big(2(s_1 - b_1), -2(s_1 + b_1), 4b_1\big), 0_{2\times 3},\ \mathrm{diag}\big(2(s_2 - b_2), -2(s_2 + b_2), 4b_2\big)\right)^T. \tag{4.34}$$

Choose $\mathcal{D}$ as ∂_t, ∂_i, and the material derivative $\partial_t + v_i^{(0)}\partial_i$, respectively. The corresponding coordinates are given by

$$\bar{q} = L\begin{pmatrix} \partial_t \mathbf{n}_1 \cdot \mathbf{n}_2 \\ \partial_t \mathbf{n}_3 \cdot \mathbf{n}_1 \\ \partial_t \mathbf{n}_2 \cdot \mathbf{n}_3 \end{pmatrix}, \quad \tilde{q}_i = L\begin{pmatrix} \partial_i \mathbf{n}_1 \cdot \mathbf{n}_2 \\ \partial_i \mathbf{n}_3 \cdot \mathbf{n}_1 \\ \partial_i \mathbf{n}_2 \cdot \mathbf{n}_3 \end{pmatrix}, \quad q = L\begin{pmatrix} \dot{\mathbf{n}}_1 \cdot \mathbf{n}_2 \\ \dot{\mathbf{n}}_3 \cdot \mathbf{n}_1 \\ \dot{\mathbf{n}}_2 \cdot \mathbf{n}_3 \end{pmatrix}. \tag{4.35}$$

Another important thing to be noticed is that (3.19) leads to $\mathcal{H}^{(0)}\mathbf{Q}^{(1)} \cdot \mathscr{L}_i(\mathbf{Q}^{(0)}) = 0$. Recall that the coordinates of $\mathcal{H}^{(0)}\mathbf{Q}^{(1)}$ is h. Thus, when writing this equation by the coordinates, we deduce that

$$L^T \widetilde{\Lambda} h = 0. \tag{4.36}$$

The calculations of the matrices M, V, N, and P involve high-order tensors, which are discussed in the supplementary materials (bif_suppm.pdf [local/web 446KB]). Here, we only present the result. To express these matrices, we introduce six constant 5×5 matrices $X_i\,(i=1,\cdots,6)$,

$$X_1 = \operatorname{diag}\left(\begin{pmatrix} -9 & 0 \\ 0 & -3 \end{pmatrix}, -12, -12, -12\right), \quad X_2 = \operatorname{diag}\left(\begin{pmatrix} -\frac{3}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}, -1, -1, 2\right),$$
$$X_3 = \operatorname{diag}\left(\begin{pmatrix} 0 & \frac{3}{2} \\ \frac{3}{2} & 0 \end{pmatrix}, -3, 3, 0\right), \quad X_4 = \operatorname{diag}\left(\begin{pmatrix} \frac{18}{35} & 0 \\ 0 & \frac{1}{35} \end{pmatrix}, -\frac{16}{35}, -\frac{16}{35}, \frac{4}{35}\right),$$
$$X_5 = \operatorname{diag}\left(\begin{pmatrix} \frac{27}{140} & -\frac{3}{28} \\ -\frac{3}{28} & \frac{19}{140} \end{pmatrix}, -\frac{16}{35}, \frac{4}{35}, -\frac{16}{35}\right),$$
$$X_6 = \operatorname{diag}\left(\begin{pmatrix} -\frac{9}{35} & \frac{3}{28} \\ \frac{3}{28} & -\frac{1}{70} \end{pmatrix}, \frac{18}{35}, -\frac{2}{35}, -\frac{2}{35}\right).$$

The blocks of the matrix M can be expressed as

$$\begin{aligned} M_{11} &= -\frac{1}{15}(\Gamma_2+\Gamma_3)X_1 + \frac{4}{7}\left((\Gamma_2 s_2 - \Gamma_3(s_1+s_2))\,X_2 + (\Gamma_2 b_2 - \Gamma_3(b_1+b_2))\,X_3\right) \\ &\quad - 4\Big((\Gamma_2(a_1+\bar{a}_1) - \Gamma_3\bar{a}_1)\,X_4 + (\Gamma_2(a_2+\bar{a}_2) - \Gamma_3\bar{a}_2)\,X_5 \\ &\quad + (\Gamma_2(a_3+\bar{a}_3) - \Gamma_3\bar{a}_3)\,X_6\Big) \\ &\stackrel{\text{def}}{=} \operatorname{diag}\left(\begin{pmatrix} \alpha_{11} & \alpha_{12} \\ \alpha_{12} & \alpha_{22} \end{pmatrix}, \alpha_{33}, \alpha_{44}, \alpha_{55}\right), \end{aligned} \tag{4.37}$$

$$\begin{aligned} M_{12} &= \frac{1}{15}\Gamma_3 X_1 + \frac{4}{7}\Gamma_3\left((s_1+s_2)X_2 + (b_1+b_2)X_3\right) - 4\Gamma_3\left(\bar{a}_1 X_4 + \bar{a}_2 X_5 + \bar{a}_3 X_6\right) \\ &\stackrel{\text{def}}{=} \operatorname{diag}\left(\begin{pmatrix} \beta_{11} & \beta_{12} \\ \beta_{12} & \beta_{22} \end{pmatrix}, \beta_{33}, \beta_{44}, \beta_{55}\right), \end{aligned} \tag{4.38}$$

$$\begin{aligned} M_{22} &= -\frac{1}{15}(\Gamma_1+\Gamma_3)X_1 + \frac{4}{7}\left((\Gamma_1 s_1 - \Gamma_3(s_1+s_2))\,X_2 + (\Gamma_1 b_1 - \Gamma_3(b_1+b_2))\,X_3\right) \\ &\quad - 4\Big((\Gamma_1(\tilde{a}_1+\bar{a}_1) - \Gamma_3\bar{a}_1)\,X_4 + (\Gamma_1(\tilde{a}_2+\bar{a}_2) - \Gamma_3\bar{a}_2)\,X_5 \\ &\quad + (\Gamma_1(\tilde{a}_3+\bar{a}_3) - \Gamma_3\bar{a}_3)\,X_6\Big) \\ &\stackrel{\text{def}}{=} \operatorname{diag}\left(\begin{pmatrix} \gamma_{11} & \gamma_{12} \\ \gamma_{12} & \gamma_{22} \end{pmatrix}, \gamma_{33}, \gamma_{44}, \gamma_{55}\right), \end{aligned} \tag{4.39}$$

where $a_i,\ \tilde{a}_i,\ \bar{a}_i\,(i=1,2,3)$ are those in (3.22). We shall keep in mind that these scalars are functions of $s_i, b_i\,(i=1,2)$. The blocks of the matrix V are expressed as

$$\begin{aligned}N_1^u &= -\frac{1}{15}e_1X_1 - \frac{2}{7}\left(\left((e_1-e_2)s_1 - 2e_2s_2\right)X_2 + \left((e_1-e_2)b_1 - 2e_2b_2\right)X_3\right)\\ &\quad - 2\left((a_1+2e_2\bar{a}_1)X_4 + (a_2+2e_2\bar{a}_2)X_5 + (a_3+2e_2\bar{a}_3)X_6\right)\\ &\overset{\text{def}}{=} \operatorname{diag}\left(\begin{pmatrix}\mu_{11} & \mu_{12}\\ \mu_{12} & \mu_{22}\end{pmatrix}, \mu_{33}, \mu_{44}, \mu_{55}\right),\end{aligned} \tag{4.40}$$

$$\begin{aligned}N_2^u &= -\frac{1}{15}e_2X_1 + \frac{2}{7}\left(\left(2e_1s_1 - (e_2-e_1)s_2\right)X_2 + \left(2e_1b_1 - (e_2-e_1)b_2\right)X_3\right)\\ &\quad - 2\left((\tilde{a}_1+2e_1\bar{a}_1)X_4 + (\tilde{a}_2+2e_1\bar{a}_2)X_5 + (\tilde{a}_3+2e_1\bar{a}_3)X_6\right)\\ &\overset{\text{def}}{=} \operatorname{diag}\left(\begin{pmatrix}\nu_{11} & \nu_{12}\\ \nu_{12} & \nu_{22}\end{pmatrix}, \nu_{33}, \nu_{44}, \nu_{55}\right),\end{aligned} \tag{4.41}$$

and

$$V = \left(\begin{array}{c|c} \begin{matrix} N_1^u \\ N_2^u \end{matrix} & \frac{1}{2}L \end{array}\right), \tag{4.42}$$

where L is given by (4.34). The matrix P can be expressed as

$$\begin{aligned}P = c\zeta\Bigg[&-\frac{1}{45}\left(I_{22}+I_{11}(1+3e_1)\right)X_1 - \frac{4}{21}\Big(\left((I_{22}+3I_{11}e_1)s_1 + I_{11}(1+3e_1)s_2\right)X_2\\ &+ \left((I_{22}+3I_{11}e_1)b_1 + I_{11}(1+3e_1)b_2\right)X_3\Big) + \left(I_{22}a_1 + I_{11}\tilde{a}_1 + 4I_{11}e_1\bar{a}_1\right)X_4\\ &+ \left(I_{22}a_2 + I_{11}\tilde{a}_2 + 4I_{11}e_1\bar{a}_2\right)X_5 + \left(I_{22}a_3 + I_{11}\tilde{a}_3 + 4I_{11}e_1\bar{a}_3\right)X_6\Bigg]\\ \overset{\text{def}}{=} \operatorname{diag}&\left(\begin{pmatrix}\vartheta_{11} & \vartheta_{12}\\ \vartheta_{12} & \vartheta_{22}\end{pmatrix}, \vartheta_{33}, \vartheta_{44}, \vartheta_{55}\right).\end{aligned} \tag{4.43}$$

In the above, we intentionally introduce notations for the components of M, V, and P, to emphasize that these matrices have specific forms. These specific forms are significant in the forthcoming derivations. We have claimed that $\mathcal{M}$ and $\mathcal{P}$ are positive definite in (4.11) and (4.10). As a result, the corresponding coefficient matrices M and P are also positive definite. We do not consider the expressions of the vectors h and g, because the terms involving them will be expressed by variational derivatives of the elastic energy.

4.4. Orthonormal frame model. We are now ready to derive the frame hydrodynamics for the biaxial nematic phase from the $O(1)$ system (4.16)–(4.18).

To begin with, we write down the elastic energy for the biaxial nematic phase. In the tensor model, the elastic energy is a functional of $\mathbf{Q}$. When $\mathbf{Q}$ takes $\mathbf{Q}^{(0)}$ that is a function of $\mathfrak{p}$, the corresponding elastic energy becomes a functional of the frame $\mathfrak{p}$, which we denote by $\mathcal{F}_{Bi}$. Generally, the biaxial elastic energy consists of twelve bulk terms [44], written as

$$\begin{aligned}\frac{\mathcal{F}_{Bi}[\mathfrak{p}]}{ck_BT} = \int \mathrm{d}\boldsymbol{x}\ \frac{1}{2}\Big(&K_{1111}D_{11}^2 + K_{2222}D_{22}^2 + K_{3333}D_{33}^2\\ &+ K_{1212}D_{12}^2 + K_{2121}D_{21}^2 + K_{2323}D_{23}^2 + K_{3232}D_{32}^2 + K_{3131}D_{31}^2 + K_{1313}D_{13}^2\\ &+ K_{1221}D_{12}D_{21} + K_{2332}D_{23}D_{32} + K_{1331}D_{13}D_{31}\Big),\end{aligned} \tag{4.44}$$

where the nine invariants $D_{ij}(i,j=1,2,3)$ are defined by (2.7). We take no account here of three surface terms, such as

$$\partial_i n_{2i}\partial_j n_{2j} - \partial_i n_{2j}\partial_j n_{2i} = 2(D_{33}D_{11} - D_{31}D_{13}). \tag{4.45}$$

The coefficients in (4.44) can be derived from the coefficients in the tensor model [44] as

$$\begin{cases} K_{1111} = J_2, \quad K_{2222} = J_1, \quad K_{3333} = J_1 + J_2 - J_3, \\ K_{1212} = K_{3232} = J_1 + J_4, \quad K_{2121} = K_{3131} = J_2 + J_5, \\ K_{2323} = K_{1313} = J_1 + J_2 - J_3 + J_4 + J_5 - J_6, \\ K_{1221} = -J_6, \quad K_{2332} = J_6 - 2J_4, \quad K_{1331} = J_6 - 2J_5, \end{cases} \tag{4.46}$$

where

(4.47)

$$\begin{cases} J_1 = 2c\left(c_{22}(s_1+b_1)^2 + c_{23}(s_2+b_2)^2 + 2c_{24}(s_1+b_1)(s_2+b_2)\right), \\ J_2 = 8c\left(c_{22}b_1^2 + c_{23}b_2^2 + 2c_{24}b_1b_2\right), \\ J_3 = 8c\left(c_{22}b_1(s_1+b_1) + c_{23}b_2(s_2+b_2) + c_{24}[b_1(s_2+b_2) + b_2(s_1+b_1)]\right), \\ J_4 = c\left(c_{28}(s_1+b_1)^2 + c_{29}(s_2+b_2)^2 + 2c_{2,10}(s_1+b_1)(s_2+b_2)\right), \\ J_5 = 4c\left(c_{28}b_1^2 + c_{29}b_2^2 + 2c_{2,10}b_1b_2\right), \\ J_6 = 4c\left(c_{28}b_1(s_1+b_1) + c_{29}b_2(s_2+b_2) + c_{2,10}[b_1(s_2+b_2) + b_2(s_1+b_1)]\right). \end{cases}$$

Using the chain rule, we deduce that

(4.48)

$$\mathscr{L}\mathcal{F}_{Bi} = \mathscr{L}\mathcal{F}_{Bi}[\mathbf{Q}^{(0)}(\mathfrak{p})] = \frac{\delta\mathcal{F}_{Bi}}{\delta\mathbf{Q}^{(0)}} \cdot \mathscr{L}\mathbf{Q}^{(0)} = ck_BT\mathcal{G}(\mathbf{Q}^{(0)}) \cdot \mathscr{L}\mathbf{Q}^{(0)} = ck_BTL^T\widetilde{\Lambda}g.$$

Therefore, it is deduced from (4.30) and (4.36) that

$$L^TM^{-1}(q - V\omega) + \frac{1}{ck_BT}\mathscr{L}\mathcal{F}_{Bi} = 0. \tag{4.49}$$

In the above, we notice that M is positive definite, thus invertible.

To calculate (4.49), we rearrange the rows and columns of the matrices so that they can be divided into blocks appropriately. To this end, we introduce a 10×10 permutation matrix

$$C = (\mathbf{E}_1, \mathbf{E}_6, \mathbf{E}_2, \mathbf{E}_7, \mathbf{E}_3, \mathbf{E}_8, \mathbf{E}_4, \mathbf{E}_9, \mathbf{E}_5, \mathbf{E}_{10}), \tag{4.50}$$

where $\mathbf{E}_j$ is the 10×1 unit vector with the jth component equal to one. We have $CC^T = I_{10}$, which is the 10×10 identity matrix. Then we have

$$C^TMC = \operatorname{diag}(M_0, M_1, M_2, M_3), \tag{4.51}$$

where the blocks $M_i\,(i = 0,1,2,3)$ are given by

$$M_0 = \begin{pmatrix} \alpha_{11} & \beta_{11} & \alpha_{12} & \beta_{12} \\ \beta_{11} & \gamma_{11} & \beta_{12} & \gamma_{12} \\ \alpha_{12} & \beta_{12} & \alpha_{22} & \beta_{22} \\ \beta_{12} & \gamma_{12} & \beta_{22} & \gamma_{22} \end{pmatrix},$$

$$M_1 = \begin{pmatrix} \alpha_{33} & \beta_{33} \\ \beta_{33} & \gamma_{33} \end{pmatrix}, \quad M_2 = \begin{pmatrix} \alpha_{44} & \beta_{44} \\ \beta_{44} & \gamma_{44} \end{pmatrix}, \quad M_3 = \begin{pmatrix} \alpha_{55} & \beta_{55} \\ \beta_{55} & \gamma_{55} \end{pmatrix}.$$

These blocks are all positive definite because M is. For the matrix V, we have

$$C^TV=\left(\begin{array}{c|cccccc} V_0 & & & & & & \\ \hline & V_1 & 0 & 0 & V_4 & 0 & 0 \\ & 0 & V_2 & 0 & 0 & V_5 & 0 \\ & 0 & 0 & V_3 & 0 & 0 & V_6 \end{array}\right), \tag{4.52}$$

where the blocks $V_i\,(i=0,1,\dots,6)$ are given by

$$V_0=\begin{pmatrix} \mu_{11} & \mu_{12} \\ \nu_{11} & \nu_{12} \\ \mu_{12} & \mu_{22} \\ \nu_{12} & \nu_{22} \end{pmatrix},\quad V_1=\begin{pmatrix} \mu_{33} \\ \nu_{33} \end{pmatrix},\quad V_2=\begin{pmatrix} \mu_{44} \\ \nu_{44} \end{pmatrix},\quad V_3=\begin{pmatrix} \mu_{55} \\ \nu_{55} \end{pmatrix},$$
$$V_4=\begin{pmatrix} s_1-b_1 \\ s_2-b_2 \end{pmatrix},\quad V_5=-\begin{pmatrix} s_1+b_1 \\ s_2+b_2 \end{pmatrix},\quad V_6=\begin{pmatrix} 2b_1 \\ 2b_2 \end{pmatrix}.$$

We also rearrange the indices of the vector q by C,

$$C^Tq=(0_{4\times 1},2(\dot{\mathbf{n}}_1\cdot\mathbf{n}_2)V_4,2(\dot{\mathbf{n}}_3\cdot\mathbf{n}_1)V_5,2(\dot{\mathbf{n}}_2\cdot\mathbf{n}_3)V_6)^T, \tag{4.53}$$

where we use $0_{N_1\times N_2}$ to represent an $N_1\times N_2$ zero matrix. The matrix L is rearranged as

$$(C^TL)^T=L^TC=(0_{3\times 4},L_1^T), \tag{4.54}$$

where $L_1^T=\mathrm{diag}(2V_4^T,2V_5^T,2V_6^T)^T$. Thus, from (4.51) and (4.54), we have

$$L^TM^{-1}C=(C^TL)^TC^TM^{-1}C=\left(\begin{array}{c|ccc} 0_{3\times 4} & 2V_4^TM_1^{-1} & & \\ & & 2V_5^TM_2^{-1} & \\ & & & 2V_6^TM_3^{-1} \end{array}\right). \tag{4.55}$$

Together with (4.55), we deduce that

$$L^TM^{-1}q=(L^TC)(C^TMC)^{-1}(C^Tq)=(\chi_3\dot{\mathbf{n}}_1\cdot\mathbf{n}_2,\chi_2\dot{\mathbf{n}}_3\cdot\mathbf{n}_1,\chi_1\dot{\mathbf{n}}_2\cdot\mathbf{n}_3)^T, \tag{4.56}$$

where the coefficients $\chi_i\,(i=1,2,3)$ are given by

$$\chi_3=4V_4^TM_1^{-1}V_4,\quad \chi_2=4V_5^TM_2^{-1}V_5,\quad \chi_1=4V_6^TM_3^{-1}V_6.$$

From (4.51), (4.52), and (4.54), we have

$$\begin{aligned} &L^TM^{-1}V\omega \\ &=\left(\eta_3\mathbf{A}_0\cdot\mathbf{s}_3+\frac{1}{2}\chi_3\mathbf{\Omega}_0\cdot\mathbf{a}_1,\ \eta_2\mathbf{A}_0\cdot\mathbf{s}_4+\frac{1}{2}\chi_2\mathbf{\Omega}_0\cdot\mathbf{a}_2,\ \eta_1\mathbf{A}_0\cdot\mathbf{s}_5+\frac{1}{2}\chi_1\mathbf{\Omega}_0\cdot\mathbf{a}_3\right)^T, \end{aligned} \tag{4.57}$$

where the coefficients $\eta_i\,(i=1,2,3)$ are expressed by

$$\eta_3=2V_4^TM_1^{-1}V_1,\quad \eta_2=2V_5^TM_2^{-1}V_2,\quad \eta_1=2V_6^TM_3^{-1}V_3.$$

Therefore, using (4.56) and (4.57), (4.49) can be reformulated as

$$\chi_1 \dot{\mathbf{n}}_2 \cdot \mathbf{n}_3 - \frac{1}{2}\chi_1 \mathbf{\Omega}_0 \cdot \mathbf{a}_3 - \eta_1 \mathbf{A}_0 \cdot \mathbf{s}_5 + \frac{1}{ck_BT}\mathscr{L}_1 \mathcal{F}_{Bi} = 0, \tag{4.58}$$

$$\chi_2 \dot{\mathbf{n}}_3 \cdot \mathbf{n}_1 - \frac{1}{2}\chi_2 \mathbf{\Omega}_0 \cdot \mathbf{a}_2 - \eta_2 \mathbf{A}_0 \cdot \mathbf{s}_4 + \frac{1}{ck_BT}\mathscr{L}_2 \mathcal{F}_{Bi} = 0, \tag{4.59}$$

$$\chi_3 \dot{\mathbf{n}}_1 \cdot \mathbf{n}_2 - \frac{1}{2}\chi_3 \mathbf{\Omega}_0 \cdot \mathbf{a}_1 - \eta_3 \mathbf{A}_0 \cdot \mathbf{s}_3 + \frac{1}{ck_BT}\mathscr{L}_3 \mathcal{F}_{Bi} = 0. \tag{4.60}$$

It remains to derive the equation of the fluid velocity $\mathbf{v}^{(0)}$. From (4.35), (4.48), and (4.36), we have

$$\tilde{q}_i^T \widetilde{\Lambda}(h+g) = \frac{1}{ck_BT}\left(\mathscr{L}_3 \mathcal{F}_{Bi} \partial_i \mathbf{n}_1 \cdot \mathbf{n}_2 + \mathscr{L}_2 \mathcal{F}_{Bi} \partial_i \mathbf{n}_3 \cdot \mathbf{n}_1 + \mathscr{L}_1 \mathcal{F}_{Bi} \partial_i \mathbf{n}_2 \cdot \mathbf{n}_3\right) \stackrel{\text{def}}{=} \mathfrak{F}_i. \tag{4.61}$$

Using this short notation $\mathfrak{F}$ for the body force, and taking (4.30) into (4.33), we deduce that

$$\begin{aligned}\rho_s \left(\frac{\partial \mathbf{v}^{(0)}}{\partial t} + \mathbf{v}^{(0)} \cdot \nabla \mathbf{v}^{(0)}\right)_i &= -\partial_i p^{(0)} + \eta \Delta v_i^{(0)} + \partial_j \left((\mathbf{s}_1, \ldots, \mathbf{s}_5) P \omega_s\right)_{ij} \\ &\quad - ck_BT \partial_j \left((\mathbf{s}_1, \ldots, \mathbf{s}_5, \mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3) N M^{-1}(q - V\omega)\right)_{ij} \\ &\quad + ck_BT \mathfrak{F}_i.\end{aligned} \tag{4.62}$$

In the above, we recall that the matrix P is given by (4.43).

Noticing $N = V^T$, and by direct matrix manipulation, we obtain that the elastic stress $\sigma_e^{(0)}$ (4.31) can be expressed as

$$\begin{aligned}\frac{1}{ck_BT}\sigma_e^{(0)} &= -(\mathbf{s}_1, \ldots, \mathbf{s}_5, \mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3) N M^{-1}(q - V\omega) \\ &= \beta_1 (\mathbf{A}_0 \cdot \mathbf{s}_1)\mathbf{s}_1 + \beta_0 (\mathbf{A}_0 \cdot \mathbf{s}_2)\mathbf{s}_1 + \beta_0 (\mathbf{A}_0 \cdot \mathbf{s}_1)\mathbf{s}_2 + \beta_2 (\mathbf{A}_0 \cdot \mathbf{s}_2)\mathbf{s}_2 \\ &\quad + \beta_3 (\mathbf{A}_0 \cdot \mathbf{s}_3)\mathbf{s}_3 - \eta_3 \left(\dot{\mathbf{n}}_1 \cdot \mathbf{n}_2 - \frac{1}{2}\mathbf{\Omega}_0 \cdot \mathbf{a}_1\right)\mathbf{s}_3 \\ &\quad + \beta_4 (\mathbf{A}_0 \cdot \mathbf{s}_4)\mathbf{s}_4 - \eta_2 \left(\dot{\mathbf{n}}_3 \cdot \mathbf{n}_1 - \frac{1}{2}\mathbf{\Omega}_0 \cdot \mathbf{a}_2\right)\mathbf{s}_4 \\ &\quad + \beta_5 (\mathbf{A}_0 \cdot \mathbf{s}_5)\mathbf{s}_5 - \eta_1 \left(\dot{\mathbf{n}}_2 \cdot \mathbf{n}_3 - \frac{1}{2}\mathbf{\Omega}_0 \cdot \mathbf{a}_3\right)\mathbf{s}_5 \\ &\quad + \frac{1}{2}\eta_3 (\mathbf{A}_0 \cdot \mathbf{s}_3)\mathbf{a}_1 - \frac{1}{2}\chi_3 \left(\dot{\mathbf{n}}_1 \cdot \mathbf{n}_2 - \frac{1}{2}\mathbf{\Omega}_0 \cdot \mathbf{a}_1\right)\mathbf{a}_1 \\ &\quad + \frac{1}{2}\eta_2 (\mathbf{A}_0 \cdot \mathbf{s}_4)\mathbf{a}_2 - \frac{1}{2}\chi_2 \left(\dot{\mathbf{n}}_3 \cdot \mathbf{n}_1 - \frac{1}{2}\mathbf{\Omega}_0 \cdot \mathbf{a}_2\right)\mathbf{a}_2 \\ &\quad + \frac{1}{2}\eta_1 (\mathbf{A}_0 \cdot \mathbf{s}_5)\mathbf{a}_3 - \frac{1}{2}\chi_1 \left(\dot{\mathbf{n}}_2 \cdot \mathbf{n}_3 - \frac{1}{2}\mathbf{\Omega}_0 \cdot \mathbf{a}_3\right)\mathbf{a}_3,\end{aligned} \tag{4.63}$$

where the coefficients β_i are given by

$$V_0^T M_0^{-1} V_0 = \begin{pmatrix} \beta_1 & \beta_0 \\ \beta_0 & \beta_2 \end{pmatrix}, \quad \beta_3 = V_1^T M_1^{-1} V_1, \quad \beta_4 = V_2^T M_2^{-1} V_2, \quad \beta_5 = V_3^T M_3^{-1} V_3. \tag{4.64}$$

Since M_0 is positive definite, the matrix $V_0^T M_0^{-1} V_0$ is symmetric positive semidefinite, yielding

$$\beta_i \geq 0,\ i=1,2, \quad \beta_0^2 \leq \beta_1\beta_2. \tag{4.65}$$

Therefore, from (4.62), the equation for $\mathbf{v}^{(0)}$ reads

$$\rho_s\left(\frac{\partial \mathbf{v}^{(0)}}{\partial t} + \mathbf{v}^{(0)}\cdot\nabla\mathbf{v}^{(0)}\right)_i = -\partial_i p^{(0)} + \partial_j\left((\sigma_v^{(0)})_{ij} + (\sigma_e^{(0)})_{ij}\right) + ck_BT\mathfrak{F}_i, \tag{4.66}$$

$$\nabla\cdot\mathbf{v}^{(0)} = 0. \tag{4.67}$$

Here, the viscous stress $\sigma_v^{(0)}$ is denoted by

$$\sigma_v^{(0)} = \eta\mathbf{A}_0 + (\mathbf{s}_1,\dots,\mathbf{s}_5)P\omega_s = (\mathbf{s}_1,\dots,\mathbf{s}_5)(\eta\Lambda^{-1}+P)\omega_s, \tag{4.68}$$

where we have used the following fact,

$$\mathbf{A}_0 = \sum_{i=1}^{5}\frac{1}{|\mathbf{s}_i|^2}(\mathbf{A}_0\cdot\mathbf{s}_i)\mathbf{s}_i = (\mathbf{s}_1,\cdots,\mathbf{s}_5)\Lambda^{-1}\omega_s.$$

To sum up, the frame hydrodynamics for the biaxial nematic phase is given by (4.58)–(4.60), (4.66), and (4.67).

Remark 4.1. Similar to the Ericksen–Leslie model, where $\mathbf{n}$ and $-\mathbf{n}$ stand for the same nematic direction, in the frame model four different frames stand for the same biaxial direction: $(\mathbf{n}_1,\mathbf{n}_2,\mathbf{n}_3)$, $(\mathbf{n}_1,-\mathbf{n}_2,-\mathbf{n}_3)$, $(-\mathbf{n}_1,\mathbf{n}_2,-\mathbf{n}_3)$, $(-\mathbf{n}_1,-\mathbf{n}_2,\mathbf{n}_3)$. Therefore, in the frame model there will also be the problem of orientability, which calls for discussion in the future.

4.5. Energy dissipation. Taking the derivative with respect to t of the biaxial elastic energy (4.44), we deduce that

$$\begin{aligned}\frac{\mathrm{d}\mathcal{F}_{Bi}}{\mathrm{d}t} &= \int\left(\frac{\delta\mathcal{F}_{Bi}}{\delta\mathbf{n}_1}\cdot\frac{\partial\mathbf{n}_1}{\partial t} + \frac{\delta\mathcal{F}_{Bi}}{\delta\mathbf{n}_2}\cdot\frac{\partial\mathbf{n}_2}{\partial t} + \frac{\delta\mathcal{F}_{Bi}}{\delta\mathbf{n}_3}\cdot\frac{\partial\mathbf{n}_3}{\partial t}\right)\mathrm{d}\mathbf{x}\\
&= \int\left(\frac{\delta\mathcal{F}_{Bi}}{\delta\mathbf{n}_1}\cdot(\mathbf{n}_2(\mathbf{n}_2\cdot\partial_t\mathbf{n}_1) + \mathbf{n}_3(\mathbf{n}_3\cdot\partial_t\mathbf{n}_1))\right.\\
&\quad + \frac{\delta\mathcal{F}_{Bi}}{\delta\mathbf{n}_2}\cdot(\mathbf{n}_1(\mathbf{n}_1\cdot\partial_t\mathbf{n}_2) + \mathbf{n}_3(\mathbf{n}_3\cdot\partial_t\mathbf{n}_2))\\
&\quad \left. + \frac{\delta\mathcal{F}_{Bi}}{\delta\mathbf{n}_3}\cdot(\mathbf{n}_1(\mathbf{n}_1\cdot\partial_t\mathbf{n}_3) + \mathbf{n}_2(\mathbf{n}_2\cdot\partial_t\mathbf{n}_3))\right)\mathrm{d}\mathbf{x}\\
&= \int\left[n_{3k}\partial_t n_{2k}\left(\mathbf{n}_3\cdot\frac{\delta\mathcal{F}_{Bi}}{\delta\mathbf{n}_2} - \mathbf{n}_2\cdot\frac{\delta\mathcal{F}_{Bi}}{\delta\mathbf{n}_3}\right) + n_{1k}\partial_t n_{3k}\left(\mathbf{n}_1\cdot\frac{\delta\mathcal{F}_{Bi}}{\delta\mathbf{n}_3} - \mathbf{n}_3\cdot\frac{\delta\mathcal{F}_{Bi}}{\delta\mathbf{n}_1}\right)\right.\\
&\quad \left. + n_{2k}\partial_t n_{1k}\left(\mathbf{n}_2\cdot\frac{\delta\mathcal{F}_{Bi}}{\delta\mathbf{n}_1} - \mathbf{n}_1\cdot\frac{\delta\mathcal{F}_{Bi}}{\delta\mathbf{n}_2}\right)\right]\mathrm{d}\mathbf{x}\\
&= \int(n_{3k}\partial_t n_{2k}\mathscr{L}_1\mathcal{F}_{Bi} + n_{1k}\partial_t n_{3k}\mathscr{L}_2\mathcal{F}_{Bi} + n_{2k}\partial_t n_{1k}\mathscr{L}_3\mathcal{F}_{Bi})\,\mathrm{d}\mathbf{x}.\end{aligned} \tag{4.69}$$

Taking the inner product on (4.66) with $\mathbf{v}^{(0)}$ and using $\nabla\cdot\mathbf{v}^{(0)}=0$, we derive that

$$\frac{\rho_s}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int|\mathbf{v}^{(0)}|^2\mathrm{d}\mathbf{x} = -\langle\sigma_v^{(0)},\mathbf{A}_0\rangle - \langle\sigma_e^{(0)},\nabla\mathbf{v}^{(0)}\rangle + ck_BT\langle\mathfrak{F},\mathbf{v}^{(0)}\rangle, \tag{4.70}$$

where

$$ck_BT\langle\mathfrak{F},\mathbf{v}^{(0)}\rangle = \int v_i^{(0)}\left(n_{3k}\partial_i n_{2k}\mathscr{L}_1\mathcal{F}_{Bi} + n_{1k}\partial_i n_{3k}\mathscr{L}_2\mathcal{F}_{Bi} + n_{2k}\partial_i n_{1k}\mathscr{L}_3\mathcal{F}_{Bi}\right)\mathrm{d}\mathbf{x}.$$

Combining (4.69) with (4.70), and using (4.58)–(4.60), we obtain the energy dissipation law,

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\rho_s}{2}\int|\mathbf{v}^{(0)}|^2\mathrm{d}\mathbf{x} + \mathcal{F}_{Bi}(\mathfrak{p})\right)\\
&\quad= -\langle\sigma_v^{(0)},\mathbf{A}_0\rangle - \langle\sigma_e^{(0)},\nabla\mathbf{v}^{(0)}\rangle\\
&\qquad+\int\left((\dot{\mathbf{n}}_2\cdot\mathbf{n}_3)\mathscr{L}_1\mathcal{F}_{Bi} + (\dot{\mathbf{n}}_3\cdot\mathbf{n}_1)\mathscr{L}_2\mathcal{F}_{Bi} + (\dot{\mathbf{n}}_1\cdot\mathbf{n}_2)\mathscr{L}_3\mathcal{F}_{Bi}\right)\mathrm{d}\mathbf{x}\\
&\quad= -\int\omega_s^T(\eta\Lambda^{-1}+P)\omega_s\mathrm{d}\mathbf{x} + ck_BT\Bigg(-\beta_1\|\mathbf{A}_0\cdot\mathbf{s}_1\|_{L^2}^2 - 2\beta_0\int(\mathbf{A}_0\cdot\mathbf{s}_1)(\mathbf{A}_0\cdot\mathbf{s}_2)\mathrm{d}\mathbf{x}\\
&\qquad-\beta_2\|\mathbf{A}_0\cdot\mathbf{s}_2\|_{L^2}^2 - \beta_3\|\mathbf{A}_0\cdot\mathbf{s}_3\|_{L^2}^2 - \beta_4\|\mathbf{A}_0\cdot\mathbf{s}_4\|_{L^2}^2 - \beta_5\|\mathbf{A}_0\cdot\mathbf{s}_5\|_{L^2}^2\\
&\qquad+2\eta_3\int\left(\dot{\mathbf{n}}_1\cdot\mathbf{n}_2 - \frac{1}{2}\mathbf{\Omega}_0\cdot\mathbf{a}_1\right)(\mathbf{A}_0\cdot\mathbf{s}_3)\mathrm{d}\mathbf{x}\\
&\qquad+2\eta_2\int\left(\dot{\mathbf{n}}_3\cdot\mathbf{n}_1 - \frac{1}{2}\mathbf{\Omega}_0\cdot\mathbf{a}_2\right)(\mathbf{A}_0\cdot\mathbf{s}_4)\mathrm{d}\mathbf{x}\\
&\qquad+2\eta_1\int\left(\dot{\mathbf{n}}_2\cdot\mathbf{n}_3 - \frac{1}{2}\mathbf{\Omega}_0\cdot\mathbf{a}_3\right)(\mathbf{A}_0\cdot\mathbf{s}_5)\mathrm{d}\mathbf{x} - \chi_1\left\|\dot{\mathbf{n}}_2\cdot\mathbf{n}_3 - \frac{1}{2}\mathbf{\Omega}_0\cdot\mathbf{a}_3\right\|_{L^2}^2\\
&\qquad-\chi_2\left\|\dot{\mathbf{n}}_3\cdot\mathbf{n}_1 - \frac{1}{2}\mathbf{\Omega}_0\cdot\mathbf{a}_2\right\|_{L^2}^2 - \chi_3\left\|\dot{\mathbf{n}}_1\cdot\mathbf{n}_2 - \frac{1}{2}\mathbf{\Omega}_0\cdot\mathbf{a}_1\right\|_{L^2}^2\Bigg).
\end{aligned}\tag{4.71}$$

The dissipation can be recognized by noticing the following facts:

- Λ and P are positive definite.
- $\beta_1,\beta_2\geq 0$ and $\beta_0^2\leq\beta_1\beta_2$. This comes from (4.65).
- $\beta_3,\chi_3\geq 0$ and $\eta_3^2\leq\beta_3\chi_3$. To realize this, we use the expressions $\beta_3 = V_1^TM_1^{-1}V_1$, $\chi_3 = 4V_4^TM_1^{-1}V_4$, and $\eta_3 = 2V_4^TM_1^{-1}V_1$, and the fact that M_1 is positive definite.

4.6. Comparison with previous formulations. In previous works, the discussion of biaxial hydrodynamics focused on the dissipation function, i.e., (4.71). If the dissipation function is determined, the hydrodynamics can be established by deriving the forces from it and applying Newton's law. For this reason, we compare the dissipation function in this work and those in previous works.

On the right-hand side of (4.71), the first integral can be merged into the six terms given by β_i, because of the special form of two matrices Λ and P. As a result, the dissipation function can be written in twelve terms, which are exactly those given in [10]. Although the dissipation function had different expressions previously, they turn out to be equivalent as claimed in [10]. While the form is identical, we manage to derive the coefficients from the physical parameters, which was not attained previously.

5. Reduction to uniaxial dynamics. In the tensor model, the minimum of the bulk energy (3.3) might be uniaxial in the form

$$Q_i = s_i\left(\mathbf{n}_1^2 - \frac{\mathfrak{i}}{3}\right),\ i=1,2.\tag{5.1}$$

In this case, the local anisotropy is axisymmetric, and the corresponding hydrodynamics is reduced to the Ericksen–Leslie theory, which we derive in the following.

The essential fact is that the form of tensors in Theorem 3.4 will be reduced (see the supplementary materials (bif_suppm.pdf [local/web 446KB]) for the proof).

THEOREM 5.1. *Assume that Q_1 and Q_2 have the uniaxial form* (5.1)*. Then, the high-order symmetric traceless tensors obtained from closure by the original entropy or the quasi-entropy have the following form:*

$$\langle \mathbf{m}_1\mathbf{m}_2\mathbf{m}_3\rangle = 0, \quad \langle (\mathbf{m}_1^4)_0\rangle = a_1(\mathbf{n}_1^4)_0, \quad \langle (\mathbf{m}_2^4)_0\rangle = \tilde{a}_1(\mathbf{n}_1^4)_0, \quad \langle (\mathbf{m}_1^2\mathbf{m}_2^2)_0\rangle = \bar{a}_1(\mathbf{n}_1^4)_0.$$

When $b_1 = b_2 = 0$, the elastic energy only depends on $\mathbf{n}_1$, denoted by $\mathcal{F}_{Un}$. We immediately obtain

$$\frac{\delta \mathcal{F}_{Un}}{\delta \mathbf{n}_2} = \frac{\delta \mathcal{F}_{Un}}{\delta \mathbf{n}_3} = 0,$$

which implies that

$$\mathscr{L}_1\mathcal{F}_{Bi} = 0, \quad \mathscr{L}_2\mathcal{F}_{Bi} = -\mathbf{n}_3\cdot\frac{\delta \mathcal{F}_{Un}}{\delta \mathbf{n}_1}, \quad \mathscr{L}_3\mathcal{F}_{Bi} = \mathbf{n}_2\cdot\frac{\delta \mathcal{F}_{Un}}{\delta \mathbf{n}_1}. \tag{5.2}$$

By $b_1, b_2 = 0$ and Theorem 5.1, in the matrices M_{ij}, N_i^u, and P (see (4.37)–(4.43)), the coefficients of X_3, X_5, X_6 are all zero. The matrices X_1, X_2, and X_4 are all diagonal matrices with their elements satisfying the following relations:

$$(X_i)_{33} = (X_i)_{44},\ (X_i)_{55} = 4(X_i)_{22}, \quad i = 1, 2, 4. \tag{5.3}$$

Thus, the blocks in (4.51) become

$$\begin{aligned} &M_0 = \begin{pmatrix} M_{01} & \\ & M_{02} \end{pmatrix},\ M_{01} \overset{\text{def}}{=} \begin{pmatrix} \alpha_{11} & \beta_{11} \\ \beta_{11} & \gamma_{11} \end{pmatrix},\ M_{02} \overset{\text{def}}{=} \begin{pmatrix} \alpha_{22} & \beta_{22} \\ \beta_{22} & \gamma_{22} \end{pmatrix}, \\ &M_1 = M_2 = \begin{pmatrix} \alpha_{33} & \beta_{33} \\ \beta_{33} & \gamma_{33} \end{pmatrix},\ M_3 = 4M_{02}. \end{aligned}$$

Similarly, the blocks in (4.52) are reduced to

$$\begin{aligned} &V_0 = \begin{pmatrix} V_{01} & \\ & V_{02} \end{pmatrix}, \quad V_{01} = \begin{pmatrix} \mu_{11} \\ \nu_{11} \end{pmatrix}, \quad V_{02} = \begin{pmatrix} \mu_{22} \\ \nu_{22} \end{pmatrix}, \quad V_1 = V_2 = \begin{pmatrix} \mu_{33} \\ \nu_{33} \end{pmatrix}, \\ &V_3 = 4\begin{pmatrix} \mu_{22} \\ \nu_{22} \end{pmatrix}, \quad V_4 = \begin{pmatrix} s_1 \\ s_2 \end{pmatrix}, \quad V_5 = -\begin{pmatrix} s_1 \\ s_2 \end{pmatrix} = -V_4, \quad V_6 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \end{aligned}$$

We know from (5.2) and that V_6 is a zero vector that (4.58) disappears. Meanwhile, noting the following relations between coefficients,

$$\chi_3 = \chi_2 = 4V_4^T M_1^{-1} V_4 > 0, \quad \eta_3 = -\eta_2 = 2V_4^T M_1^{-1} V_1,$$

we could simplify the equations (4.59) and (4.60) as

$$\begin{cases} \chi_2\left(\dot{\mathbf{n}}_3\cdot\mathbf{n}_1 - \frac{1}{2}\mathbf{\Omega}_0\cdot\mathbf{a}_2\right) - \eta_2\mathbf{A}_0\cdot\mathbf{s}_4 - \frac{1}{ck_BT}\mathbf{n}_3\cdot\frac{\delta\mathcal{F}_{Un}}{\delta\mathbf{n}_1} = 0, \\ \chi_2\left(\dot{\mathbf{n}}_1\cdot\mathbf{n}_2 - \frac{1}{2}\mathbf{\Omega}_0\cdot\mathbf{a}_1\right) + \eta_2\mathbf{A}_0\cdot\mathbf{s}_3 + \frac{1}{ck_BT}\mathbf{n}_2\cdot\frac{\delta\mathcal{F}_{Un}}{\delta\mathbf{n}_1} = 0. \end{cases} \tag{5.4}$$

Denote the rotational derivative of the director and the molecular field as, respectively,

$$\mathbf{N}_1 = \dot{\mathbf{n}}_1 - \Omega_{ij}^{(0)} n_{1j}, \quad \mathbf{h}_1 = -\frac{1}{ck_BT}\frac{\delta \mathcal{F}_{Un}}{\delta \mathbf{n}_1}.$$

Then, (5.4) can be rewritten as

$$\mathbf{n}_1 \times (\mathbf{h}_1 - \chi_2 \mathbf{N}_1 - \eta_2 \mathbf{A}_0 \mathbf{n}_1) = 0. \tag{5.5}$$

It remains to reduce (4.66) to the unixial case. It follows from the derivations above of the blocks in M and V that

$$\beta_0 = 0, \quad \eta_1 = 0, \quad \chi_1 = 0, \quad \chi_2 = \chi_3, \quad \eta_2 = -\eta_3, \quad \beta_3 = \beta_4, \quad \beta_5 = 4\beta_2,$$

and the coefficients $\beta_1, \beta_2, \beta_3$ are given by

$$\beta_1 = V_{01}^T M_{01}^{-1} V_{01}, \quad \beta_2 = V_{02}^T M_{02}^{-1} V_{02}, \quad \beta_3 = V_1^T M_1^{-1} V_1.$$

Then, by a direct calculation, we obtain

$$\begin{aligned}\sigma_v^{(0)} + \sigma_e^{(0)} = {} & \alpha_1 (\mathbf{A}_0 \cdot \mathbf{n}_1^2)\mathbf{n}_1^2 + \alpha_2 \mathbf{n}_1 \otimes \mathbf{N}_1 + \alpha_3 \mathbf{N}_1 \otimes \mathbf{n}_1 + \alpha_4 \mathbf{A}_0 \\ & + \alpha_5 n_{1i} n_{1k} A_{kj}^{(0)} + \alpha_6 A_{ik}^{(0)} n_{1k} n_{1j},\end{aligned} \tag{5.6}$$

where we have neglected the term $(\mathbf{A}_0 \cdot \mathbf{n}_1^2)\mathbf{i}$, since it can be absorbed into the pressure. The coefficients α_i $(i = 1, \ldots, 6)$ are given by

$$\begin{aligned}&\alpha_1 = \vartheta_{11} + \vartheta_{22} - \vartheta_{33} + ck_BT(\beta_1 + \beta_2 - \beta_3),\\ &\alpha_2 = -\frac{1}{2} ck_BT(\chi_2 + \eta_2), \quad \alpha_3 = \frac{1}{2} ck_BT(\chi_2 - \eta_2), \quad \alpha_4 = \eta + 2\vartheta_{22} + 2ck_BT\beta_2,\\ &\alpha_5 = \frac{1}{2}\left(\vartheta_{33} + ck_BT(\beta_3 - \eta_2)\right) - 2(\vartheta_{22} + ck_BT\beta_2),\\ &\alpha_6 = \frac{1}{2}\left(\vartheta_{33} + ck_BT(\beta_3 + \eta_2)\right) - 2(\vartheta_{22} + ck_BT\beta_2),\end{aligned}$$

which satisfy the following relations:

$$\alpha_2 + \alpha_3 = \alpha_6 - \alpha_5, \quad ck_BT\chi_2 = \alpha_3 - \alpha_2, \quad ck_BT\eta_2 = \alpha_6 - \alpha_5.$$

Using $\frac{\delta \mathcal{F}_{Un}}{\delta \mathbf{n}_2} = \frac{\delta \mathcal{F}_{Un}}{\delta \mathbf{n}_3} = 0$, the body force can be simplified as

$$ck_BT\mathfrak{F}_i = \partial_i n_{1k} \frac{\delta \mathcal{F}_{Un}}{\delta n_{1k}} = \partial_j \sigma_{ij}^E, \tag{5.7}$$

where $\sigma_{ij}^E = -\frac{\partial \mathcal{F}_{Un}}{\partial(\partial_j n_{1k})}\partial_i n_{1k}$ is called the Ericksen stress. Therefore, from (5.6) and (5.7), the equation of the fluid velocity $\mathbf{v}^{(0)}$ for the uniaxial case is given by

$$\rho_s \left(\frac{\partial \mathbf{v}^{(0)}}{\partial t} + \mathbf{v}^{(0)} \cdot \nabla \mathbf{v}^{(0)} \right)_i = -\partial_i p^{(0)} + \partial_j (\sigma_{ij}^L + \sigma_{ij}^E), \tag{5.8}$$

where the Leslie stress $\sigma^L = \sigma_v^{(0)} + \sigma_e^{(0)}$.

Equations (5.5) and (5.8) give the Ericksen–Leslie system, which also keep the following energy dissipation:

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\rho_s}{2}\int|\mathbf{v}^{(0)}|^2\mathrm{d}\mathbf{x}+\mathcal{F}_{Un}(\mathbf{n}_1)\right)\\ &\quad=-\int\left(\alpha_1'|\mathbf{A}_0\cdot\mathbf{n}_1^2|^2+\alpha_2'|\mathbf{A}_0|^2+\alpha_3'|\mathbf{A}_0\mathbf{n}_1|^2+ck_BT\frac{1}{\chi_2}|\mathbf{n}_1\times\mathbf{h}_1|^2\right)\mathrm{d}\mathbf{x},\end{aligned}\tag{5.9}$$

where

$$\alpha_1'=\alpha_1+ck_BT\frac{\eta_2^2}{\chi_2},\quad \alpha_2'=\alpha_4,\quad \alpha_3'=\alpha_5+\alpha_6-ck_BT\frac{\eta_2^2}{\chi_2}.$$

It can be seen from Proposition 2.2 in [34] that the first three terms in (5.9) are negative semidefinite if and only if

$$\alpha_2'\geq 0,\quad 2\alpha_2'+\alpha_3'\geq 0,\quad \frac{3}{2}\alpha_2'+\alpha_3'+\alpha_1'\geq 0.$$

It is easy to verify that (5.9) is indeed nonnegative, since we have $\eta>0$, $\vartheta_{11},\vartheta_{22},\vartheta_{33}>0$ from the positive definiteness of P, and $\beta_1,\beta_2,\beta_3>0,\beta_3\chi_2-\eta_2^2>0$ from the positive definiteness of M.

6. Conclusion. Using the Hilbert expansion, we derive a frame hydrodynamics for the biaxial nematic phase from a molecular-theory-based tensor model. Its coefficients are all expressed as those in the tensor model, and the energy dissipation is maintained. The model is further reduced to the Ericksen–Leslie model if the bulk energy minimum becomes uniaxial.

The key ingredient is to recognize the form of the high-order tensors from the properties of the original entropy or the quasi-entropy. This technique is also applicable to other mesoscopic symmetries. It calls for expressions of tensors under other symmetries [38, 39, 40], which we aim to investigate in future works.

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SUPPLEMENTARY MATERIALS: FRAME HYDRODYNAMICS OF BIAXIAL NEMATICS FROM MOLECULAR-THEORY-BASED TENSOR MODELS*

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SM1. Symmetric traceless tensors. As we have mentioned, any tensor can be decomposed into symmetric traceless tensors. To carry out calculations of high-order tensors, it is necessary to discuss some fundamental ingredients of symmetric traceless tensors.

For a tensor U expressed in the basis generated by $\mathfrak{q} = (\mathbf{m}_1, \mathbf{m}_2, \mathbf{m}_3)$, let us denote it as a function of $\mathfrak{q}$, i.e. $U(\mathfrak{q})$, to allow $\mathfrak{q}$ to vary. For example, let us consider a tensor $U(\mathfrak{q}) = 3\mathbf{m}_1 \otimes \mathbf{m}_3 - \mathbf{m}_3 \otimes \mathbf{m}_2$. For another orthonormal frame $\mathfrak{q}' = (\mathbf{m}'_1, \mathbf{m}'_2, \mathbf{m}'_3)$, we mean $U(\mathfrak{q}') = 3\mathbf{m}'_1 \otimes \mathbf{m}'_3 - \mathbf{m}'_3 \otimes \mathbf{m}'_2$.

SM1.1. Basis of symmetric traceless tensors. Any symmetric tensor can generate a symmetric traceless tensor in the form (2.2). To write down a basis of symmetric traceless tensors of certain order, we could choose those generated by monomials. Their expressions are derived previously [SM2]. Below, we list the third-order and fourth-order tensors that we will make use of.

A basis of third-order symmetric traceless tensors can be given by

$$(\mathbf{m}_1^3)_0,\ (\mathbf{m}_1^2\mathbf{m}_2)_0,\ (\mathbf{m}_1\mathbf{m}_2^2)_0,\ (\mathbf{m}_2^3)_0,$$
$$(\mathbf{m}_1^2\mathbf{m}_3)_0,\ (\mathbf{m}_1\mathbf{m}_2\mathbf{m}_3)_0,\ (\mathbf{m}_2^2\mathbf{m}_3)_0.$$

Their expressions are given by

$$(\mathbf{m}_1\mathbf{m}_2\mathbf{m}_3)_0 = \mathbf{m}_1\mathbf{m}_2\mathbf{m}_3,$$
$$(\mathbf{m}_1^3)_0 = \mathbf{m}_1^3 - \frac{3}{5}\mathbf{m}_1\mathfrak{i},$$
$$(\mathbf{m}_1^2\mathbf{m}_2)_0 = \mathbf{m}_1^2\mathbf{m}_2 - \frac{1}{5}\mathbf{m}_2\mathfrak{i}.$$

The others can be written down by changing the indices. A basis of fourth-order symmetric traceless tensors can be given by

$$(\mathbf{m}_1^4)_0,\ (\mathbf{m}_1^3\mathbf{m}_2)_0,\ (\mathbf{m}_1^2\mathbf{m}_2^2)_0,\ (\mathbf{m}_1\mathbf{m}_2^3)_0,\ (\mathbf{m}_2^4)_0,$$
$$(\mathbf{m}_1^3\mathbf{m}_3)_0,\ (\mathbf{m}_1^2\mathbf{m}_2\mathbf{m}_3)_0,\ (\mathbf{m}_1\mathbf{m}_2^2\mathbf{m}_3)_0,\ (\mathbf{m}_2^3\mathbf{m}_3)_0.$$

Their expressions are given by

$$(\mathbf{m}_1^4)_0 = \mathbf{m}_1^4 - \frac{6}{7}\mathbf{m}_1^2\mathfrak{i} + \frac{3}{35}\mathfrak{i}^2,$$
$$(\mathbf{m}_1^3\mathbf{m}_2)_0 = \mathbf{m}_1^3\mathbf{m}_2 - \frac{3}{7}\mathbf{m}_1\mathbf{m}_2\mathfrak{i},$$

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$$(\mathbf{m}_1^2\mathbf{m}_2^2)_0 = \mathbf{m}_1^2\mathbf{m}_2^2 - \frac{1}{7}(\mathbf{m}_1^2+\mathbf{m}_2^2)\mathfrak{i} + \frac{1}{35}\mathfrak{i}^2,$$
$$(\mathbf{m}_1^2\mathbf{m}_2\mathbf{m}_3)_0 = \mathbf{m}_1^2\mathbf{m}_2\mathbf{m}_3 - \frac{1}{7}\mathbf{m}_2\mathbf{m}_3\mathfrak{i}.$$

An additional note is that for a monomial with the power of $\mathbf{m}_3$ not less than two, we could substitute it by $\mathbf{m}_3^2 = \mathfrak{i} - \mathbf{m}_1^2 - \mathbf{m}_2^2$ to obtain equations such as (cf. the uniqueness of W in (2.2))

$$(\mathbf{m}_3^2)_0 = (\mathfrak{i} - \mathbf{m}_1^2 - \mathbf{m}_2^2)_0 = (-\mathbf{m}_1^2 - \mathbf{m}_2^2)_0, \quad (\mathbf{m}_3^4)_0 = \big((\mathbf{m}_1^2+\mathbf{m}_2^2)^2\big)_0.$$

For our discussion afterwards, we introduce the group $\mathscr{D}_2$ that has four elements,

$$\mathfrak{i} = \mathrm{diag}(1,1,1),\ \mathfrak{b}_1 = \mathrm{diag}(1,-1,-1),\ \mathfrak{b}_2 = \mathrm{diag}(-1,1,-1),\ \mathfrak{b}_3 = \mathrm{diag}(-1,-1,1).$$

The tensor U is called invariant of $\mathscr{D}_2$ if $U(\mathfrak{q}\mathfrak{b}_i) = U(\mathfrak{q})$ (recall the notation at the beginning of Appendix). All the invariant tensors of the order n form a linear subspace of nth-order symmetric traceless tensors, denoted by $\mathbb{A}^{\mathscr{D}_2,n}$. According to a short discussion in [SM2], its orthogonal complement $(\mathbb{A}^{\mathscr{D}_2,n})^\perp$ consists of all the nth-order symmetric traceless tensors U such that $U(\mathfrak{q}) + U(\mathfrak{q}\mathfrak{b}_1) + U(\mathfrak{q}\mathfrak{b}_2) + U(\mathfrak{q}\mathfrak{b}_3) = 0$.

It is evident that $\mathfrak{q}\mathfrak{b}_i$ transforms two of $\mathbf{m}_1$, $\mathbf{m}_2$, $\mathbf{m}_3$ to their opposites. From the expressions of symmetric traceless tensors written above, we can easily identify the decomposition $\mathbb{A}^{\mathscr{D}_2,n}$ and $(\mathbb{A}^{\mathscr{D}_2,n})^\perp$. For $n = 1,2,3,4$, they are listed below,

$$\begin{aligned}
&\mathbb{A}^{\mathscr{D}_2,1} = \{0\}, \quad (\mathbb{A}^{\mathscr{D}_2,1})^\perp = \mathrm{span}\{\mathbf{m}_1,\mathbf{m}_2,\mathbf{m}_3\},\\
&\mathbb{A}^{\mathscr{D}_2,2} = \mathrm{span}\{(\mathbf{m}_1^2)_0,(\mathbf{m}_2^2)_0\}, \quad (\mathbb{A}^{\mathscr{D}_2,2})^\perp = \mathrm{span}\{\mathbf{m}_1\mathbf{m}_2,\mathbf{m}_1\mathbf{m}_3,\mathbf{m}_2\mathbf{m}_3\},\\
&\mathbb{A}^{\mathscr{D}_2,3} = \mathrm{span}\{\mathbf{m}_1\mathbf{m}_2\mathbf{m}_3\},\\
&(\mathbb{A}^{\mathscr{D}_2,3})^\perp = \mathrm{span}\{(\mathbf{m}_1^3)_0,(\mathbf{m}_1^2\mathbf{m}_2)_0,(\mathbf{m}_1\mathbf{m}_2^2)_0,(\mathbf{m}_2^3)_0,(\mathbf{m}_1^2\mathbf{m}_3)_0,(\mathbf{m}_2^2\mathbf{m}_3)_0\},\\
&\mathbb{A}^{\mathscr{D}_2,4} = \mathrm{span}\{(\mathbf{m}_1^4)_0,(\mathbf{m}_1^2\mathbf{m}_2^2)_0,(\mathbf{m}_2^4)_0\},\\
&(\mathbb{A}^{\mathscr{D}_2,4})^\perp = \mathrm{span}\{(\mathbf{m}_1^3\mathbf{m}_2)_0,(\mathbf{m}_1\mathbf{m}_2^3)_0,(\mathbf{m}_1^3\mathbf{m}_3)_0,\\
&\qquad (\mathbf{m}_1^2\mathbf{m}_2\mathbf{m}_3)_0,(\mathbf{m}_1\mathbf{m}_2^2\mathbf{m}_3)_0,(\mathbf{m}_2^3\mathbf{m}_3)_0\}.
\end{aligned} \tag{SM1.1}$$

Let us write down some equalities to be used later. Define

$$\mathbf{S}_1 = \mathbf{m}_1^2 - \mathfrak{i}/3,\ \mathbf{S}_2 = \mathbf{m}_2^2 - \mathbf{m}_3^2,\ \mathbf{S}_3 = \mathbf{m}_1\mathbf{m}_2,\ \mathbf{S}_4 = \mathbf{m}_1\mathbf{m}_3,\ \mathbf{S}_5 = \mathbf{m}_2\mathbf{m}_3. \tag{SM1.2}$$

For third-order tensors, we have

$$\begin{aligned}
\mathbf{m}_1\mathbf{m}_2\mathbf{m}_3\cdot\mathbf{m}_i\otimes\mathbf{S}_j &= 0, \quad \text{if } (i,j)\neq\{(1,5),(2,4),(3,3)\},\\
\epsilon^{ils}(\mathbf{m}_1\mathbf{m}_2\mathbf{m}_3)_{jks}(\mathbf{S}_\nu\otimes\mathbf{S}_{\nu'})_{ijkl} &= 0, \quad \text{if } i\neq j \text{ and } \{\nu,\nu'\}\neq\{1,2\}.
\end{aligned} \tag{SM1.3}$$

If $U \in (\mathbb{A}^{\mathscr{D}_2,3})^\perp$, then

$$\begin{aligned}
&U\cdot\mathbf{m}_i\otimes\mathbf{S}_j = 0, \quad \text{if } (i,j)=\{(1,5),(2,4),(3,3)\},\\
&\epsilon^{ils}U_{jks}(\mathbf{S}_\nu\otimes\mathbf{S}_\nu)_{ijkl} = \epsilon^{ils}U_{jks}(\mathbf{S}_1\otimes\mathbf{S}_2)_{ijkl} = \epsilon^{ils}U_{jks}(\mathbf{S}_2\otimes\mathbf{S}_1)_{ijkl} = 0.
\end{aligned} \tag{SM1.4}$$

For fourth-order tensors, if $U \in \mathbb{A}^{\mathscr{D}_2,4}$, then

$$U\cdot\mathbf{S}_i\otimes\mathbf{S}_j = 0, \quad \text{if } i\neq j \text{ and } \{i,j\}\neq\{1,2\}. \tag{SM1.5}$$

If $U \in (\mathbb{A}^{\mathscr{D}_2,4})^{\perp}$, then

$$U \cdot \mathbf{S}_i \otimes \mathbf{S}_i = (\mathbf{m}_1^3\mathbf{m}_2)_0 \cdot \mathbf{S}_1 \otimes \mathbf{S}_2 = 0. \tag{SM1.6}$$

The equalities (SM1.3)–(SM1.6) can be recognized straightforwardly by expanding the tensors into several terms of tensor products of $\mathbf{m}_i$. The Levi-Civita symbol can be expanded as

$$\begin{aligned}\epsilon^{ijk} = &(\mathbf{m}_1 \otimes \mathbf{m}_2 \otimes \mathbf{m}_3 + \mathbf{m}_2 \otimes \mathbf{m}_3 \otimes \mathbf{m}_1 + \mathbf{m}_3 \otimes \mathbf{m}_1 \otimes \mathbf{m}_2\\ &- \mathbf{m}_1 \otimes \mathbf{m}_3 \otimes \mathbf{m}_2 - \mathbf{m}_3 \otimes \mathbf{m}_2 \otimes \mathbf{m}_1 - \mathbf{m}_2 \otimes \mathbf{m}_1 \otimes \mathbf{m}_3)_{ijk}.\end{aligned}$$

The equations above hold independent of the orthonormal frame we choose. In particular, they are valid if we substitute $\mathbf{m}_i$ with $\mathbf{n}_i$ and correspondingly $\mathbf{S}_i$ with $\mathbf{s}_i$ (recall (4.19)).

SM1.2. Expressing tensors by symmetric traceless tensors. There are complicated linear relations between high-order tensors. To figure out the linear relations, we shall express them by symmetric traceless tensors that completely give linearly independent components. These linear relations are inherited by averaged high-order tensors. The special forms of averaged high-order tensors are also revealed in this way.

To express a general tensor U by symmetric traceless tensors, we first decompose it as $U = U_{\text{sym}} + (U - U_{\text{sym}})$. The anti-symmetric part $U - U_{\text{sym}}$ can be written as the sum of several terms of the form

$$U_{\dots i \dots j \dots} - U_{\dots j \dots i \dots} = \epsilon^{ijk} W_{k \dots},$$

where W is an $(n-1)$th-order tensor (but notice that $\epsilon^{ijk}W_{k\dots}$ is an nth-order tensor). Thus, U is expressed by a symmetric tensor of nth-order and some tensors of lower order. Next, for each W occurring in the expression, we could do the similar decomposition. Carry out this action repeatedly until we express U by symmetric tensors. Then, each symmetric tensor can be expressed by a symmetric traceless tensor and several symmetric tensors of lower order. Also do it repeatedly to finally express U by symmetric traceless tensors. This procedure can be better understood shortly in our calculations below.

In what follows, we use this procedure to deal with the tensors

$$\Big(\mathbf{m}_1^2 - \frac{\mathfrak{i}}{3}\Big) \otimes \Big(\mathbf{m}_1^2 - \frac{\mathfrak{i}}{3}\Big),\ \Big(\mathbf{m}_1^2 - \frac{\mathfrak{i}}{3}\Big) \otimes (\mathbf{m}_2^2 - \mathbf{m}_3^2),\ (\mathbf{m}_2^2 - \mathbf{m}_3^2) \otimes (\mathbf{m}_2^2 - \mathbf{m}_3^2),$$
$$\mathbf{m}_1\mathbf{m}_2 \otimes \mathbf{m}_1\mathbf{m}_2,\ \mathbf{m}_1\mathbf{m}_3 \otimes \mathbf{m}_1\mathbf{m}_3,\ \mathbf{m}_2\mathbf{m}_3 \otimes \mathbf{m}_2\mathbf{m}_3.$$

From the expressions of symmetric traceless tensors, we can derive that

$$\begin{aligned}\mathbf{m}_1^4 &= (\mathbf{m}_1^4)_0 + \frac{6}{7}\mathbf{m}_1^2\mathfrak{i} - \frac{3}{35}\mathfrak{i}^2\\ &= (\mathbf{m}_1^4)_0 + \frac{6}{7}\Big(\mathbf{m}_1^2 - \frac{\mathfrak{i}}{3}\Big)\mathfrak{i} + \Big(\frac{2}{7} - \frac{3}{35}\Big)\mathfrak{i}^2\\ &= (\mathbf{m}_1^4)_0 + \frac{6}{7}(\mathbf{m}_1^2)_0\mathfrak{i} + \frac{1}{5}\mathfrak{i}^2, \qquad \text{(SM1.7)}\\ \mathbf{m}_1^2\mathbf{m}_2^2 &= (\mathbf{m}_1^2\mathbf{m}_2^2)_0 + \frac{1}{7}(\mathbf{m}_1^2 + \mathbf{m}_2^2)\mathfrak{i} - \frac{1}{35}\mathfrak{i}^2\\ &= (\mathbf{m}_1^2\mathbf{m}_2^2)_0 + \frac{1}{7}\Big(\frac{\mathfrak{i}}{3} - \mathbf{m}_3^2\Big)\mathfrak{i} + \Big(\frac{2}{21} - \frac{1}{35}\Big)\mathfrak{i}^2\\ &= (\mathbf{m}_1^2\mathbf{m}_2^2)_0 - \frac{1}{7}(\mathbf{m}_3^2)_0\mathfrak{i} + \frac{1}{15}\mathfrak{i}^2. \qquad \text{(SM1.8)}\end{aligned}$$

For a second-order tensor U, define

$$\mathcal{A}(U)_{ijkl} \stackrel{\text{def}}{=} \delta_{kl}U_{ij} + \delta_{ij}U_{kl} - \frac{3}{4}\big(\delta_{ik}U_{jl} + \delta_{jl}U_{ik} + \delta_{il}U_{jk} + \delta_{jk}U_{il}\big),$$
$$\mathcal{B}(U)_{ijkl} \stackrel{\text{def}}{=} U_{ki}\delta_{jl} - U_{kj}\delta_{il} + U_{li}\delta_{jk} - U_{lj}\delta_{ik}.$$

Using the expressions of symmetric traceless tensors and (SM1.7), it follows that

(SM1.9)
$$\begin{aligned}
&\Big(\mathbf{m}_1^2 - \frac{1}{3}\mathfrak{i}\Big)_{ij}\Big(\mathbf{m}_1^2 - \frac{1}{3}\mathfrak{i}\Big)_{kl} \\
&= \Big((\mathbf{m}_1^4)_0 + \frac{6}{7}(\mathbf{m}_1^2)_0\mathfrak{i} + \frac{1}{5}\mathfrak{i}^2\Big)_{ijkl} - \frac{1}{3}\delta_{ij}(\mathbf{m}_1^2)_{kl} - \frac{1}{3}\delta_{kl}(\mathbf{m}_1^2)_{ij} + \frac{1}{9}\delta_{ij}\delta_{kl} \\
&= \Big((\mathbf{m}_1^4)_0 + \frac{6}{7}(\mathbf{m}_1^2)_0\mathfrak{i} + \frac{1}{5}\mathfrak{i}^2\Big)_{ijkl} - \frac{1}{3}\delta_{ij}\big((\mathbf{m}_1^2)_0\big)_{kl} - \frac{1}{3}\delta_{kl}\big((\mathbf{m}_1^2)_0\big)_{ij} - \frac{1}{9}\delta_{ij}\delta_{kl} \\
&= \big((\mathbf{m}_1^4)_0\big)_{ijkl} - \frac{4}{21}\mathcal{A}\big((\mathbf{m}_1^2)_0\big)_{ijkl} - \frac{1}{45}(2\delta_{ij}\delta_{kl} - 3\delta_{ik}\delta_{jl} - 3\delta_{il}\delta_{jk}).
\end{aligned}$$

The symmetric tensor $\mathbf{m}_1^2\mathbf{m}_2^2$ is expressed by

$$\begin{aligned}
(\mathbf{m}_1^2\mathbf{m}_2^2)_{ijkl} = \frac{1}{6}\Big(&m_{1i}m_{1j}m_{2k}m_{2l} + m_{2i}m_{2j}m_{1k}m_{1l} \\
&+ (m_{1i}m_{2j} + m_{2i}m_{1j})(m_{1k}m_{2l} + m_{2k}m_{1l})\Big).
\end{aligned} \tag{SM1.10}$$

Then we obtain from (SM1.10) that

$$\begin{aligned}
&(\mathbf{m}_1\mathbf{m}_2 \otimes \mathbf{m}_1\mathbf{m}_2)_{ijkl} - (\mathbf{m}_1^2\mathbf{m}_2^2)_{ijkl} \\
&\quad = -\frac{1}{12}\Big(2m_{1i}m_{1j}m_{2k}m_{2l} + 2m_{2i}m_{2j}m_{1k}m_{1l} \\
&\qquad - (m_{1i}m_{2j} + m_{2i}m_{1j})(m_{1k}m_{2l} + m_{2k}m_{1l})\Big).
\end{aligned} \tag{SM1.11}$$

Using the equality

$$m_{1i}m_{2j} - m_{2i}m_{1j} = \epsilon^{ijs}m_{3s}, \tag{SM1.12}$$

the tensor in the big parenthesis of (SM1.11) can be calculated as

(SM1.13)
$$\begin{aligned}
&m_{1i}m_{2l}(m_{1j}m_{2k} - m_{2j}m_{1k}) + m_{1i}m_{2k}(m_{1j}m_{2l} - m_{2j}m_{1l}) \\
&\quad + m_{2i}m_{1l}(m_{2j}m_{1k} - m_{1j}m_{2k}) + m_{2i}m_{1k}(m_{2j}m_{1l} - m_{1j}m_{2l}) \\
&= (m_{1i}m_{2l} - m_{2i}m_{1l})(m_{1j}m_{2k} - m_{2j}m_{1k}) + (m_{1i}m_{2k} - m_{2i}m_{1k})(m_{1j}m_{2l} - m_{2j}m_{1l}) \\
&= (\epsilon^{ils}\epsilon^{jkt} + \epsilon^{iks}\epsilon^{jlt})(\mathbf{m}_3^2)_{st} \\
&= 2\delta_{ij}\delta_{kl} - \delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk} \\
&\quad - 2\delta_{ij}(\mathbf{m}_3^2)_{kl} - 2\delta_{kl}(\mathbf{m}_3^2)_{ij} + \delta_{ik}(\mathbf{m}_3^2)_{jl} + \delta_{il}(\mathbf{m}_3^2)_{jk} + \delta_{jk}(\mathbf{m}_3^2)_{il} + \delta_{jl}(\mathbf{m}_3^2)_{ik} \\
&= \frac{1}{3}\big(2\delta_{ij}\delta_{kl} - \delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk}\big) - 2\delta_{ij}\big((\mathbf{m}_3^2)_0\big)_{kl} - 2\delta_{kl}\big((\mathbf{m}_3^2)_0\big)_{ij} \\
&\quad + \delta_{ik}\big((\mathbf{m}_3^2)_0\big)_{jl} + \delta_{il}\big((\mathbf{m}_3^2)_0\big)_{jk} + \delta_{jk}\big((\mathbf{m}_3^2)_0\big)_{il} + \delta_{jl}\big((\mathbf{m}_3^2)_0\big)_{ik}.
\end{aligned}$$

Thus, combining (SM1.8), (SM1.11) and (SM1.13) yields

$$(\mathbf{m}_1\mathbf{m}_2 \otimes \mathbf{m}_1\mathbf{m}_2)_{ijkl} = \big((\mathbf{m}_1^2\mathbf{m}_2^2)_0\big)_{ijkl} + \frac{1}{7}\mathcal{A}\big((\mathbf{m}_3^2)_0\big)_{ijkl} - \frac{1}{60}(2\delta_{ij}\delta_{kl} - 3\delta_{ik}\delta_{jl} - 3\delta_{il}\delta_{jk}). \tag{SM1.14}$$

Similar to the calculation of (SM1.14), we obtain

$$(\mathbf{m}_1\mathbf{m}_3 \otimes \mathbf{m}_1\mathbf{m}_3)_{ijkl} = \big((\mathbf{m}_1^2\mathbf{m}_3^2)_0\big)_{ijkl} + \frac{1}{7}\mathcal{A}\big((\mathbf{m}_2^2)_0\big)_{ijkl} - \frac{1}{60}(2\delta_{ij}\delta_{kl} - 3\delta_{ik}\delta_{jl} - 3\delta_{il}\delta_{jk}), \tag{SM1.15}$$

$$(\mathbf{m}_2\mathbf{m}_3 \otimes \mathbf{m}_2\mathbf{m}_3)_{ijkl} = \big((\mathbf{m}_2^2\mathbf{m}_3^2)_0\big)_{ijkl} + \frac{1}{7}\mathcal{A}\big((\mathbf{m}_1^2)_0\big)_{ijkl} - \frac{1}{60}(2\delta_{ij}\delta_{kl} - 3\delta_{ik}\delta_{jl} - 3\delta_{il}\delta_{jk}). \tag{SM1.16}$$

In the same way, we have

$$\begin{aligned}\big((\mathbf{m}_2^2 - \mathbf{m}_3^2) \otimes (\mathbf{m}_2^2 - \mathbf{m}_3^2)\big)_{ijkl} &- (\mathbf{m}_2^4 - 2\mathbf{m}_2^2\mathbf{m}_3^2 + \mathbf{m}_3^4)_{ijkl} \\ = -\frac{1}{3}\Big(&2m_{2i}m_{2j}m_{3k}m_{3l} + 2m_{3i}m_{3j}m_{2k}m_{2l} \\ &- (m_{2i}m_{3j} + m_{3i}m_{2j})(m_{2k}m_{3l} + m_{3k}m_{2l})\Big).\end{aligned} \tag{SM1.17}$$

Similar to the calculation of (SM1.13), we obtain

$$\begin{aligned}&2m_{2i}m_{2j}m_{3k}m_{3l} + 2m_{3i}m_{3j}m_{2k}m_{2l} - (m_{2i}m_{3j} + m_{3i}m_{2j})(m_{2k}m_{3l} + m_{3k}m_{2l}) \\ =\,& m_{2i}m_{3l}(m_{2j}m_{3k} - m_{3j}m_{2k}) + m_{2i}m_{3k}(m_{2j}m_{3l} - m_{3j}m_{2l}) \\ &+ m_{3i}m_{2l}(m_{3j}m_{2k} - m_{2j}m_{3k}) + m_{3i}m_{2k}(m_{3j}m_{2l} - m_{2j}m_{3l}) \\ =\,& (m_{2i}m_{3l} - m_{3i}m_{2l})(m_{2j}m_{3k} - m_{3j}m_{2k}) + (m_{2i}m_{3k} - m_{3i}m_{2k})(m_{2j}m_{3l} - m_{3j}m_{2l}) \\ =\,& (\epsilon^{ils}\epsilon^{jkt} + \epsilon^{iks}\epsilon^{jlt})(\mathbf{m}_1^2)_{st} \\ =\,& 2\delta_{ij}\delta_{kl} - \delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk} - 2\delta_{ij}(\mathbf{m}_1^2)_{kl} - 2\delta_{kl}(\mathbf{m}_1^2)_{ij} \\ &+ \delta_{ik}(\mathbf{m}_1^2)_{jl} + \delta_{il}(\mathbf{m}_1^2)_{jk} + \delta_{jk}(\mathbf{m}_1^2)_{il} + \delta_{jl}(\mathbf{m}_1^2)_{ik} \\ =\,& \frac{1}{3}\big(2\delta_{ij}\delta_{kl} - \delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk}\big) - 2\delta_{ij}\big((\mathbf{m}_1^2)_0\big)_{kl} - 2\delta_{kl}\big((\mathbf{m}_1^2)_0\big)_{ij} \\ &+ \delta_{ik}\big((\mathbf{m}_1^2)_0\big)_{jl} + \delta_{il}\big((\mathbf{m}_1^2)_0\big)_{jk} + \delta_{jk}\big((\mathbf{m}_1^2)_0\big)_{il} + \delta_{jl}\big((\mathbf{m}_1^2)_0\big)_{ik}.\end{aligned} \tag{SM1.18}$$

Note that

$$\begin{aligned}&\mathbf{m}_2^4 - 2\mathbf{m}_2^2\mathbf{m}_3^2 + \mathbf{m}_3^4 \\ &= (\mathbf{m}_2^4 - 2\mathbf{m}_2^2\mathbf{m}_3^2 + \mathbf{m}_3^4)_0 + \frac{6}{7}(\mathbf{m}_2^2 + \mathbf{m}_3^2)_0\mathfrak{i} + \frac{2}{7}(\mathbf{m}_1^2)_0\mathfrak{i} + \frac{4}{15}\mathfrak{i}^2 \\ &= (\mathbf{m}_2^4 - 2\mathbf{m}_2^2\mathbf{m}_3^2 + \mathbf{m}_3^4)_0 - \frac{4}{7}(\mathbf{m}_1^2)_0\mathfrak{i} + \frac{4}{15}\mathfrak{i}^2.\end{aligned}$$

Then, from (SM1.17) and (SM1.18), we deduce

$$\begin{aligned}\big((\mathbf{m}_2^2 - \mathbf{m}_3^2) \otimes (\mathbf{m}_2^2 - \mathbf{m}_3^2)\big)_{ijkl} = \big((\mathbf{m}_2^4 - 2\mathbf{m}_2^2\mathbf{m}_3^2 + \mathbf{m}_3^4)_0\big)_{ijkl} &+ \frac{4}{7}\mathcal{A}\big((\mathbf{m}_1^2)_0\big)_{ijkl} \\ &- \frac{1}{15}(2\delta_{ij}\delta_{kl} - 3\delta_{ik}\delta_{jl} - 3\delta_{il}\delta_{jk}).\end{aligned} \tag{SM1.19}$$

The next task is to calculate the fourth-order tensor $(\mathbf{m}_1^2)_0 \otimes (\mathbf{m}_2^2 - \mathbf{m}_3^2)$. A direct calculation gives

$$\begin{aligned}
&m_{1i}m_{1j}m_{2k}m_{2l} - m_{2i}m_{2j}m_{1k}m_{1l}\\
&\quad = m_{1i}m_{2l}(m_{1j}m_{2k} - m_{2j}m_{1k}) + m_{2j}m_{1k}(m_{1i}m_{2l} - m_{2i}m_{1l})\\
&\quad = \epsilon^{jks}m_{1i}m_{2l}m_{3s} + \epsilon^{ils}m_{1k}m_{2j}m_{3s}.
\end{aligned} \tag{SM1.20}$$

Furthermore, the asymmetric part of (SM1.20) can be calculated as follows:

(SM1.21)

$$\begin{aligned}
&\epsilon^{jks}m_{1i}m_{2l}m_{3s} + \epsilon^{ils}m_{1k}m_{2j}m_{3s} - \epsilon^{jks}(\mathbf{m}_1\mathbf{m}_2\mathbf{m}_3)_{ils} - \epsilon^{ils}(\mathbf{m}_1\mathbf{m}_2\mathbf{m}_3)_{kjs}\\
&= \frac{1}{6}\epsilon^{jks}\Big(m_{1i}m_{2l}m_{3s} - m_{2i}m_{3l}m_{1s} + m_{1i}m_{2l}m_{3s} - m_{3i}m_{1l}m_{2s}\\
&\quad + m_{1i}(m_{2l}m_{3s} - m_{3l}m_{2s}) + (m_{1i}m_{2l} - m_{2i}m_{1l})m_{3s} + (m_{1i}m_{3s} - m_{3i}m_{1s})m_{2l}\Big)\\
&\quad + \frac{1}{6}\epsilon^{ils}\Big(m_{1k}m_{2j}m_{3s} - m_{2k}m_{3j}m_{1s} + m_{1k}m_{2j}m_{3s} - m_{3k}m_{1j}m_{2s}\\
&\quad + m_{1k}(m_{2j}m_{3s} - m_{3j}m_{2s}) + (m_{1k}m_{2j} - m_{2k}m_{1j})m_{3s} + (m_{1k}m_{3s} - m_{3k}m_{1s})m_{2j}\Big)\\
&= \frac{1}{6}\epsilon^{jks}\Big(3\epsilon^{ilt}m_{3t}m_{3s} + \epsilon^{slt}m_{2i}m_{2t} + \epsilon^{ist}m_{1t}m_{1l} + \epsilon^{lst}m_{1i}m_{1t} + \epsilon^{sit}m_{2t}m_{2l}\Big)\\
&\quad + \frac{1}{6}\epsilon^{ils}\Big(3\epsilon^{kjt}m_{3t}m_{3s} + \epsilon^{sjt}m_{2k}m_{2t} + \epsilon^{kst}m_{1t}m_{1j} + \epsilon^{jst}m_{1k}m_{1t} + \epsilon^{skt}m_{2t}m_{2j}\Big)\\
&= \frac{1}{2}\epsilon^{jks}\epsilon^{ilt}(\mathbf{m}_3^2)_{ts} + \frac{1}{6}\Big((\delta_{jl}\delta_{kt} - \delta_{jt}\delta_{kl})m_{2i}m_{2t} + (\delta_{jt}\delta_{ki} - \delta_{ji}\delta_{kt})m_{1t}m_{1l}\\
&\quad + (\delta_{jt}\delta_{kl} - \delta_{jl}\delta_{kt})m_{1i}m_{1t} + (\delta_{ji}\delta_{kt} - \delta_{jt}\delta_{ki})m_{2t}m_{2l}\Big)\\
&\quad + \frac{1}{2}\epsilon^{ils}\epsilon^{kjt}(\mathbf{m}_3^2)_{ts} + \frac{1}{6}\Big((\delta_{ij}\delta_{lt} - \delta_{it}\delta_{lj})m_{2k}m_{2t} + (\delta_{it}\delta_{lk} - \delta_{ik}\delta_{lt})m_{1t}m_{1j}\\
&\quad + (\delta_{it}\delta_{lj} - \delta_{ij}\delta_{lt})m_{1k}m_{1t} + (\delta_{ik}\delta_{lt} - \delta_{it}\delta_{lk})m_{2t}m_{2j}\Big)\\
&= \frac{1}{2}(\epsilon^{jks}\epsilon^{ilt} + \epsilon^{ils}\epsilon^{kjt})(\mathbf{m}_3^2)_{ts} + \frac{1}{3}\Big(\delta_{kl}(\mathbf{m}_1^2)_{ij} - \delta_{ij}(\mathbf{m}_1^2)_{kl} + \delta_{ij}(\mathbf{m}_2^2)_{kl} - \delta_{kl}(\mathbf{m}_2^2)_{ij}\Big)\\
&= \frac{1}{3}\Big(\delta_{kl}(\mathbf{m}_1^2)_{ij} - \delta_{ij}(\mathbf{m}_1^2)_{kl} + \delta_{ij}(\mathbf{m}_2^2)_{kl} - \delta_{kl}(\mathbf{m}_2^2)_{ij}\Big),
\end{aligned}$$

where we have used the fact that

$$\begin{aligned}
&(\epsilon^{jks}\epsilon^{ilt} + \epsilon^{ils}\epsilon^{kjt})(\mathbf{m}_3^2)_{ts}\\
&\quad = \Big(\delta_{ji}\delta_{kl}\delta_{st} + \delta_{jl}\delta_{kt}\delta_{si} + \delta_{jt}\delta_{ki}\delta_{sl} - \delta_{ji}\delta_{sl}\delta_{kt} - \delta_{jl}\delta_{ki}\delta_{st} - \delta_{jt}\delta_{kl}\delta_{si}\\
&\qquad + \delta_{ik}\delta_{lj}\delta_{st} + \delta_{ij}\delta_{lt}\delta_{sk} + \delta_{it}\delta_{lk}\delta_{sj} - \delta_{ik}\delta_{sj}\delta_{lt} - \delta_{ij}\delta_{lk}\delta_{st} - \delta_{it}\delta_{lj}\delta_{sk}\Big)(\mathbf{m}_3^2)_{ts}\\
&\quad = \delta_{jl}(\mathbf{m}_3^2)_{ik} + \delta_{ik}(\mathbf{m}_3^2)_{jl} - \delta_{ij}(\mathbf{m}_3^2)_{kl} - \delta_{kl}(\mathbf{m}_3^2)_{ij}\\
&\qquad + \delta_{ij}(\mathbf{m}_3^2)_{kl} + \delta_{kl}(\mathbf{m}_3^2)_{ij} - \delta_{ik}(\mathbf{m}_3^2)_{jl} - \delta_{jl}(\mathbf{m}_3^2)_{ik}\\
&\quad = 0.
\end{aligned}$$

Then, using (SM1.10), (SM1.7)-(SM1.8), (SM1.14), (SM1.20)-(SM1.21) and the relation $\mathbf{m}_1^2 + \mathbf{m}_2^2 + \mathbf{m}_3^2 = \mathfrak{i}$, we obtain

(SM1.22)

$$\Big(\mathbf{m}_1^2 - \frac{\mathfrak{i}}{3}\Big)_{ij}(\mathbf{m}_2^2 - \mathbf{m}_3^2)_{kl} = \Big(\mathbf{m}_1^2 - \frac{\mathfrak{i}}{3}\Big)_{ij}(2\mathbf{m}_2^2 + \mathbf{m}_1^2 - \mathfrak{i})_{kl}$$

$$
\begin{aligned}
&= 2m_{1i}m_{1j}m_{2k}m_{2l} + (\mathbf{m}_1^4)_{ijkl} - \delta_{kl}(\mathbf{m}_1^2)_{ij} - \frac{2}{3}\delta_{ij}(\mathbf{m}_2^2)_{kl} - \frac{1}{3}\delta_{ij}(\mathbf{m}_1^2)_{kl} + \frac{1}{3}\delta_{ij}\delta_{kl}\\
&= m_{1i}m_{1j}m_{2k}m_{2l} - m_{2i}m_{2j}m_{1k}m_{1l} + 6(\mathbf{m}_1^2\mathbf{m}_2^2)_{ijkl} - 4(\mathbf{m}_1\mathbf{m}_2 \otimes \mathbf{m}_1\mathbf{m}_2)_{ijkl}\\
&\quad + (\mathbf{m}_1^4)_{ijkl} - \delta_{kl}(\mathbf{m}_1^2)_{ij} - \frac{2}{3}\delta_{ij}(\mathbf{m}_2^2)_{kl} - \frac{1}{3}\delta_{ij}(\mathbf{m}_1^2)_{kl} + \frac{1}{3}\delta_{ij}\delta_{kl}\\
&= \epsilon^{jks}(\mathbf{m}_1\mathbf{m}_2\mathbf{m}_3)_{ils} + \epsilon^{ils}(\mathbf{m}_1\mathbf{m}_2\mathbf{m}_3)_{kjs}\\
&\quad + \frac{1}{3}\Big(\delta_{kl}\big((\mathbf{m}_1^2)_0\big)_{ij} - \delta_{ij}\big((\mathbf{m}_1^2)_0\big)_{kl} + \delta_{ij}\big((\mathbf{m}_2^2)_0\big)_{kl} - \delta_{kl}\big((\mathbf{m}_2^2)_0\big)_{ij}\Big)\\
&\quad + 6\big((\mathbf{m}_1^2\mathbf{m}_2^2)_0\big)_{ijkl} - \frac{6}{7}\big((\mathbf{m}_3^2)_0\mathfrak{i}\big)_{ijkl} + \frac{2}{5}(\mathfrak{i}^2)_{ijkl}\\
&\quad - 4\big((\mathbf{m}_1^2\mathbf{m}_2^2)_0\big)_{ijkl} - \frac{4}{7}\mathcal{A}\big((\mathbf{m}_3^2)_0\big)_{ijkl} + \frac{1}{15}(2\delta_{ij}\delta_{kl} - 3\delta_{ik}\delta_{jl} - 3\delta_{il}\delta_{jk})\\
&\quad + \big((\mathbf{m}_1^4)_0\big)_{ijkl} + \frac{6}{7}\big((\mathbf{m}_1^2)_0\mathfrak{i}\big)_{ijkl} + \frac{1}{5}(\mathfrak{i}^2)_{ijkl}\\
&\quad - \delta_{kl}\big((\mathbf{m}_1^2)_0\big)_{ij} - \frac{2}{3}\delta_{ij}\big((\mathbf{m}_2^2)_0\big)_{kl} - \frac{1}{3}\delta_{ij}\big((\mathbf{m}_1^2)_0\big)_{kl} - \frac{1}{3}\delta_{ij}\delta_{kl}\\
&= \epsilon^{jks}(\mathbf{m}_1\mathbf{m}_2\mathbf{m}_3)_{ils} + \epsilon^{ils}(\mathbf{m}_1\mathbf{m}_2\mathbf{m}_3)_{kjs} + 2\big((\mathbf{m}_1^2\mathbf{m}_2^2)_0\big)_{ijkl} + \big((\mathbf{m}_1^4)_0\big)_{ijkl}\\
&\quad + \frac{4}{21}\mathcal{A}\big((\mathbf{m}_1^2)_0\big)_{ijkl} + \frac{8}{21}\mathcal{A}\big((\mathbf{m}_2^2)_0\big)_{ijkl},
\end{aligned}
$$

where we have also used the following fact

$$
\begin{aligned}
&\frac{1}{3}\Big(\delta_{kl}\big((\mathbf{m}_1^2)_0\big)_{ij} - \delta_{ij}\big((\mathbf{m}_1^2)_0\big)_{kl} + \delta_{ij}\big((\mathbf{m}_2^2)_0\big)_{kl} - \delta_{kl}\big((\mathbf{m}_2^2)_0\big)_{ij}\Big)\\
&- \delta_{kl}\big((\mathbf{m}_1^2)_0\big)_{ij} - \frac{2}{3}\delta_{ij}\big((\mathbf{m}_2^2)_0\big)_{kl} - \frac{1}{3}\delta_{ij}\big((\mathbf{m}_1^2)_0\big)_{kl} - \frac{6}{7}\big((\mathbf{m}_3^2)_0\mathfrak{i}\big)_{ijkl} + \frac{2}{5}(\mathfrak{i}^2)_{ijkl}\\
&+ \frac{6}{7}\big((\mathbf{m}_1^2)_0\mathfrak{i}\big)_{ijkl} + \frac{1}{5}(\mathfrak{i}^2)_{ijkl} - \frac{1}{3}\delta_{ij}\delta_{kl}\\
&= -\frac{1}{3}\Big(2\delta_{kl}\big((\mathbf{m}_1^2)_0\big)_{ij} + 2\delta_{ij}\big((\mathbf{m}_1^2)_0\big)_{kl} + \delta_{kl}\big((\mathbf{m}_2^2)_0\big)_{ij} + \delta_{ij}\big((\mathbf{m}_2^2)_0\big)_{kl}\Big)\\
&\quad + \frac{12}{7}\big((\mathbf{m}_1^2)_0\mathfrak{i}\big)_{ijkl} + \frac{6}{7}\big((\mathbf{m}_2^2)_0\mathfrak{i}\big)_{ijkl} - \frac{1}{15}(2\delta_{ij}\delta_{kl} - 3\delta_{ik}\delta_{jl} - 3\delta_{il}\delta_{jk})\\
&= -\frac{8}{21}\mathcal{A}\big((\mathbf{m}_1^2)_0\big)_{ijkl} - \frac{4}{21}\mathcal{A}\big((\mathbf{m}_2^2)_0\big)_{ijkl} - \frac{1}{15}(2\delta_{ij}\delta_{kl} - 3\delta_{ik}\delta_{jl} - 3\delta_{il}\delta_{jk}).
\end{aligned}
$$

Note that $\mathbf{m}_2^2 - \mathbf{m}_3^2 = (2\mathbf{m}_2^2 + \mathbf{m}_1^2)_0$. It follows that

$$
\begin{aligned}
(\mathbf{m}_2^2)_0 \otimes (\mathbf{m}_2^2)_0 &= \frac{1}{4}\big(\mathbf{m}_2^2 - \mathbf{m}_3^2 - (\mathbf{m}_1^2)_0\big) \otimes \big(\mathbf{m}_2^2 - \mathbf{m}_3^2 - (\mathbf{m}_2^2)_0\big)\\
&= \frac{1}{4}\Big((\mathbf{m}_2^2 - \mathbf{m}_3^2) \otimes (\mathbf{m}_2^2 - \mathbf{m}_3^2) - (\mathbf{m}_2^2 - \mathbf{m}_3^2) \otimes (\mathbf{m}_1^2)_0\\
&\quad - (\mathbf{m}_1^2)_0 \otimes (\mathbf{m}_2^2 - \mathbf{m}_3^2) + (\mathbf{m}_1^2)_0 \otimes (\mathbf{m}_1^2)_0\Big).
\end{aligned}
\tag{SM1.23}
$$

Thus, combining (SM1.23) with (SM1.9), (SM1.19) and (SM1.22), we obtain

(SM1.24)

$$
\begin{aligned}
&\Big(\mathbf{m}_2^2 - \frac{1}{3}\mathfrak{i}\Big)_{ij}\Big(\mathbf{m}_2^2 - \frac{1}{3}\mathfrak{i}\Big)_{kl}\\
&= \frac{1}{4}\Big(\big((\mathbf{m}_2^4 - 2\mathbf{m}_2^2\mathbf{m}_3^2 + \mathbf{m}_3^4)_0\big)_{ijkl} - \frac{4}{7}\mathcal{A}\big((\mathbf{m}_1^2)_0\big)_{ijkl} - \frac{1}{15}(2\delta_{ij}\delta_{kl} - 3\delta_{ik}\delta_{jl} - 3\delta_{il}\delta_{jk})
\end{aligned}
$$

$$
\begin{aligned}
&+\big((\mathbf{m}_1^4)_0\big)_{ijkl}-\frac{4}{21}\mathcal{A}\big((\mathbf{m}_1^2)_0\big)_{ijkl}-\frac{1}{45}(2\delta_{ij}\delta_{kl}-3\delta_{ik}\delta_{jl}-3\delta_{il}\delta_{jk})\\
&-4\big((\mathbf{m}_1^2\mathbf{m}_2^2)_0\big)_{ijkl}-2\big((\mathbf{m}_1^4)_0\big)_{ijkl}-\frac{8}{21}\mathcal{A}\big((\mathbf{m}_1^2)_0\big)_{ijkl}-\frac{16}{21}\mathcal{A}\big((\mathbf{m}_2^2)_0\big)_{ijkl}\Big)\\
=&\big((\mathbf{m}_2^4)_0\big)_{ijkl}-\frac{4}{21}\mathcal{A}\big((\mathbf{m}_2^2)_0\big)_{ijkl}-\frac{1}{45}(2\delta_{ij}\delta_{kl}-3\delta_{ik}\delta_{jl}-3\delta_{il}\delta_{jk}),
\end{aligned}
$$

where we have employed the cancellation relation

$$
\begin{aligned}
&\epsilon^{jks}(\mathbf{m}_1\mathbf{m}_2\mathbf{m}_3)_{ils}+\epsilon^{ils}(\mathbf{m}_1\mathbf{m}_2\mathbf{m}_3)_{kjs}\\
&\quad+\epsilon^{lis}(\mathbf{m}_1\mathbf{m}_2\mathbf{m}_3)_{kjs}+\epsilon^{kjs}(\mathbf{m}_1\mathbf{m}_2\mathbf{m}_3)_{ils}=0.
\end{aligned}
$$

Next, we calculate the three tensors

$$
\mathbf{m}_1\otimes\mathbf{m}_2\mathbf{m}_3,\quad \mathbf{m}_2\otimes\mathbf{m}_1\mathbf{m}_3,\quad \mathbf{m}_3\otimes\mathbf{m}_1\mathbf{m}_2.
$$

It turns out that

$$
\begin{aligned}
&\frac{1}{2}m_{1i}(m_{2j}m_{3k}+m_{3j}m_{2k})\\
&\quad=(\mathbf{m}_1\mathbf{m}_2\mathbf{m}_3)_{ijk}+\frac{1}{6}\Big((m_{1i}m_{2j}-m_{2i}m_{1j})m_{3k}+(m_{1i}m_{3j}-m_{3i}m_{1j})m_{2k}\\
&\qquad+(m_{1i}m_{2k}-m_{2i}m_{1k})m_{3j}+(m_{1i}m_{3k}-m_{3i}m_{1k})m_{3j}\Big)
\end{aligned}
$$

(SM1.25)
$$
\quad=(\mathbf{m}_1\mathbf{m}_2\mathbf{m}_3)_{ijk}+\frac{1}{6}\Big(\epsilon^{ijs}\big((\mathbf{m}_3^2)_0-(\mathbf{m}_2^2)_0\big)_{ks}+\epsilon^{iks}\big((\mathbf{m}_3^2)_0-(\mathbf{m}_2^2)_0\big)_{js}\Big),
$$

$$
\frac{1}{2}m_{2i}(m_{1j}m_{3k}+m_{3j}m_{1k})
$$

(SM1.26)
$$
\quad=(\mathbf{m}_1\mathbf{m}_2\mathbf{m}_3)_{ijk}+\frac{1}{6}\Big(\epsilon^{ijs}\big((\mathbf{m}_1^2)_0-(\mathbf{m}_3^2)_0\big)_{ks}+\epsilon^{iks}\big((\mathbf{m}_1^2)_0-(\mathbf{m}_3^2)_0\big)_{js}\Big),
$$

$$
\frac{1}{2}m_{3i}(m_{1j}m_{2k}+m_{2j}m_{1k})
$$

(SM1.27)
$$
\quad=(\mathbf{m}_1\mathbf{m}_2\mathbf{m}_3)_{ijk}+\frac{1}{6}\Big(\epsilon^{ijs}\big((\mathbf{m}_2^2)_0-(\mathbf{m}_1^2)_0\big)_{ks}+\epsilon^{iks}\big((\mathbf{m}_2^2)_0-(\mathbf{m}_1^2)_0\big)_{js}\Big).
$$

The equations (SM1.25)–(SM1.27) also hold if we replace $\mathbf{m}_i$ with $\mathbf{n}_i$, which we also need to use later.

To deal with $\mathcal{V}^{(0)}$ in the subsection 4.1, we need to calculate

$$
\begin{aligned}
&(\mathbf{m}_1\otimes\mathbf{m}_2)\otimes\mathbf{m}_1\mathbf{m}_2,\quad (\mathbf{m}_2\otimes\mathbf{m}_1)\otimes\mathbf{m}_1\mathbf{m}_2,\\
&(\mathbf{m}_1\otimes\mathbf{m}_3)\otimes\mathbf{m}_1\mathbf{m}_3,\quad (\mathbf{m}_2\otimes\mathbf{m}_3)\otimes\mathbf{m}_2\mathbf{m}_3.
\end{aligned}
$$

Using the definition of $\mathcal{R}_i^{(0)}(i=3,4,5)$, it follows that

$$
\begin{aligned}
2\langle m_{1i}m_{2j}(\mathbf{m}_1\mathbf{m}_2)_{kl}\rangle&=\frac{1}{2}\mathcal{R}_3^{(0)}+\big\langle(m_{1i}m_{2j}-m_{2i}m_{1j})(\mathbf{m}_1\mathbf{m}_2)_{kl}\big\rangle,\\
2\langle m_{2i}m_{1j}(\mathbf{m}_1\mathbf{m}_2)_{kl}\rangle&=\frac{1}{2}\mathcal{R}_3^{(0)}-\big\langle(m_{1i}m_{2j}-m_{2i}m_{1j})(\mathbf{m}_1\mathbf{m}_2)_{kl}\big\rangle,\\
2\langle m_{1i}m_{3j}(\mathbf{m}_1\mathbf{m}_3)_{kl}\rangle&=\frac{1}{2}\mathcal{R}_4^{(0)}+\big\langle(m_{1i}m_{3j}-m_{3i}m_{1j})(\mathbf{m}_1\mathbf{m}_3)_{kl}\big\rangle,\\
2\langle m_{2i}m_{3j}(\mathbf{m}_2\mathbf{m}_3)_{kl}\rangle&=\frac{1}{2}\mathcal{R}_5^{(0)}+\big\langle(m_{2i}m_{3j}-m_{3i}m_{2j})(\mathbf{m}_2\mathbf{m}_3)_{kl}\big\rangle.
\end{aligned}
$$

In order to calculate the above tensor moments, it is desirable to utilize the following relation:

$$\epsilon^{ijk}\epsilon^{ist} = \delta_{js}\delta_{kt} - \delta_{jt}\delta_{ks}. \tag{SM1.28}$$

Then, using (SM1.12) and (SM1.28), we derive that

(SM1.29)

$$\begin{aligned}
&(m_{1i}m_{2j} - m_{2i}m_{1j})(\mathbf{m}_1\mathbf{m}_2)_{kl}\\
&= \frac{1}{2}\epsilon^{ijs}m_{3s}(m_{1k}m_{2l} + m_{2k}m_{1l})\\
&= \epsilon^{ijs}\Big((\mathbf{m}_1\mathbf{m}_2\mathbf{m}_3)_{kls} + \frac{1}{6}m_{1k}(m_{2l}m_{3s} - m_{3l}m_{2s}) + \frac{1}{6}m_{2l}(m_{1k}m_{3s} - m_{3k}m_{1s})\\
&\quad + \frac{1}{6}m_{2k}(m_{1l}m_{3s} - m_{3l}m_{1s}) + \frac{1}{6}m_{1l}(m_{2k}m_{3s} - m_{3k}m_{2s})\Big)\\
&= \epsilon^{ijs}\Big((\mathbf{m}_1\mathbf{m}_2\mathbf{m}_3)_{kls} + \frac{1}{6}\big(m_{1k}m_{1t}\epsilon^{lst} + m_{2l}m_{2t}\epsilon^{skt} + m_{2k}m_{2t}\epsilon^{slt} + m_{1l}m_{1t}\epsilon^{kst}\big)\Big)\\
&= \epsilon^{ijs}(\mathbf{m}_1\mathbf{m}_2\mathbf{m}_3)_{kls} + \frac{1}{6}\Big(m_{1k}m_{1t}(\delta_{it}\delta_{jl} - \delta_{il}\delta_{jt}) + m_{2l}m_{2t}(\delta_{ik}\delta_{jt} - \delta_{it}\delta_{jk})\\
&\quad + m_{2k}m_{2t}(\delta_{il}\delta_{jt} - \delta_{it}\delta_{jl}) + m_{1l}m_{1t}(\delta_{it}\delta_{jk} - \delta_{ik}\delta_{jt})\Big)\\
&= \epsilon^{ijs}(\mathbf{m}_1\mathbf{m}_2\mathbf{m}_3)_{kls} + \frac{1}{6}\Big(\mathcal{B}\big((\mathbf{m}_1^2)_0\big)_{ijkl} + \mathcal{B}\big((\mathbf{m}_2^2)_0\big)_{ijkl}\Big).
\end{aligned}$$

In the above, we have encountered several symmetric traceless tensors. They have the following relations.

$$\begin{aligned}
&(\mathbf{m}_3^2)_0 = -(\mathbf{m}_1^2)_0 - (\mathbf{m}_2^2)_0,\\
&(\mathbf{m}_1^2\mathbf{m}_3^2)_0 = -(\mathbf{m}_1^4)_0 - (\mathbf{m}_1^2\mathbf{m}_2^2)_0,\\
&(\mathbf{m}_2^2\mathbf{m}_3^2)_0 = -(\mathbf{m}_2^4)_0 - (\mathbf{m}_1^2\mathbf{m}_2^2)_0.
\end{aligned}$$

When averaged tensors are considered, the linear relations obtained above still hold. Therefore, we only need to focus on the following tensors that are the linearly independent:

$$\langle(\mathbf{m}_1^2\mathbf{m}_2^2)_0\rangle,\ \langle(\mathbf{m}_1^2\mathbf{m}_3^2)_0\rangle,\ \langle(\mathbf{m}_2^2\mathbf{m}_3^2)_0\rangle,\ \langle(\mathbf{m}_i^2)_0\rangle,\ i = 1,2,3.$$

SM1.3. Expression involving low-order tensors. When $Q_i = Q_i^{(0)}$, we will encounter a few terms only involving second-order tensors, which we provide alternative expressions below. They will be useful for matrix manipulations in the main text, and the discussion afterwards.

Let us look into the last tensor in (SM3.2). Using the relation $\mathfrak{i} = \mathbf{n}_1^2 + \mathbf{n}_2^2 + \mathbf{n}_3^2$, we deduce that

$$\begin{aligned}
&2\delta_{ij}\delta_{kl} - 3\delta_{ik}\delta_{jl} - 3\delta_{il}\delta_{jk}\\
&= 2(\mathbf{n}_1^2 + \mathbf{n}_2^2 + \mathbf{n}_3^2)_{ij}(\mathbf{n}_1^2 + \mathbf{n}_2^2 + \mathbf{n}_3^2)_{kl} - 3(\mathbf{n}_1^2 + \mathbf{n}_2^2 + \mathbf{n}_3^2)_{ik}(\mathbf{n}_1^2 + \mathbf{n}_2^2 + \mathbf{n}_3^2)_{jl}\\
&\quad - 3(\mathbf{n}_1^2 + \mathbf{n}_2^2 + \mathbf{n}_3^2)_{il}(\mathbf{n}_1^2 + \mathbf{n}_2^2 + \mathbf{n}_3^2)_{jk}\\
&= 2\sum_{\alpha\neq\beta}\mathbf{n}_\alpha^2\otimes\mathbf{n}_\beta^2 - 4\sum_{\alpha=1}^{3}\mathbf{n}_\alpha^4\\
&\quad - 12(\mathbf{n}_1\mathbf{n}_2\otimes\mathbf{n}_1\mathbf{n}_2 + \mathbf{n}_1\mathbf{n}_3\otimes\mathbf{n}_1\mathbf{n}_3 + \mathbf{n}_2\mathbf{n}_3\otimes\mathbf{n}_2\mathbf{n}_3),
\end{aligned}$$

where we have used the fact that $\mathbf{n}_1\mathbf{n}_2 = \frac{1}{2}(\mathbf{n}_1 \otimes \mathbf{n}_2 + \mathbf{n}_2 \otimes \mathbf{n}_1)$. The terms in the second line are expressed linearly by $\mathbf{s}_i \otimes \mathbf{s}_j$ We would also like to express the first line in this form. Note that

$$\mathbf{n}_1^2 - \frac{\mathfrak{i}}{3} = \frac{1}{3}(2\mathbf{n}_1^2 - \mathbf{n}_2^2 - \mathbf{n}_3^2). \tag{SM1.30}$$

Thus, fitting with a term $\mathbf{n}^2 - \mathfrak{i}/3$ in (SM1.30) yields

$$\begin{aligned} -9\mathbf{s}_1 \otimes \mathbf{s}_1 =& -9(\mathbf{n}_1^2 - \frac{\mathfrak{i}}{3}) \otimes (\mathbf{n}_1^2 - \frac{\mathfrak{i}}{3}) \\ =& -(2\mathbf{n}_1^2 - \mathbf{n}_2^2 - \mathbf{n}_3^2) \otimes (2\mathbf{n}_1^2 - \mathbf{n}_2^2 - \mathbf{n}_3^2) \\ =& -4\mathbf{n}_1^4 + 2\big(\mathbf{n}_1^2 \otimes (\mathbf{n}_2^2 + \mathbf{n}_3^2) + (\mathbf{n}_2^2 + \mathbf{n}_3^2) \otimes \mathbf{n}_1^2\big) - (\mathbf{n}_2^2 + \mathbf{n}_3^2) \otimes (\mathbf{n}_2^2 + \mathbf{n}_3^2). \end{aligned} \tag{SM1.31}$$

Then the remaining terms are given by

$$\begin{aligned} & -4\mathbf{n}_2^4 - 4\mathbf{n}_3^4 + 2(\mathbf{n}_2^2 \otimes \mathbf{n}_3^2 + \mathbf{n}_3^2 \otimes \mathbf{n}_2^2) + (\mathbf{n}_2^2 + \mathbf{n}_3^2) \otimes (\mathbf{n}_2^2 + \mathbf{n}_3^2) \\ &= -3(\mathbf{n}_2^2 - \mathbf{n}_3^2) \otimes (\mathbf{n}_2^2 - \mathbf{n}_3^2) = -3\mathbf{s}_2 \otimes \mathbf{s}_2. \end{aligned}$$

Therefore, we arrive at

$$2\delta_{ij}\delta_{kl} - 3\delta_{ik}\delta_{jl} - 3\delta_{il}\delta_{jk} = -9\mathbf{s}_1 \otimes \mathbf{s}_1 - 3\mathbf{s}_2 \otimes \mathbf{s}_2 - 12(\mathbf{s}_3 \otimes \mathbf{s}_3 + \mathbf{s}_4 \otimes \mathbf{s}_4 + \mathbf{s}_5 \otimes \mathbf{s}_5), \tag{SM1.32}$$

where the corresponding coordinate X_1 is given by

$$X_1 = \begin{pmatrix} -9 & 0 & & & \\ 0 & -3 & & & \\ & & -12 & & \\ & & & -12 & \\ & & & & -12 \end{pmatrix}.$$

We note that

$$\begin{aligned} \mathbf{s}_2 \otimes \mathbf{s}_2 &= (\mathbf{n}_2^2 - \mathbf{n}_3^2) \otimes (\mathbf{n}_2^2 - \mathbf{n}_3^2) \\ &= \mathbf{n}_2^4 + \mathbf{n}_3^4 - (\mathbf{n}_2^2 \otimes \mathbf{n}_3^2 + \mathbf{n}_3^2 \otimes \mathbf{n}_2^2). \end{aligned} \tag{SM1.33}$$

Then $\mathcal{A}\big((\mathbf{n}_1^2)_0\big)_{ijkl}$ can be calculated as follows:

$$\begin{aligned} \mathcal{A}\big((\mathbf{n}_1^2)_0\big)_{ijkl} =& (\mathbf{n}_1^2 + \mathbf{n}_2^2 + \mathbf{n}_3^2)_{kl}\Big(\mathbf{n}_1^2 - \frac{\mathfrak{i}}{3}\Big)_{ij} + (\mathbf{n}_1^2 + \mathbf{n}_2^2 + \mathbf{n}_3^2)_{ij}\Big(\mathbf{n}_1^2 - \frac{\mathfrak{i}}{3}\Big)_{kl} \\ & - \frac{3}{4}(\mathbf{n}_1^2 + \mathbf{n}_2^2 + \mathbf{n}_3^2)_{ik}\Big(\mathbf{n}_1^2 - \frac{\mathfrak{i}}{3}\Big)_{jl} - \frac{3}{4}(\mathbf{n}_1^2 + \mathbf{n}_2^2 + \mathbf{n}_3^2)_{jl}\Big(\mathbf{n}_1^2 - \frac{\mathfrak{i}}{3}\Big)_{ik} \\ & - \frac{3}{4}(\mathbf{n}_1^2 + \mathbf{n}_2^2 + \mathbf{n}_3^2)_{il}\Big(\mathbf{n}_1^2 - \frac{\mathfrak{i}}{3}\Big)_{jk} - \frac{3}{4}(\mathbf{n}_1^2 + \mathbf{n}_2^2 + \mathbf{n}_3^2)_{jk}\Big(\mathbf{n}_1^2 - \frac{\mathfrak{i}}{3}\Big)_{il} \\ =& \frac{1}{3}\Big((2\mathbf{n}_1^2 - \mathbf{n}_2^2 - \mathbf{n}_3^2) \otimes (\mathbf{n}_1^2 + \mathbf{n}_2^2 + \mathbf{n}_3^2) \\ & + (\mathbf{n}_1^2 + \mathbf{n}_2^2 + \mathbf{n}_3^2) \otimes (2\mathbf{n}_1^2 - \mathbf{n}_2^2 - \mathbf{n}_3^2)\Big) \\ & - (2\mathbf{n}_1^4 - \mathbf{n}_2^4 - \mathbf{n}_3^4) - (\mathbf{n}_1\mathbf{n}_2 \otimes \mathbf{n}_1\mathbf{n}_2 + \mathbf{n}_1\mathbf{n}_3 \otimes \mathbf{n}_1\mathbf{n}_3 - 2\mathbf{n}_2\mathbf{n}_3 \otimes \mathbf{n}_2\mathbf{n}_3), \end{aligned}$$

where we have used the relation $\mathfrak{i} = \mathbf{n}_1^2 + \mathbf{n}_2^2 + \mathbf{n}_3^2$. Using (SM1.31) and (SM1.33), we get

$$\begin{aligned}
&\frac{1}{3}\Big((2\mathbf{n}_1^2 - \mathbf{n}_2^2 - \mathbf{n}_3^2) \otimes (\mathbf{n}_1^2 + \mathbf{n}_2^2 + \mathbf{n}_3^2) + (\mathbf{n}_1^2 + \mathbf{n}_2^2 + \mathbf{n}_3^2) \otimes (2\mathbf{n}_1^2 - \mathbf{n}_2^2 - \mathbf{n}_3^2)\Big) \\
&\quad - (2\mathbf{n}_1^4 - \mathbf{n}_2^4 - \mathbf{n}_3^4) \\
&= \mathbf{n}_2^4 + \mathbf{n}_3^4 + \frac{1}{3}\Big(- 2\mathbf{n}_1^4 + \mathbf{n}_1^2 \otimes (\mathbf{n}_2^2 + \mathbf{n}_3^2) + (\mathbf{n}_2^2 + \mathbf{n}_3^2) \otimes \mathbf{n}_1^2 - 2(\mathbf{n}_2^2 + \mathbf{n}_3^2) \otimes (\mathbf{n}_2^2 + \mathbf{n}_3^2)\Big) \\
&= -\frac{3}{2}(\mathbf{n}_1^2 - \frac{\mathfrak{i}}{3}) \otimes (\mathbf{n}_1^2 - \frac{\mathfrak{i}}{3}) + \frac{1}{2}(\mathbf{n}_2^2 - \mathbf{n}_3^2) \otimes (\mathbf{n}_2^2 - \mathbf{n}_3^2) \\
&= -\frac{3}{2}\mathbf{s}_1 \otimes \mathbf{s}_1 + \frac{1}{2}\mathbf{s}_2 \otimes \mathbf{s}_2.
\end{aligned}$$

Consequently, we obtain

$$\mathcal{A}\big((\mathbf{n}_1^2)_0\big)_{ijkl} = -\frac{3}{2}\mathbf{s}_1 \otimes \mathbf{s}_1 + \frac{1}{2}\mathbf{s}_2 \otimes \mathbf{s}_2 - (\mathbf{s}_3 \otimes \mathbf{s}_3 + \mathbf{s}_4 \otimes \mathbf{s}_4 - 2\mathbf{s}_5 \otimes \mathbf{s}_5), \tag{SM1.34}$$

where the corresponding coordinate X_2 is written by

$$X_2 = \begin{pmatrix} -\frac{3}{2} & 0 & & & \\ 0 & \frac{1}{2} & & & \\ & & -1 & & \\ & & & -1 & \\ & & & & 2 \end{pmatrix}.$$

Next we deal with the term $\mathcal{A}\big(\mathbf{n}_2^2 - \mathbf{n}_3^2\big)_{ijkl}$. Note that

$$\begin{aligned}
\frac{3}{2}(\mathbf{s}_1 \otimes \mathbf{s}_2 + \mathbf{s}_2 \otimes \mathbf{s}_1) &= \frac{3}{2}\Big((\mathbf{n}_1^2 - \frac{\mathfrak{i}}{3}) \otimes (\mathbf{n}_2^2 - \mathbf{n}_3^2) + (\mathbf{n}_2^2 - \mathbf{n}_3^2) \otimes (\mathbf{n}_1^2 - \frac{\mathfrak{i}}{3})\Big) \\
&= -(\mathbf{n}_2^4 - \mathbf{n}_3^4) + (\mathbf{n}_1^2 \otimes \mathbf{n}_2^2 + \mathbf{n}_2^2 \otimes \mathbf{n}_1^2) - (\mathbf{n}_1^2 \otimes \mathbf{n}_3^2 + \mathbf{n}_3^2 \otimes \mathbf{n}_1^2).
\end{aligned}$$

Then, $\mathcal{A}\big(\mathbf{n}_2^2 - \mathbf{n}_3^2\big)_{ijkl}$ can be calculated as

$$\begin{aligned}
\mathcal{A}\big(\mathbf{n}_2^2 - \mathbf{n}_3^2\big)_{ijkl} &= (\mathbf{n}_1^2 + \mathbf{n}_2^2 + \mathbf{n}_3^2)_{kl}(\mathbf{n}_2^2 - \mathbf{n}_3^2)_{ij} + (\mathbf{n}_1^2 + \mathbf{n}_2^2 + \mathbf{n}_3^2)_{ij}(\mathbf{n}_2^2 - \mathbf{n}_3^2)_{kl} \\
&\quad - \frac{3}{4}(\mathbf{n}_1^2 + \mathbf{n}_2^2 + \mathbf{n}_3^2)_{ik}(\mathbf{n}_2^2 - \mathbf{n}_3^2)_{jl} - \frac{3}{4}(\mathbf{n}_1^2 + \mathbf{n}_2^2 + \mathbf{n}_3^2)_{jl}(\mathbf{n}_2^2 - \mathbf{n}_3^2)_{ik} \\
&\quad - \frac{3}{4}(\mathbf{n}_1^2 + \mathbf{n}_2^2 + \mathbf{n}_3^2)_{il}(\mathbf{n}_2^2 - \mathbf{n}_3^2)_{jk} - \frac{3}{4}(\mathbf{n}_1^2 + \mathbf{n}_2^2 + \mathbf{n}_3^2)_{jk}(\mathbf{n}_2^2 - \mathbf{n}_3^2)_{il} \\
&= 2(\mathbf{n}_2^4 - \mathbf{n}_3^4) + (\mathbf{n}_1^2 \otimes \mathbf{n}_2^2 + \mathbf{n}_2^2 \otimes \mathbf{n}_1^2) - (\mathbf{n}_1^2 \otimes \mathbf{n}_3^2 + \mathbf{n}_3^2 \otimes \mathbf{n}_1^2) \\
&\quad - 3\big(\mathbf{n}_2^4 - \mathbf{n}_3^4 + \mathbf{n}_1\mathbf{n}_2 \otimes \mathbf{n}_1\mathbf{n}_2 - \mathbf{n}_1\mathbf{n}_3 \otimes \mathbf{n}_1\mathbf{n}_3\big) \\
&= \frac{3}{2}\Big(\Big(\mathbf{n}_1^2 - \frac{\mathfrak{i}}{3}\Big) \otimes (\mathbf{n}_2^2 - \mathbf{n}_3^2) + (\mathbf{n}_2^2 - \mathbf{n}_3^2) \otimes \Big(\mathbf{n}_1^2 - \frac{\mathfrak{i}}{3}\Big)\Big) \\
&\quad - 3(\mathbf{n}_1\mathbf{n}_2 \otimes \mathbf{n}_1\mathbf{n}_2 - \mathbf{n}_1\mathbf{n}_3 \otimes \mathbf{n}_1\mathbf{n}_3) \\
&= \frac{3}{2}(\mathbf{s}_1 \otimes \mathbf{s}_2 + \mathbf{s}_2 \otimes \mathbf{s}_1) - 3(\mathbf{s}_3 \otimes \mathbf{s}_3 - \mathbf{s}_4 \otimes \mathbf{s}_4),
\end{aligned} \tag{SM1.35}$$

where the corresponding coordinate X_3 is written by

$$X_3 = \begin{pmatrix} 0 & \frac{3}{2} & & & \\ \frac{3}{2} & 0 & & & \\ & & -3 & & \\ & & & 3 & \\ & & & & 0 \end{pmatrix}.$$

SM2. Closure approximation: Theorem 3.3. We discuss Theorem 3.3 that recognizes the form of high-order tensors. Theorem 3.3 is stated for the original entropy and the quasi-entropy. So we need to consider them separately.

Theorem 3.3 is actually a special case in previous works: for the original entropy, it is a special case of Theorem 5.2 in [SM2]; for quasi-entropy, it is a special case of Theorem 4.8 in [SM3]. Nevertheless, both of them were shown for general cases of symmetry and the explicit form (3.22) is not provided. For this reason, we shall explain how those theorems are applied to the current work to obtain Theorem 3.3, and at places show some results.

SM2.1. Original entropy. We first discuss the closure by the original entropy. The following result has been shown in Appendix in [SM4].

LEMMA SM2.1. *If s_i, b_i satisfy* (3.20)*, then there exists a unique density function*

$$\rho(\mathfrak{q}) = \frac{1}{Z}\exp\left(\sum_{i,j=1,2}\lambda_{ij}(\mathbf{m}_i\cdot\mathbf{n}_j)^2\right),$$

such that $\langle(\mathbf{m}_i^2)_0\rangle = s_i(\mathbf{n}_1^2)_0 + b_i(\mathbf{n}_2^2-\mathbf{n}_3^2)$. It minimizes $\int_{SO(3)}\rho\ln\rho\mathrm{d}\mathfrak{q}$ when Q_i is fixed.

Recall that $\mathfrak{q} = (\mathbf{m}_1, \mathbf{m}_2, \mathbf{m}_3)$ and $\mathfrak{p} = (\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3)$. The density function satisfies $\rho(\mathfrak{p}\mathfrak{b}_k\mathfrak{p}^T\mathfrak{q}) = \rho(\mathfrak{q})$ for $k = 1, 2, 3$. This can be seen by noticing that $\mathbf{m}_i\cdot\mathbf{n}_j$ is the (j, i) element of $\mathfrak{p}^T\mathfrak{q}$. Thus, when $\mathfrak{q}$ is replaced by $\mathfrak{p}\mathfrak{b}_k\mathfrak{p}^T\mathfrak{q}$, the dot product $\mathbf{m}_i\cdot\mathbf{n}_j$ becomes the (j, i) element of $\mathfrak{p}^T(\mathfrak{p}\mathfrak{b}_k\mathfrak{p}^T\mathfrak{q}) = \mathfrak{b}_k\mathfrak{p}^T\mathfrak{q} = (\mathfrak{p}\mathfrak{b}_k^T)^T\mathfrak{q}$. It suffices to notice the equalities like $\mathfrak{p}\mathfrak{b}_1^T = (\mathbf{n}_1, -\mathbf{n}_2, -\mathbf{n}_3)$.

By Theorem 5.2 in [SM2] and the related discussions before the theorem, when an nth-order symmetric traceless tensor is calculated from the density function above, it could be expressed as $W(\mathfrak{p})$ for some $W \in \mathbb{A}^{\mathscr{D}_2,n}$. Using the decomposition written down in (SM1.1), we arrive at the expression in Theorem 3.3.

The positive-definiteness of the averaged tensors $\mathcal{R}_i$ in (4.1) is obvious because they are calculated from a positive density function.

SM2.2. Quasi-entropy. To illustrate some ideas, let us start from the second-order quasi-entropy Ξ_2. Denote by $\mathbf{r}_1$ the vector formed by 1 and $\mathbf{m}_i\cdot\mathbf{n}_j$, $1 \le i, j \le 3$, which is a 10×1 vector. For a first-order tensor U, we define a row vector as

$$\Phi_1(U)_j = (U\cdot\mathbf{n}_j).$$

For a second-order tensor U, we define a matrix as

$$\Psi_2(U)_{ij} = (U\cdot\mathbf{n}_i\otimes\mathbf{n}_j). \tag{SM2.1}$$

The general second-order quasi-entropy, denoted by $\widetilde{\Xi}_2$, is defined as the minus log-determinant of the second moment of $\mathbf{r}_1$ (hereafter we omit the free parameter ν introduced in (3.17)),

(SM2.2)
$$\begin{aligned}\widetilde{\Xi}_2 =& -\ln\det\langle\mathbf{r}_1\mathbf{r}_1^T\rangle\\ =& -\ln\det\begin{pmatrix} 1 & \Phi_1(\langle\mathbf{m}_1\rangle) & \Phi_1(\langle\mathbf{m}_2\rangle) & \Phi_1(\langle\mathbf{m}_3\rangle)\\ \Phi_1(\langle\mathbf{m}_1\rangle)^T & \Psi_2(\langle\mathbf{m}_1^2\rangle) & \Psi_2(\langle\mathbf{m}_1\otimes\mathbf{m}_2\rangle) & \Psi_2(\langle\mathbf{m}_1\otimes\mathbf{m}_3\rangle)\\ \Phi_1(\langle\mathbf{m}_2\rangle)^T & \Psi_2(\langle\mathbf{m}_2\otimes\mathbf{m}_1\rangle) & \Psi_2(\langle\mathbf{m}_2^2\rangle) & \Psi_2(\langle\mathbf{m}_2\otimes\mathbf{m}_3\rangle)\\ \Phi_1(\langle\mathbf{m}_3\rangle)^T & \Psi_2(\langle\mathbf{m}_3\otimes\mathbf{m}_1\rangle) & \Psi_2(\langle\mathbf{m}_3\otimes\mathbf{m}_2\rangle) & \Psi_2(\langle\mathbf{m}_3^2\rangle)\end{pmatrix}.\end{aligned}$$

In [SM3], the second moment of $\mathbf{r}_1$ is replaced by the covariance matrix of the 9×1 vector formed by the last nine components of $\mathbf{r}_1$. It can be seen that these two formulations are equivalent.

Here, we need to emphasize that the notation $\langle\cdot\rangle$ does not assume that they are averaged by certain positive density function, but only implies that the tensors obey linear relations such as what we have obtained in Appendix SM1.2. For second-order tensors not symmetric, we express them using symmetric traceless tensors, such as $\langle\mathbf{m}_1\otimes\mathbf{m}_2\rangle_{ij} = \langle\mathbf{m}_1\mathbf{m}_2\rangle_{ij} + \epsilon^{ijk}\langle\mathbf{m}_3\rangle_k$. Thus, $\widetilde{\Xi}_2$ is a function of symmetric traceless tensors up to second order. If we choose a basis of symmetric traceless tensors, their 'average' are independent variables in $\widetilde{\Xi}_2$.

Now, for our problem, the tensors specified are Q_1 and Q_2, which determine $\langle\mathbf{m}_1^2\rangle = Q_1 + \mathfrak{i}/3$, $\langle\mathbf{m}_2^2\rangle = Q_2 + \mathfrak{i}/3$, $\langle\mathbf{m}_3^2\rangle = -Q_1 - Q_2 + \mathfrak{i}/3$. To obtain the quasi-entropy Ξ_2 about Q_1 and Q_2 only, we shall minimize $\widetilde{\Xi}_2$ with Q_1 and Q_2 fixed. At the minimizer many tensors vanish, because we have the following lemma.

Lemma SM2.2. *For a symmetric positive-definite matrix K, suppose that it is given in blocks as*

(SM2.3)
$$K = \begin{pmatrix} K_1 & A\\ A^T & K_2\end{pmatrix}.$$

Then we have

(SM2.4)
$$\det K \le \det K_1 \det K_2.$$

The equality holds if and only if $A = 0$.

Notice that off-diagonal blocks are functions of $\langle\mathbf{m}_i\rangle$ and $\langle\mathbf{m}_i\mathbf{m}_j\rangle$ for $i\neq j$, which are independent of Q_1 and Q_2. Using this lemma, we immediately deduce that the minimizer is attained when all the off-diagonal blocks are zero. In this way, we obtain the quasi-entropy Ξ_2 in (3.17).

It is worthy noting that for Q_1 and Q_2, $\mathbf{m}_1^2 - \mathfrak{i}/3$ and $\mathbf{m}_2^2 - \mathfrak{i}/3$ are invariant under $\mathscr{D}_2$. On the other hand, the off-diagonal blocks vanish when averaged over $\mathscr{D}_2$, since in these blocks the times of $\mathbf{m}_1$, $\mathbf{m}_2$, $\mathbf{m}_3$ appearing are not all odd or not all even. This result actually holds for quasi-entropy up to arbitrary order, as indicated by Theorem 4.8 in [SM3].

The ideas above are also useful when discussing the fourth-order quasi-entropy Ξ_4. Denote by $\mathbf{r}_2$ the vector formed by 1, $\mathbf{m}_i\cdot\mathbf{n}_j$, $1\le i,j\le 3$ and $\mathbf{S}_i\cdot\mathbf{s}_j$ $1\le i,j\le 5$, which has the size 35×1. The fourth-order quasi-entropy is defined as the minus log-determinant of $\langle\mathbf{r}_2\mathbf{r}_2^T\rangle$. It is a function of symmetric traceless tensors up to fourth order.

The closure approximation minimizes the quasi-entropy with Q_1 and Q_2 fixed. Still, if the times of $\mathbf{m}_1$, $\mathbf{m}_2$, $\mathbf{m}_3$ are not all odd or not all even, then the tensor vanishes when averaged over $\mathscr{D}_2$. Theorem 4.8 in [SM3] guarantees that when seeking the minimizer with Q_1 and Q_2 fixed, these tensors are zero. After setting these tensors as zero in the quasi-entropy, we could get a reduced expression, which we write down below.

For a second-order tensor U, we define a 1×5 row vector as

$$\Phi_2(U)_j = (U\cdot \mathbf{s}_j).$$

For a third-order tensor U, we define a 3×5 matrix,

$$\Psi_3(U)_{ij} = (U\cdot \mathbf{n}_i\otimes \mathbf{s}_j).$$

For a fourth order tensor U, we define a 5×5 matrix,

$$\Psi_4(U)_{ij} = (U\cdot \mathbf{s}_i\otimes \mathbf{s}_j).$$

The reduced quasi-entropy is given by

$$\begin{aligned}
&\Xi_4 = \\
&-\ln\det\begin{pmatrix} 1 & \Phi_2(\langle \mathbf{m}_1^2-\frac{\mathrm{i}}{3}\rangle) & \Phi_2(\langle \mathbf{m}_2^2-\mathbf{m}_3^2\rangle) \\ \Phi_2(\langle \mathbf{m}_1^2-\frac{\mathrm{i}}{3}\rangle)^T & \Psi_4\big(\langle(\mathbf{m}_1^2-\frac{\mathrm{i}}{3})\otimes(\mathbf{m}_1^2-\frac{\mathrm{i}}{3})\rangle\big) & \Psi_4\big(\langle(\mathbf{m}_2^2-\mathbf{m}_3^2)\otimes(\mathbf{m}_1^2-\frac{\mathrm{i}}{3})\rangle\big) \\ \Phi_2(\langle \mathbf{m}_2^2-\mathbf{m}_3^2\rangle)^T & \Psi_4\big(\langle(\mathbf{m}_2^2-\mathbf{m}_3^2)\otimes(\mathbf{m}_1^2-\frac{\mathrm{i}}{3})\rangle\big)^T & \Psi_4\big(\langle(\mathbf{m}_2^2-\mathbf{m}_3^2)\otimes(\mathbf{m}_2^2-\mathbf{m}_3^2)\rangle\big) \end{pmatrix} \\
&-\ln\det\begin{pmatrix} \Psi_2(\langle \mathbf{m}_1^2\rangle) & \Psi_3(\langle \mathbf{m}_1\otimes\mathbf{m}_2\mathbf{m}_3\rangle) \\ \Psi_3(\langle \mathbf{m}_1\otimes\mathbf{m}_2\mathbf{m}_3\rangle)^T & \Psi_4(\langle \mathbf{m}_2\mathbf{m}_3\otimes\mathbf{m}_2\mathbf{m}_3\rangle) \end{pmatrix} \\
&-\ln\det\begin{pmatrix} \Psi_2(\langle \mathbf{m}_2^2\rangle) & \Psi_3(\langle \mathbf{m}_2\otimes\mathbf{m}_1\mathbf{m}_3\rangle) \\ \Psi_3(\langle \mathbf{m}_2\otimes\mathbf{m}_1\mathbf{m}_3\rangle)^T & \Psi_4(\langle \mathbf{m}_1\mathbf{m}_3\otimes\mathbf{m}_1\mathbf{m}_3\rangle) \end{pmatrix} \\
&-\ln\det\begin{pmatrix} \Psi_2(\langle \mathbf{m}_3^2\rangle) & \Psi_3(\langle \mathbf{m}_3\otimes\mathbf{m}_1\mathbf{m}_2\rangle) \\ \Psi_3(\langle \mathbf{m}_3\otimes\mathbf{m}_1\mathbf{m}_2\rangle)^T & \Psi_4(\langle \mathbf{m}_1\mathbf{m}_2\otimes\mathbf{m}_1\mathbf{m}_2\rangle) \end{pmatrix}.
\end{aligned} \tag{SM2.5}$$

The first matrix is 11×11, while the other three are 8×8. The blocks can be expressed by symmetric traceless tensors as we have calculated in Appendix SM1.2.

The quasi-entropy Ξ_4 is defined on the domain such that the four matrices in Ξ_4 are positive definite. Thus, we conclude that if the high-order tensors are calculated from the constrained minimization of Ξ_4, the tensors $\mathcal{R}_i$ in (4.4) are positive definite in the sense of (4.10). This is because that many of $\mathcal{R}_1,\mathcal{R}_3,\mathcal{R}_4,\mathcal{R}_5$ are diagonal blocks of Ξ_4, and for $\mathcal{R}_2$ we use (SM1.23).

Now, let us assume that Q_i has the biaxial form (3.18). First, we claim that the domain of quasi-entropy Ξ_4 is not empty when s_i,b_i are fixed with the conditions (3.20). This is because that the high-order tensors calculated from any positive density function must make the covariance matrix positive definite. Such a density function exists because of Lemma SM2.1.

We are now ready to show Theorem 3.3. By (SM1.25)–(SM1.27), (SM1.32), (SM1.34) and (SM1.35), the zeroth- and second-order tensors could fill the following entries in the quasi-entropy. In the 11×11 matrix, they are labelled as

$$\left(\begin{array}{c|ccccc|ccccc}
1 & * & * & & & & * & * & & & \\
\hline
* & * & * & & & & * & * & & & \\
* & * & * & & & & * & * & & & \\
 & & & * & & & & & * & & \\
 & & & & * & & & & & * & \\
 & & & & & * & & & & & * \\
\hline
* & * & * & & & & * & * & & & \\
* & * & * & & & & * & * & & & \\
 & & & * & & & & & * & & \\
 & & & & * & & & & & * & \\
 & & & & & * & & & & & *
\end{array}\right). \tag{SM2.6}$$

In the three 8×8 matrices, they are labelled as

$$\left(\begin{array}{ccc|ccccc}
* & & & & & & & * \\
 & * & & & & & * & \\
 & & * & & & * & & \\
\hline
 & & & * & * & & & \\
 & & & * & * & & & \\
 & & * & & & * & & \\
 & * & & & & & * & \\
* & & & & & & & *
\end{array}\right). \tag{SM2.7}$$

The third-order and fourth-order symmetric traceless tensors are expressed by the bases,

$$\begin{aligned}
\langle \mathbf{m}_1\mathbf{m}_2\mathbf{m}_3 \rangle &= z\mathbf{n}_1\mathbf{n}_2\mathbf{n}_3 + z_1'(\mathbf{n}_1^3)_0 + z_2'(\mathbf{n}_1^2\mathbf{n}_2)_0 + z_3'(\mathbf{n}_1\mathbf{n}_2^2)_0 \\
&\quad + z_4'(\mathbf{n}_2^3)_0 + z_5'(\mathbf{n}_1^2\mathbf{n}_3)_0 + z_6'(\mathbf{n}_2^2\mathbf{n}_3)_0, \\
\langle (\mathbf{m}_1^4)_0 \rangle &= a_1(\mathbf{n}_1^4)_0 + a_2(\mathbf{n}_2^4)_0 + a_3(\mathbf{n}_1^2\mathbf{n}_2^2)_0 \\
&\quad + a_4(\mathbf{n}_1^3\mathbf{n}_2)_0 + a_5(\mathbf{n}_1^3\mathbf{n}_3)_0 + a_6(\mathbf{n}_1^2\mathbf{n}_2\mathbf{n}_3)_0 \\
&\quad + a_7(\mathbf{n}_1\mathbf{n}_2^3)_0 + a_8(\mathbf{n}_1\mathbf{n}_2^2\mathbf{n}_3)_0 + a_9(\mathbf{n}_2^3\mathbf{n}_3)_0, \\
\langle (\mathbf{m}_2^4)_0 \rangle &= \tilde{a}_1(\mathbf{n}_1^4)_0 + \tilde{a}_2(\mathbf{n}_2^4)_0 + \tilde{a}_3(\mathbf{n}_1^2\mathbf{n}_2^2)_0 \\
&\quad + \tilde{a}_4(\mathbf{n}_1^3\mathbf{n}_2)_0 + \tilde{a}_5(\mathbf{n}_1^3\mathbf{n}_3)_0 + \tilde{a}_6(\mathbf{n}_1^2\mathbf{n}_2\mathbf{n}_3)_0 \\
&\quad + \tilde{a}_7(\mathbf{n}_1\mathbf{n}_2^3)_0 + \tilde{a}_8(\mathbf{n}_1\mathbf{n}_2^2\mathbf{n}_3)_0 + \tilde{a}_9(\mathbf{n}_2^3\mathbf{n}_3)_0, \\
\langle (\mathbf{m}_1^2\mathbf{m}_2^2)_0 \rangle &= \bar{a}_1(\mathbf{n}_1^4)_0 + \bar{a}_2(\mathbf{n}_2^4)_0 + \bar{a}_3(\mathbf{n}_1^2\mathbf{n}_2^2)_0 \\
&\quad + \bar{a}_4(\mathbf{n}_1^3\mathbf{n}_2)_0 + \bar{a}_5(\mathbf{n}_1^3\mathbf{n}_3)_0 + \bar{a}_6(\mathbf{n}_1^2\mathbf{n}_2\mathbf{n}_3)_0 \\
&\quad + \bar{a}_7(\mathbf{n}_1\mathbf{n}_2^3)_0 + \bar{a}_8(\mathbf{n}_1\mathbf{n}_2^2\mathbf{n}_3)_0 + \bar{a}_9(\mathbf{n}_2^3\mathbf{n}_3)_0.
\end{aligned} \tag{SM2.8}$$

Using (SM1.3)–(SM1.6), the terms $a_i, \tilde{a}_i, \bar{a}_i$ for $i = 1, 2, 3$ and z contribute only to the starred entries, while the terms z_i' and $a_j, \tilde{a}_j, \bar{a}_j$ for $4 \le j \le 9$ contribute only to the non-starred entries. Meanwhile, as long as the starred entries form a positive definite matrix, the determinant reaches its unique maximum when the non-starred entries are zero. This can be observed by rearranging the rows and columns of the four matrices in Ξ_4. In the 11×11 matrix, we group the indices as $\{1, 2, 3, 7, 8\}$, $\{4, 9\}$, $\{5, 10\}$ and $\{6, 11\}$. In the three 8×8 matrices, we group the indices as $\{1, 8\}$, $\{2, 7\}$, $\{3, 6\}$, $\{4, 5\}$. After rearrangement, these matrices become block diagonal. Thus, the determinant must be no less than that the off-diagonal blocks are zero. Therefore, at the minimizer of Ξ_4 we must have $z_i' = 0$ and $a_i = \tilde{a}_i = \bar{a}_i = 0$, $i = 4, \cdots, 9$.

SM3. Explicit expression with biaxial Q_i. Next, we calculate the blocks in (SM2.2) when the tensors take (3.22). They also give the matrices in Section 4.3.

Using (3.22) and the average of (SM1.14) with respect to the density function, we derive that

$$\begin{aligned}
&\langle \mathbf{m}_1\mathbf{m}_2 \otimes \mathbf{m}_1\mathbf{m}_2\rangle_{ijkl}\\
&\quad = \big(\bar{a}_1(\mathbf{n}_1^4)_0 + \bar{a}_2(\mathbf{n}_2^4)_0 + \bar{a}_3(\mathbf{n}_1^2\mathbf{n}_2^2)_0\big)_{ijkl} - \frac{1}{7}\mathcal{A}\big(Q_1^{(0)} + Q_2^{(0)}\big)_{ijkl}\\
&\qquad - \frac{1}{60}(2\delta_{ij}\delta_{kl} - 3\delta_{ik}\delta_{jl} - 3\delta_{il}\delta_{jk})\\
&\quad = \big(\bar{a}_1(\mathbf{n}_1^4)_0 + \bar{a}_2(\mathbf{n}_2^4)_0 + \bar{a}_3(\mathbf{n}_1^2\mathbf{n}_2^2)_0\big)_{ijkl} - \frac{1}{7}\Big((s_1+s_2)\mathcal{A}\big((\mathbf{n}_1^2)_0\big)_{ijkl}\\
&\qquad + (b_1+b_2)\mathcal{A}\big(\mathbf{n}_2^2 - \mathbf{n}_3^2\big)_{ijkl}\Big) - \frac{1}{60}(2\delta_{ij}\delta_{kl} - 3\delta_{ik}\delta_{jl} - 3\delta_{il}\delta_{jk}).
\end{aligned} \tag{SM3.1}$$

From here, we can see that we shall need to express the six tensors below in the basis of $\mathbf{s}_i \otimes \mathbf{s}_j$,

$$2\delta_{ij}\delta_{kl} - 3\delta_{ik}\delta_{jl} - 3\delta_{il}\delta_{jk},\ \mathcal{A}\big((\mathbf{n}_1^2)_0\big)_{ijkl},\ \mathcal{A}\big(\mathbf{n}_2^2 - \mathbf{n}_3^2\big)_{ijkl},\ (\mathbf{n}_1^4)_0,\ (\mathbf{n}_2^4)_0,\ (\mathbf{n}_1^2\mathbf{n}_2^2)_0. \tag{SM3.2}$$

Actually, we will see that they only have the following terms:

$$\mathbf{s}_1\otimes\mathbf{s}_1,\quad \mathbf{s}_1\otimes\mathbf{s}_2,\quad \mathbf{s}_2\otimes\mathbf{s}_1,\quad \mathbf{s}_2\otimes\mathbf{s}_2,\quad \mathbf{s}_3\otimes\mathbf{s}_3,\quad \mathbf{s}_4\otimes\mathbf{s}_4,\quad \mathbf{s}_5\otimes\mathbf{s}_5.$$

The first three tensors in (SM3.2) have been discussed in Appendix SM1.3. In what follows, we calculate the other three tensors.

For the calculation of the term $(\mathbf{n}_1^4)_0$, employing (SM1.33) and the following equality

$$2\sum_{\alpha\neq\beta}\mathbf{n}_\alpha^2\otimes\mathbf{n}_\beta^2 - 4\sum_{\alpha=1}^{3}\mathbf{n}_\alpha^4 = -9\mathbf{s}_1\otimes\mathbf{s}_1 - 3\mathbf{s}_2\otimes\mathbf{s}_2, \tag{SM3.3}$$

we deduce that

$$\begin{aligned}
(\mathbf{n}_1^4)_0 &= \mathbf{n}_1^4 - \frac{6}{7}\mathbf{n}_1^2\mathbf{i} + \frac{3}{35}\mathbf{i}^2\\
&= \mathbf{n}_1^4 - \frac{1}{7}\Big(n_{1i}n_{1j}\delta_{kl} + n_{1i}n_{1k}\delta_{jl} + n_{1i}n_{1l}\delta_{jk} + n_{1j}n_{1k}\delta_{il} + n_{1j}n_{1l}\delta_{ik} + n_{1k}n_{1l}\delta_{ij}\Big)\\
&\quad + \frac{1}{35}\big(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\big)\\
&= \frac{1}{7}\Big(\mathbf{n}_1^4 - (\mathbf{n}_1^2\otimes\mathbf{n}_2^2 + \mathbf{n}_2^2\otimes\mathbf{n}_1^2 + \mathbf{n}_1^2\otimes\mathbf{n}_3^2 + \mathbf{n}_3^2\otimes\mathbf{n}_1^2)\\
&\quad - 4(\mathbf{n}_1\mathbf{n}_2\otimes\mathbf{n}_1\mathbf{n}_2 + \mathbf{n}_1\mathbf{n}_3\otimes\mathbf{n}_1\mathbf{n}_3)\Big)\\
&\quad + \frac{1}{35}\Bigg(\sum_{\alpha\neq\beta}\mathbf{n}_\alpha^2\otimes\mathbf{n}_\beta^2 + 3\sum_{\alpha=1}^{3}\mathbf{n}_\alpha^4 + 4(\mathbf{n}_1\mathbf{n}_2\otimes\mathbf{n}_1\mathbf{n}_2\\
&\quad + \mathbf{n}_1\mathbf{n}_3\otimes\mathbf{n}_1\mathbf{n}_3 + \mathbf{n}_2\mathbf{n}_3\otimes\mathbf{n}_2\mathbf{n}_3)\Bigg)\\
&= \frac{18}{35}\mathbf{s}_1\otimes\mathbf{s}_1 + \frac{1}{35}\mathbf{s}_2\otimes\mathbf{s}_2 - \frac{16}{35}(\mathbf{s}_3\otimes\mathbf{s}_3 + \mathbf{s}_4\otimes\mathbf{s}_4) + \frac{4}{35}\mathbf{s}_5\otimes\mathbf{s}_5,
\end{aligned} \tag{SM3.4}$$

where the corresponding matrix X_4 is given by

$$X_4 = \begin{pmatrix} \frac{18}{35} & 0 & & & \\ 0 & \frac{1}{35} & & & \\ & & -\frac{16}{35} & & \\ & & & -\frac{16}{35} & \\ & & & & \frac{4}{35} \end{pmatrix}.$$

Similarly, from (SM3.3) and (SM1.33), we derive that

(SM3.5)

$$\begin{aligned}
(\mathbf{n}_2^4)_0 =& \mathbf{n}_2^4 - \frac{6}{7}\mathbf{n}_2^2\mathbf{i} + \frac{3}{35}\mathbf{i}^2 \\
=& \mathbf{n}_2^4 - \frac{1}{7}\Big(n_{2i}n_{2j}\delta_{kl} + n_{2i}n_{2k}\delta_{jl} + n_{2i}n_{2l}\delta_{jk} + n_{2j}n_{2k}\delta_{il} + n_{2j}n_{2l}\delta_{ik} + n_{2k}n_{2l}\delta_{ij}\Big) \\
&+ \frac{1}{35}\big(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\big) \\
=& \frac{1}{7}\Big(\mathbf{n}_2^4 - (\mathbf{n}_1^2 \otimes \mathbf{n}_2^2 + \mathbf{n}_2^2 \otimes \mathbf{n}_1^2 + \mathbf{n}_2^2 \otimes \mathbf{n}_3^2 + \mathbf{n}_3^2 \otimes \mathbf{n}_2^2) \\
&- 4(\mathbf{n}_1\mathbf{n}_2 \otimes \mathbf{n}_1\mathbf{n}_2 + \mathbf{n}_2\mathbf{n}_3 \otimes \mathbf{n}_2\mathbf{n}_3)\Big) \\
&+ \frac{1}{35}\Bigg(\sum_{\alpha\neq\beta} \mathbf{n}_\alpha^2 \otimes \mathbf{n}_\beta^2 + 3\sum_{\alpha=1}^{3} \mathbf{n}_\alpha^4 \\
&+ 4(\mathbf{n}_1\mathbf{n}_2 \otimes \mathbf{n}_1\mathbf{n}_2 + \mathbf{n}_1\mathbf{n}_3 \otimes \mathbf{n}_1\mathbf{n}_3 + \mathbf{n}_2\mathbf{n}_3 \otimes \mathbf{n}_2\mathbf{n}_3)\Bigg) \\
=& \frac{27}{140}\mathbf{s}_1 \otimes \mathbf{s}_1 + \frac{19}{140}\mathbf{s}_2 \otimes \mathbf{s}_2 - \frac{3}{28}(\mathbf{s}_1 \otimes \mathbf{s}_2 + \mathbf{s}_2 \otimes \mathbf{s}_1) \\
&- \frac{16}{35}(\mathbf{s}_3 \otimes \mathbf{s}_3 + \mathbf{s}_5 \otimes \mathbf{s}_5) + \frac{4}{35}\mathbf{s}_4 \otimes \mathbf{s}_4,
\end{aligned}$$

where the corresponding matrix X_5 is given by

$$X_5 = \begin{pmatrix} \frac{27}{140} & -\frac{3}{28} & & & \\ -\frac{3}{28} & \frac{19}{140} & & & \\ & & -\frac{16}{35} & & \\ & & & \frac{4}{35} & \\ & & & & -\frac{16}{35} \end{pmatrix}.$$

We may now proceed to deal with the term $(\mathbf{n}_1^2\mathbf{n}_2^2)_0$. Analogously, we have

$$\begin{aligned}
(\mathbf{n}_1^2\mathbf{n}_2^2)_0 =& \mathbf{n}_1^2\mathbf{n}_2^2 - \frac{1}{7}(\mathbf{n}_1^2 + \mathbf{n}_2^2)\mathbf{i} + \frac{1}{35}\mathbf{i}^2 \\
=& \frac{1}{6}\Big(n_{1i}n_{1j}n_{2k}n_{2l} + n_{1i}n_{2j}n_{1k}n_{2l} + n_{1i}n_{2j}n_{2k}n_{1l} \\
&+ n_{2i}n_{1j}n_{1k}n_{2l} + n_{2i}n_{1j}n_{2k}n_{1l} + n_{2i}n_{2j}n_{1k}n_{1l}\Big) \\
&- \frac{1}{42}\Big(n_{1i}n_{1j}\delta_{kl} + n_{1i}n_{1k}\delta_{jl}
\end{aligned}$$

$$
\begin{aligned}
&+ n_{1i}n_{1l}\delta_{jk} + n_{1j}n_{1k}\delta_{il} + n_{1j}n_{1l}\delta_{ik} + n_{1k}n_{1l}\delta_{ij}\Big) \\
&- \frac{1}{42}\Big(n_{2i}n_{2j}\delta_{kl} + n_{2i}n_{2k}\delta_{jl} \\
&+ n_{2i}n_{2l}\delta_{jk} + n_{2j}n_{2k}\delta_{il} + n_{2j}n_{2l}\delta_{ik} + n_{2k}n_{2l}\delta_{ij}\Big) \\
&+ \frac{1}{105}\big(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\big) \\
=& \frac{1}{6}\big(\mathbf{n}_1^2 \otimes \mathbf{n}_2^2 + \mathbf{n}_2^2 \otimes \mathbf{n}_1^2 + 4\mathbf{n}_1\mathbf{n}_2 \otimes \mathbf{n}_1\mathbf{n}_2\big) \\
&- \frac{1}{42}\Bigg(6\mathbf{n}_1^4 + \sum_{\alpha\neq\beta} \mathbf{n}_\alpha^2 \otimes \mathbf{n}_\beta^2 - (\mathbf{n}_2^2 \otimes \mathbf{n}_3^2 + \mathbf{n}_3^2 \otimes \mathbf{n}_2^2) \\
&+ 4(\mathbf{n}_1\mathbf{n}_2 \otimes \mathbf{n}_1\mathbf{n}_2 + \mathbf{n}_1\mathbf{n}_3 \otimes \mathbf{n}_1\mathbf{n}_3)\Bigg) \\
&- \frac{1}{42}\Bigg(6\mathbf{n}_2^4 + \sum_{\alpha\neq\beta} \mathbf{n}_\alpha^2 \otimes \mathbf{n}_\beta^2 - (\mathbf{n}_1^2 \otimes \mathbf{n}_3^2 + \mathbf{n}_3^2 \otimes \mathbf{n}_1^2) \\
&+ 4(\mathbf{n}_1\mathbf{n}_2 \otimes \mathbf{n}_1\mathbf{n}_2 + \mathbf{n}_2\mathbf{n}_3 \otimes \mathbf{n}_2\mathbf{n}_3)\Bigg) \\
&+ \frac{1}{105}\Bigg(\sum_{\alpha\neq\beta} \mathbf{n}_\alpha^2 \otimes \mathbf{n}_\beta^2 + 3\sum_{\alpha=1}^{3} \mathbf{n}_\alpha^4 \\
&+ 4(\mathbf{n}_1\mathbf{n}_2 \otimes \mathbf{n}_1\mathbf{n}_2 + \mathbf{n}_1\mathbf{n}_3 \otimes \mathbf{n}_1\mathbf{n}_3 + \mathbf{n}_2\mathbf{n}_3 \otimes \mathbf{n}_2\mathbf{n}_3)\Bigg) \\
=& -\frac{9}{35}\mathbf{s}_1 \otimes \mathbf{s}_1 - \frac{1}{70}\mathbf{s}_2 \otimes \mathbf{s}_2 + \frac{3}{28}(\mathbf{s}_1 \otimes \mathbf{s}_2 + \mathbf{s}_2 \otimes \mathbf{s}_1) \\
&+ \frac{18}{35}\mathbf{s}_3 \otimes \mathbf{s}_3 - \frac{2}{35}(\mathbf{s}_4 \otimes \mathbf{s}_4 + \mathbf{s}_5 \otimes \mathbf{s}_5), \qquad \text{(SM3.6)}
\end{aligned}
$$

where the corresponding matrix X_6 is given by

$$
X_6 = \begin{pmatrix} -\frac{9}{35} & \frac{3}{28} & & & \\ \frac{3}{28} & -\frac{1}{70} & & & \\ & & \frac{18}{35} & & \\ & & & -\frac{2}{35} & \\ & & & & -\frac{2}{35} \end{pmatrix}.
$$

A direct calculation leads to

$$
\epsilon^{ilt}(\mathbf{n}_1\mathbf{n}_2\mathbf{n}_3)_{jkt} + \epsilon^{jkt}(\mathbf{n}_1\mathbf{n}_2\mathbf{n}_3)_{ilt} = \frac{3}{2}(\mathbf{s}_1 \otimes \mathbf{s}_2 - \mathbf{s}_2 \otimes \mathbf{s}_1), \qquad \text{(SM3.7)}
$$

where the associated coefficient matrix Π is given by

$$
\Pi = \begin{pmatrix} 0 & \frac{3}{2} & & & \\ -\frac{3}{2} & 0 & & & \\ & & 0 & & \\ & & & 0 & \\ & & & & 0 \end{pmatrix}. \qquad \text{(SM3.8)}
$$

Based on the above calculations, we immediately give the expressions of $\mathcal{R}_i^{(0)}(i = 1,\cdots,6)$ under the basis $\mathbf{s}_i\otimes\mathbf{s}_j$. Using (3.22) and the averages of (SM1.9) with respect to the density function, we deduce that

$$\begin{aligned}\mathcal{R}_1^{(0)} =& \Big\langle\Big(\mathbf{m}_1^2-\frac{1}{3}\mathfrak{i}\Big)\otimes\Big(\mathbf{m}_1^2-\frac{1}{3}\mathfrak{i}\Big)\Big\rangle_{ijkl}\\ =&\big\langle(\mathbf{m}_1^4)_0\big\rangle_{ijkl}-\frac{4}{21}\mathcal{A}\big(Q_1^{(0)}\big)_{ijkl}-\frac{1}{45}(2\delta_{ij}\delta_{kl}-3\delta_{ik}\delta_{jl}-3\delta_{il}\delta_{jk}).\end{aligned}$$

In the light of Theorem 3.3, and from (SM1.32), (SM3.4)-(SM3.6), we deduce that

$$\begin{aligned}\mathcal{R}_1^{(0)} =& a_1(\mathbf{n}_1^4)_0+a_2(\mathbf{n}_2^4)_0+a_3(\mathbf{n}_1^2\mathbf{n}_2^2)_0-\frac{4}{21}\Big(s_1\mathcal{A}\big((\mathbf{n}_1^2)_0\big)_{ijkl}+b_1\mathcal{A}\big(\mathbf{n}_2^2-\mathbf{n}_3^2\big)_{ijkl}\Big)\\ &-\frac{1}{45}(2\delta_{ij}\delta_{kl}-3\delta_{ik}\delta_{jl}-3\delta_{il}\delta_{jk}),\end{aligned}\tag{SM3.9}$$

for which the matrix R_1 is written as

$$R_1 = -\frac{1}{45}X_1-\frac{4}{21}(s_1X_2+b_1X_3)+a_1X_4+a_2X_5+a_3X_6.\tag{SM3.10}$$

Similarly, for $\mathcal{R}_2^{(0)}$, it follows that

$$\begin{aligned}\mathcal{R}_2^{(0)} =& \Big\langle\Big(\mathbf{m}_2^2-\frac{1}{3}\mathfrak{i}\Big)\otimes\Big(\mathbf{m}_2^2-\frac{1}{3}\mathfrak{i}\Big)\Big\rangle\\ =&\big\langle(\mathbf{m}_2^4)_0\big\rangle-\frac{4}{21}\mathcal{A}\big(Q_2^{(0)}\big)-\frac{1}{45}(2\delta_{ij}\delta_{kl}-3\delta_{ik}\delta_{jl}-3\delta_{il}\delta_{jk})\\ =&\tilde{a}_1(\mathbf{n}_1^4)_0+\tilde{a}_2(\mathbf{n}_2^4)_0+\tilde{a}_3(\mathbf{n}_1^2\mathbf{n}_2^2)_0-\frac{4}{21}\Big(s_2\mathcal{A}\big((\mathbf{n}_1^2)_0\big)_{ijkl}+b_2\mathcal{A}\big(\mathbf{n}_2^2-\mathbf{n}_3^2\big)_{ijkl}\Big)\\ &-\frac{1}{45}(2\delta_{ij}\delta_{kl}-3\delta_{ik}\delta_{jl}-3\delta_{il}\delta_{jk}),\end{aligned}\tag{SM3.11}$$

for which the matrix R_2 is written as

$$R_2 = -\frac{1}{45}X_1-\frac{4}{21}(s_2X_2+b_2X_3)+\tilde{a}_1X_4+\tilde{a}_2X_5+\tilde{a}_3X_6.\tag{SM3.12}$$

Combining (SM3.1) with (SM3.4)-(SM3.6), the tensor $\mathcal{R}_3^{(0)}$ is expressed by

$$\begin{aligned}\mathcal{R}_3^{(0)} =& 4\big(\bar{a}_1(\mathbf{n}_1^4)_0+\bar{a}_2(\mathbf{n}_2^4)_0+\bar{a}_3(\mathbf{n}_1^2\mathbf{n}_2^2)_0\big)_{ijkl}-\frac{4}{7}\Big((s_1+s_2)\mathcal{A}\big((\mathbf{n}_1^2)_0\big)_{ijkl}\\ &+(b_1+b_2)\mathcal{A}\big(\mathbf{n}_2^2-\mathbf{n}_3^2\big)_{ijkl}\Big)-\frac{1}{15}(2\delta_{ij}\delta_{kl}-3\delta_{ik}\delta_{jl}-3\delta_{il}\delta_{jk}),\end{aligned}\tag{SM3.13}$$

for which the matrix R_3 is denoted by

$$R_3 = -\frac{1}{15}X_1-\frac{4}{7}\big((s_1+s_2)X_2+(b_1+b_2)X_3\big)+4\big(\bar{a}_1X_4+\bar{a}_2X_5+\bar{a}_3X_6\big).\tag{SM3.14}$$

Analogously, the tensor moment $\mathcal{R}_4^{(0)}$ can be expressed by

$$\begin{aligned}\mathcal{R}_4^{(0)} =& -4\Big((a_1+\bar{a}_1)(\mathbf{n}_1^4)_0+(a_2+\bar{a}_2)(\mathbf{n}_2^4)_0+(a_3+\bar{a}_3)(\mathbf{n}_1^2\mathbf{n}_2^2)_0\Big)_{ijkl}\\ &+\frac{4}{7}\Big(s_2\mathcal{A}\big((\mathbf{n}_1^2)_0\big)_{ijkl}+b_2\mathcal{A}\big(\mathbf{n}_2^2-\mathbf{n}_3^2\big)_{ijkl}\Big)-\frac{1}{15}(2\delta_{ij}\delta_{kl}-3\delta_{ik}\delta_{jl}-3\delta_{il}\delta_{jk}),\end{aligned}\tag{SM3.15}$$

for which the matrix R_4 is denoted by

(SM3.16)
$$R_4 = -\frac{1}{15}X_1 + \frac{4}{7}(s_2X_2 + b_2X_3) - 4\big((a_1+\bar{a}_1)X_4 + (a_2+\bar{a}_2)X_5 + (a_3+\bar{a}_3)X_6\big).$$

In the same way, we obtain

(SM3.17)
$$\begin{aligned}\mathcal{R}_5^{(0)} =& -4\Big((\tilde{a}_1+\bar{a}_1)(\mathbf{n}_1^4)_0 + (\tilde{a}_2+\bar{a}_2)(\mathbf{n}_2^4)_0 + (\tilde{a}_3+\bar{a}_3)(\mathbf{n}_1^2\mathbf{n}_2^2)_0\Big)_{ijkl}\\ &+\frac{4}{7}\Big(s_1\mathcal{A}\big((\mathbf{n}_1^2)_0\big)_{ijkl} + b_1\mathcal{A}\big(\mathbf{n}_2^2-\mathbf{n}_3^2\big)_{ijkl}\Big) - \frac{1}{15}(2\delta_{ij}\delta_{kl} - 3\delta_{ik}\delta_{jl} - 3\delta_{il}\delta_{jk}),\end{aligned}$$

for which the matrix R_5 is denoted as

(SM3.18)
$$R_5 = -\frac{1}{15}X_1 + \frac{4}{7}(s_1X_2 + b_1X_3) - 4\big((\tilde{a}_1+\bar{a}_1)X_4 + (\tilde{a}_2+\bar{a}_2)X_5 + (\tilde{a}_3+\bar{a}_3)X_6\big).$$

By

$$(\mathbf{m}_3^4)_0 = (\mathbf{m}_1^4)_0 + (\mathbf{m}_2^4)_0 + 2(\mathbf{m}_1^2\mathbf{m}_2^2)_0, \quad (\mathbf{m}_2^2\mathbf{m}_3^2)_0 = -(\mathbf{m}_2^4)_0 - (\mathbf{m}_1^2\mathbf{m}_2^2)_0,$$

we derive from (SM1.19) that

(SM3.19)
$$\begin{aligned}\mathcal{R}_6 =& \langle(\mathbf{m}_2^2-\mathbf{m}_3^2)\otimes(\mathbf{m}_2^2-\mathbf{m}_3^2)\rangle\\ =& \langle(\mathbf{m}_1^4)_0\rangle + 4\langle(\mathbf{m}_2^4)_0\rangle + 4\langle(\mathbf{m}_1^2\mathbf{m}_2^2)_0\rangle + \frac{4}{7}\mathcal{A}\big(Q_1^{(0)}\big)\\ &-\frac{1}{15}(2\delta_{ij}\delta_{kl} - 3\delta_{ik}\delta_{jl} - 3\delta_{il}\delta_{jk})\\ =& (a_1+4\tilde{a}_1+4\bar{a}_1)(\mathbf{n}_1^4)_0 + (a_2+4\tilde{a}_2+4\bar{a}_2)(\mathbf{n}_2^4)_0 + (a_3+4\tilde{a}_3+4\bar{a}_3)(\mathbf{n}_1^2\mathbf{n}_2^2)_0\\ &+\frac{4}{7}\Big(s_1\mathcal{A}\big((\mathbf{n}_1^2)_0\big)_{ijkl} + b_1\mathcal{A}\big(\mathbf{n}_2^2-\mathbf{n}_3^2\big)_{ijkl}\Big) - \frac{1}{15}(2\delta_{ij}\delta_{kl} - 3\delta_{ik}\delta_{jl} - 3\delta_{il}\delta_{jk}),\end{aligned}$$

for which the matrix R_6 is given by

(SM3.20)
$$\begin{aligned}R_6 =& -\frac{1}{15}X_1 + \frac{4}{7}(s_1X_2 + b_1X_3) + (a_1+4\tilde{a}_1+4\bar{a}_1)X_4\\ &+(a_2+4\tilde{a}_2+4\bar{a}_2)X_5 + (a_3+4\tilde{a}_3+4\bar{a}_3)X_6.\end{aligned}$$

We turn to the term $\langle(\mathbf{m}_1^2)_0\otimes(\mathbf{m}_2^2-\mathbf{m}_3^2)\rangle$. By (SM1.22), we have

(SM3.21)
$$\begin{aligned}\mathcal{S} =& \langle(\mathbf{m}_1^2)_0\otimes(\mathbf{m}_2^2-\mathbf{m}_3^2)\rangle\\ =& \epsilon^{jks}\langle\mathbf{m}_1\mathbf{m}_2\mathbf{m}_3\rangle_{ils} + \epsilon^{ils}\langle\mathbf{m}_1\mathbf{m}_2\mathbf{m}_3\rangle_{kjs} + 2\langle(\mathbf{m}_1^2\mathbf{m}_2^2)_0\rangle + \langle(\mathbf{m}_1^4)_0\rangle\\ &+\frac{4}{21}\mathcal{A}\big(Q_1^{(0)}\big) + \frac{8}{21}\mathcal{A}\big(Q_2^{(0)}\big)\\ =& z\epsilon^{jks}(\mathbf{n}_1\mathbf{n}_2\mathbf{n}_3)_{ils} + z\epsilon^{ils}(\mathbf{n}_1\mathbf{n}_2\mathbf{n}_3)_{kjs}\\ &+(a_1+2\bar{a}_1)(\mathbf{n}_1^4)_0 + (a_2+2\bar{a}_2)(\mathbf{n}_2^4)_0 + (a_3+2\bar{a}_3)(\mathbf{n}_1^2\mathbf{n}_2^2)_0\\ &+\frac{4}{21}\Big((s_1+2s_2)\mathcal{A}\big((\mathbf{n}_1^2)_0\big)_{ijkl} + (b_1+2b_2)\mathcal{A}\big(\mathbf{n}_2^2-\mathbf{n}_3^2\big)_{ijkl}\Big),\end{aligned}$$

where the coefficient matrix S is given by

$$S = z\Pi + \frac{4}{21}\Big((s_1+2s_2)X_2 + (b_1+2b_2)X_3\Big) + (a_1+2\bar{a}_1)X_4 + (a_2+2\bar{a}_2)X_5 + (a_3+2\bar{a}_3)X_6.$$

We are now able to give the matrices M and P. By (4.3) and (4.5), the corresponding coordinates M_{11}, M_{12} and M_{22} are

$$M_{11} = \Gamma_2 R_4 + \Gamma_3 R_3, \quad M_{12} = -\Gamma_3 R_3, \quad M_{22} = \Gamma_1 R_5 + \Gamma_3 R_3, \tag{SM3.22}$$

$$P = c\zeta(I_{22}R_1 + I_{11}R_2 + I_{11}e_1 R_3). \tag{SM3.23}$$

Using the expressions of R_i, we arrive at (4.37)–(4.39) and (4.43).

The remaining part is to express averages of fourth-order antisymmetric traceless tensors and third-order tensors. From (SM1.29), we deduce that

(SM3.24)

$$\begin{aligned}
&\big\langle (m_{1i}m_{2j} - m_{2i}m_{1j})(\mathbf{m}_1\mathbf{m}_2)_{kl}\big\rangle \\
&= z\epsilon^{ijs}(\mathbf{n}_1\mathbf{n}_2\mathbf{n}_3)_{kls} + \frac{1}{6}\Big(\mathcal{B}\big(Q_1^{(0)}\big)_{ijkl} + \mathcal{B}\big(Q_2^{(0)}\big)_{ijkl}\Big) \\
&= z\epsilon^{ijs}(\mathbf{n}_1\mathbf{n}_2\mathbf{n}_3)_{kls} + \frac{1}{6}\Big((s_1-s_2)\mathcal{B}\big((\mathbf{n}_1^2)_0\big)_{ijkl} + (b_1-b_2)\mathcal{B}\big(\mathbf{n}_2^2-\mathbf{n}_3^2\big)_{ijkl}\Big).
\end{aligned}$$

We would like to express the above tensors linearly by the three tensors below,

$$\begin{aligned}
\mathbf{a}_1\otimes\mathbf{s}_3 &= (\mathbf{n}_1\otimes\mathbf{n}_2 - \mathbf{n}_2\otimes\mathbf{n}_1)\otimes\mathbf{n}_1\mathbf{n}_2, \\
\mathbf{a}_2\otimes\mathbf{s}_4 &= (\mathbf{n}_3\otimes\mathbf{n}_1 - \mathbf{n}_1\otimes\mathbf{n}_3)\otimes\mathbf{n}_1\mathbf{n}_3, \\
\mathbf{a}_3\otimes\mathbf{s}_5 &= (\mathbf{n}_2\otimes\mathbf{n}_3 - \mathbf{n}_3\otimes\mathbf{n}_2)\otimes\mathbf{n}_2\mathbf{n}_3.
\end{aligned}$$

Direct calculations lead to

$$\begin{aligned}
\mathcal{B}\big((\mathbf{n}_1^2)_0\big)_{ijkl} =& \frac{1}{3}\Big((2\mathbf{n}_1^2-\mathbf{n}_2^2-\mathbf{n}_3^2)_{ki}(\mathbf{n}_1^2+\mathbf{n}_2^2+\mathbf{n}_3^2)_{jl} \\
&- (2\mathbf{n}_1^2-\mathbf{n}_2^2-\mathbf{n}_3^2)_{kj}(\mathbf{n}_1^2+\mathbf{n}_2^2+\mathbf{n}_3^2)_{il} \\
&+ (2\mathbf{n}_1^2-\mathbf{n}_2^2-\mathbf{n}_3^2)_{li}(\mathbf{n}_1^2+\mathbf{n}_2^2+\mathbf{n}_3^2)_{jk} \\
&- (2\mathbf{n}_1^2-\mathbf{n}_2^2-\mathbf{n}_3^2)_{lj}(\mathbf{n}_1^2+\mathbf{n}_2^2+\mathbf{n}_3^2)_{ik}\Big) \\
=& 2(\mathbf{n}_1\otimes\mathbf{n}_2 - \mathbf{n}_2\otimes\mathbf{n}_1)\otimes\mathbf{n}_1\mathbf{n}_2 + 2(\mathbf{n}_1\otimes\mathbf{n}_3 - \mathbf{n}_3\otimes\mathbf{n}_1)\otimes\mathbf{n}_1\mathbf{n}_3 \\
=& 2(\mathbf{a}_1\otimes\mathbf{s}_3 - \mathbf{a}_2\otimes\mathbf{s}_4), \qquad \text{(SM3.25)}\\
\mathcal{B}\big(\mathbf{n}_2^2-\mathbf{n}_3^2\big)_{ijkl} =& \big(\mathbf{n}_2^2-\mathbf{n}_3^2\big)_{ki}(\mathbf{n}_1^2+\mathbf{n}_2^2+\mathbf{n}_3^2)_{jl} - \big(\mathbf{n}_2^2-\mathbf{n}_3^2\big)_{kj}(\mathbf{n}_1^2+\mathbf{n}_2^2+\mathbf{n}_3^2)_{il} \\
&+ \big(\mathbf{n}_2^2-\mathbf{n}_3^2\big)_{li}(\mathbf{n}_1^2+\mathbf{n}_2^2+\mathbf{n}_3^2)_{jk} - \big(\mathbf{n}_2^2-\mathbf{n}_3^2\big)_{lj}(\mathbf{n}_1^2+\mathbf{n}_2^2+\mathbf{n}_3^2)_{ik} \\
=& -2(\mathbf{n}_1\otimes\mathbf{n}_2 - \mathbf{n}_2\otimes\mathbf{n}_1)\otimes\mathbf{n}_1\mathbf{n}_2 + 2(\mathbf{n}_1\otimes\mathbf{n}_3 - \mathbf{n}_3\otimes\mathbf{n}_1)\otimes\mathbf{n}_1\mathbf{n}_3 \\
&+ 4(\mathbf{n}_2\otimes\mathbf{n}_3 - \mathbf{n}_3\otimes\mathbf{n}_2)\otimes\mathbf{n}_2\mathbf{n}_3 \\
=& -2(\mathbf{a}_1\otimes\mathbf{s}_3 + \mathbf{a}_2\otimes\mathbf{s}_4) + 4\mathbf{a}_3\otimes\mathbf{s}_5. \qquad \text{(SM3.26)}
\end{aligned}$$

By virtue of the definition of symmetric tensors and (SM1.12), it follows that

(SM3.27)

$$\begin{aligned}
&\epsilon^{ijs}(\mathbf{n}_1\mathbf{n}_2\mathbf{n}_3)_{kls}\\
&=\frac{1}{6}\epsilon^{ijs}\Big(n_{1k}n_{2l}n_{3s}+n_{2k}n_{3l}n_{1s}+n_{3k}n_{1l}n_{2s}+n_{1k}n_{3l}n_{2s}+n_{2k}n_{1l}n_{3s}+n_{3k}n_{2l}n_{1s}\Big)\\
&=\frac{1}{6}\Big((n_{1i}n_{2j}-n_{2i}n_{1j})n_{1k}n_{2l}+(n_{2i}n_{3j}-n_{3i}n_{2j})n_{2k}n_{3l}+(n_{3i}n_{1j}-n_{1i}n_{3j})n_{3k}n_{1l}\\
&\quad+(n_{3i}n_{1j}-n_{1i}n_{3j})n_{1k}n_{3l}+(n_{1i}n_{2j}-n_{2i}n_{1j})n_{2k}n_{1l}+(n_{2i}n_{3j}-n_{3i}n_{2j})n_{3k}n_{2l}\Big)\\
&=\frac{1}{3}(\mathbf{a}_1\otimes\mathbf{s}_3+\mathbf{a}_2\otimes\mathbf{s}_4+\mathbf{a}_3\otimes\mathbf{s}_5).
\end{aligned}$$

Rotation of the indices leads to

$$\epsilon^{jis}(\mathbf{n}_1\mathbf{n}_2\mathbf{n}_3)_{ksl}=-\frac{1}{3}(\mathbf{a}_1\otimes\mathbf{s}_3+\mathbf{a}_2\otimes\mathbf{s}_4+\mathbf{a}_3\otimes\mathbf{s}_5), \tag{SM3.28}$$

$$\epsilon^{ijs}(\mathbf{n}_1\mathbf{n}_2\mathbf{n}_3)_{skl}=\frac{1}{3}(\mathbf{a}_1\otimes\mathbf{s}_3+\mathbf{a}_2\otimes\mathbf{s}_4+\mathbf{a}_3\otimes\mathbf{s}_5). \tag{SM3.29}$$

Analogous to the derivation of (SM3.24), it holds

(SM3.30)

$$\begin{aligned}
&\langle(m_{1i}m_{3j}-m_{3i}m_{1j})(\mathbf{m}_1\mathbf{m}_3)_{kl}\rangle\\
&\quad=z\epsilon^{jis}(\mathbf{n}_1\mathbf{n}_2\mathbf{n}_3)_{ksl}+\frac{1}{6}\Big(2\mathcal{B}\big(Q_1^{(0)}\big)_{ijkl}-\mathcal{B}\big(Q_2^{(0)}\big)_{ijkl}\Big)\\
&\quad=z\epsilon^{jis}(\mathbf{n}_1\mathbf{n}_2\mathbf{n}_3)_{ksl}+\frac{1}{6}\Big((2s_1+s_2)\mathcal{B}\big((\mathbf{n}_1^2)_0\big)_{ijkl}+(2b_1+b_2)\mathcal{B}\big(\mathbf{n}_2^2-\mathbf{n}_3^2\big)_{ijkl}\Big),
\end{aligned}$$

(SM3.31)

$$\begin{aligned}
&\langle(m_{2i}m_{3j}-m_{3i}m_{2j})(\mathbf{m}_2\mathbf{m}_3)_{kl}\rangle\\
&\quad=z\epsilon^{ijs}(\mathbf{n}_1\mathbf{n}_2\mathbf{n}_3)_{skl}+\frac{1}{6}\Big(\mathcal{B}\big(Q_1^{(0)}\big)_{ijkl}-2\mathcal{B}\big(Q_2^{(0)}\big)_{ijkl}\Big)\\
&\quad=z\epsilon^{ijs}(\mathbf{n}_1\mathbf{n}_2\mathbf{n}_3)_{skl}+\frac{1}{6}\Big((s_1+2s_2)\mathcal{B}\big((\mathbf{n}_1^2)_0\big)_{ijkl}+(b_1+2b_2)\mathcal{B}\big(\mathbf{n}_2^2-\mathbf{n}_3^2\big)_{ijkl}\Big).
\end{aligned}$$

Therefore, taking advantage of the definition of $\mathcal{N}_{Q_1}^{(0)}$ and combining (SM3.13) and (SM3.15) with (SM3.24)–(SM3.28) and (SM3.31), and using $1-e_1-e_2=0$, we deduce that

(SM3.32)

$$\begin{aligned}
\mathcal{N}_{Q_1}^{(0)}&=\frac{1}{2}\mathcal{R}_4^{(0)}+\frac{1}{2}(e_1-e_2)\mathcal{R}_3^{(0)}-\frac{z}{3}(\mathbf{a}_1\otimes\mathbf{s}_3+\mathbf{a}_2\otimes\mathbf{s}_4+\mathbf{a}_3\otimes\mathbf{s}_5)\\
&\qquad+(e_1+e_2)\frac{z}{3}(\mathbf{a}_1\otimes\mathbf{s}_3+\mathbf{a}_2\otimes\mathbf{s}_4+\mathbf{a}_3\otimes\mathbf{s}_5)\\
&\qquad+\frac{1}{6}\Big((2s_1+s_2)\mathcal{B}\big((\mathbf{n}_1^2)_0\big)_{ijkl}+(2b_1+b_2)\mathcal{B}\big(\mathbf{n}_2^2-\mathbf{n}_3^2\big)_{ijkl}\Big)\\
&\qquad+(e_1+e_2)\frac{1}{6}\Big((s_1-s_2)\mathcal{B}\big((\mathbf{n}_1^2)_0\big)_{ijkl}+(b_1-b_2)\mathcal{B}\big(\mathbf{n}_2^2-\mathbf{n}_3^2\big)_{ijkl}\Big)\\
&=\frac{1}{2}\mathcal{R}_4^{(0)}+\frac{1}{2}(e_1-e_2)\mathcal{R}_3^{(0)}+(s_1-b_1)\mathbf{a}_1\otimes\mathbf{s}_3-(s_1+b_1)\mathbf{a}_2\otimes\mathbf{s}_4+2b_1\mathbf{a}_3\otimes\mathbf{s}_5.
\end{aligned}$$

Similarly, combining (SM3.13) and (SM3.17) with (SM3.24)-(SM3.27), (SM3.29) and (SM3), then we have

(SM3.33)
$$
\begin{aligned}
\mathcal{N}_{Q_2}^{(0)} = & \frac{1}{2}\mathcal{R}_5^{(0)} + \frac{1}{2}(e_2 - e_1)\mathcal{R}_3^{(0)} + \frac{z}{3}(\mathbf{a}_1 \otimes \mathbf{s}_3 + \mathbf{a}_2 \otimes \mathbf{s}_4 + \mathbf{a}_3 \otimes \mathbf{s}_5) \\
& - (e_1 + e_2)\frac{z}{3}(\mathbf{a}_1 \otimes \mathbf{s}_3 + \mathbf{a}_2 \otimes \mathbf{s}_4 + \mathbf{a}_3 \otimes \mathbf{s}_5) \\
& + \frac{1}{6}\Big((s_1 + 2s_2)\mathcal{B}\big((\mathbf{n}_1^2)_0\big)_{ijkl} + (b_1 + 2b_2)\mathcal{B}\big(\mathbf{n}_2^2 - \mathbf{n}_3^2\big)_{ijkl}\Big) \\
& - (e_1 + e_2)\frac{1}{6}\Big((s_1 - s_2)\mathcal{B}\big((\mathbf{n}_1^2)_0\big)_{ijkl} + (b_1 - b_2)\mathcal{B}\big(\mathbf{n}_2^2 - \mathbf{n}_3^2\big)_{ijkl}\Big) \\
= & \frac{1}{2}\mathcal{R}_5^{(0)} + \frac{1}{2}(e_2 - e_1)\mathcal{R}_3^{(0)} + (s_2 - b_2)\mathbf{a}_1 \otimes \mathbf{s}_3 - (s_2 + b_2)\mathbf{a}_2 \otimes \mathbf{s}_4 + 2b_2\mathbf{a}_3 \otimes \mathbf{s}_5.
\end{aligned}
$$

The equations (4.40)–(4.42) then come from (SM3.32) and (SM3.33).

Finally, we deal with the third-order tensors. By a direct calculation, we get

$$
\begin{aligned}
(\mathbf{n}_1\mathbf{n}_2\mathbf{n}_3)_{ijk} = & \frac{1}{6}\Big(n_{1i}(n_{2j}n_{3k} + n_{3j}n_{2k}) + n_{2i}(n_{1j}n_{3k} + n_{3j}n_{1k}) \\
& + n_{3i}(n_{1j}n_{2k} + n_{2j}n_{1k})\Big) \\
= & \frac{1}{3}\big(\mathbf{n}_1 \otimes \mathbf{s}_5 + \mathbf{n}_2 \otimes \mathbf{s}_4 + \mathbf{n}_3 \otimes \mathbf{s}_3\big).
\end{aligned}
$$

Meanwhile, we also easily deduce that

$$
\begin{aligned}
\epsilon^{ijs}\big((\mathbf{n}_1^2)_0\big)_{ks} + \epsilon^{iks}\big((\mathbf{n}_1^2)_0\big)_{js} = & (n_{2i}n_{3j} - n_{3i}n_{2j})n_{1k} + (n_{2i}n_{3k} - n_{3i}n_{2k})n_{1j} \\
= & 2(\mathbf{n}_2 \otimes \mathbf{s}_4 - \mathbf{n}_3 \otimes \mathbf{s}_3), \\
\epsilon^{ijs}(\mathbf{n}_2^2 - \mathbf{n}_3^2)_{ks} + \epsilon^{iks}(\mathbf{n}_2^2 - \mathbf{n}_3^2)_{js} = & n_{2k}(n_{3i}n_{1j} - n_{1i}n_{3j}) - n_{3k}(n_{1i}n_{2j} - n_{2i}n_{1j}) \\
& + n_{2j}(n_{3i}n_{1k} - n_{1i}n_{3k}) - n_{3j}(n_{1i}n_{2k} - n_{2i}n_{1k}) \\
= & 2\big(\mathbf{n}_3 \otimes \mathbf{s}_3 - 2\mathbf{n}_1 \otimes \mathbf{s}_5 + \mathbf{n}_2 \otimes \mathbf{s}_4\big).
\end{aligned}
$$

Hence, by using (SM1.25), we derive from Theorem 3.3 that

$$
\begin{aligned}
\langle \mathbf{m}_1 \otimes \mathbf{m}_2\mathbf{m}_3\rangle_{ijk} = & \langle \mathbf{m}_1\mathbf{m}_2\mathbf{m}_3\rangle_{ijk} + \frac{1}{6}\Big(\epsilon^{ijs}\big(\langle(\mathbf{m}_3^2)_0\rangle - \langle(\mathbf{m}_2^2)_0\rangle\big)_{ks} \\
& + \epsilon^{iks}\big(\langle(\mathbf{m}_3^2)_0\rangle - \langle(\mathbf{m}_2^2)_0\rangle\big)_{js}\Big) \\
= & z(\mathbf{n}_1\mathbf{n}_2\mathbf{n}_3)_{ijk} - \frac{1}{6}\Big(\epsilon^{ijs}\big(Q_1^{(0)} + 2Q_2^{(0)}\big)_{ks} + \epsilon^{iks}\big(Q_1^{(0)} + 2Q_2^{(0)}\big)_{js}\Big) \\
= & z(\mathbf{n}_1\mathbf{n}_2\mathbf{n}_3)_{ijk} - \frac{1}{6}(s_1 + 2s_2)\Big(\epsilon^{ijs}\big((\mathbf{n}_1^2)_0\big)_{ks} + \epsilon^{iks}\big((\mathbf{n}_1^2)_0\big)_{js}\Big) \\
& - \frac{1}{6}(b_1 + 2b_2)\Big(\epsilon^{ijs}(\mathbf{n}_2^2 - \mathbf{n}_3^2)_{ks} + \epsilon^{iks}(\mathbf{n}_2^2 - \mathbf{n}_3^2)_{js}\Big) \\
= & \frac{1}{3}(z + 2b_1 + 4b_2)\mathbf{n}_1 \otimes \mathbf{s}_5 + \frac{1}{3}(z - s_1 - 2s_2 - b_1 - 2b_2)\mathbf{n}_2 \otimes \mathbf{s}_4 \\
& + \frac{1}{3}(z + s_1 + 2s_2 - b_1 - 2b_2)\mathbf{n}_3 \otimes \mathbf{s}_3,
\end{aligned}
\tag{SM3.34}
$$

for which the coefficient matrix T_1 under the basis $\mathbf{n}_i \otimes \mathbf{s}_j$ is given by

$$T_1 = \begin{pmatrix} 0 & 0 & 0 & 0 & \frac{1}{3}(z+2b_1+4b_2) \\ 0 & 0 & 0 & \begin{matrix}\frac{1}{3}(z-s_1-2s_2 \\ -b_1-2b_2)\end{matrix} & 0 \\ 0 & 0 & \begin{matrix}\frac{1}{3}(z+s_1+2s_2 \\ -b_1-2b_2)\end{matrix} & 0 & 0 \end{pmatrix}. \tag{SM3.35}$$

Following the same procedure, we obtain

$$\begin{aligned}
\langle \mathbf{m}_2 \otimes \mathbf{m}_1\mathbf{m}_3\rangle_{ijk} &= \langle \mathbf{m}_1\mathbf{m}_2\mathbf{m}_3\rangle_{ijk} + \frac{1}{6}\Big(\epsilon^{ijs}\big(\langle(\mathbf{m}_1^2)_0\rangle - \langle(\mathbf{m}_3^2)_0\rangle\big)_{ks} \\
&\quad + \epsilon^{iks}\big(\langle(\mathbf{m}_1^2)_0\rangle - \langle(\mathbf{m}_3^2)_0\rangle\big)_{js}\Big) \\
&= z(\mathbf{n}_1\mathbf{n}_2\mathbf{n}_3)_{ijk} + \frac{1}{6}(2s_1+s_2)\Big(\epsilon^{ijs}\big((\mathbf{n}_1^2)_0\big)_{ks} + \epsilon^{iks}\big((\mathbf{n}_1^2)_0\big)_{js}\Big) \\
&\quad + \frac{1}{6}(2b_1+b_2)\Big(\epsilon^{ijs}(\mathbf{n}_2^2-\mathbf{n}_3^2)_{ks} + \epsilon^{iks}(\mathbf{n}_2^2-\mathbf{n}_3^2)_{js}\Big) \\
&= \frac{1}{3}(z-4b_1-2b_2)\mathbf{n}_1\otimes\mathbf{s}_5 + \frac{1}{3}(z+2s_1+s_2+2b_1+b_2)\mathbf{n}_2\otimes\mathbf{s}_4 \\
&\quad + \frac{1}{3}(z-2s_1-s_2+2b_1+b_2)\mathbf{n}_3\otimes\mathbf{s}_3,
\end{aligned} \tag{SM3.36}$$

$$\begin{aligned}
\langle \mathbf{m}_3 \otimes \mathbf{m}_1\mathbf{m}_2\rangle_{ijk} &= \langle \mathbf{m}_1\mathbf{m}_2\mathbf{m}_3\rangle_{ijk} + \frac{1}{6}\Big(\epsilon^{ijs}\big(\langle(\mathbf{m}_2^2)_0\rangle - \langle(\mathbf{m}_1^2)_0\rangle\big)_{ks} \\
&\quad + \epsilon^{iks}\big(\langle(\mathbf{m}_2^2)_0\rangle - \langle(\mathbf{m}_1^2)_0\rangle\big)_{js}\Big) \\
&= z(\mathbf{n}_1\mathbf{n}_2\mathbf{n}_3)_{ijk} - \frac{1}{6}(s_1-s_2)\Big(\epsilon^{ijs}\big((\mathbf{n}_1^2)_0\big)_{ks} + \epsilon^{iks}\big((\mathbf{n}_1^2)_0\big)_{js}\Big) \\
&\quad - \frac{1}{6}(b_1-b_2)\Big(\epsilon^{ijs}(\mathbf{n}_2^2-\mathbf{n}_3^2)_{ks} + \epsilon^{iks}(\mathbf{n}_2^2-\mathbf{n}_3^2)_{js}\Big) \\
&= \frac{1}{3}(z+2b_1-2b_2)\mathbf{n}_1\otimes\mathbf{s}_5 + \frac{1}{3}(z-s_1+s_2-b_1+b_2)\mathbf{n}_2\otimes\mathbf{s}_4 \\
&\quad + \frac{1}{3}(z+s_1-s_2-b_1+b_2)\mathbf{n}_3\otimes\mathbf{s}_3,
\end{aligned} \tag{SM3.37}$$

where the associated coefficient matrices T_2, T_3 in (SM3.36) and (SM3.37) can be written as

$$T_2 = \begin{pmatrix} 0 & 0 & 0 & 0 & \frac{1}{3}(z-4b_1-2b_2) \\ 0 & 0 & 0 & \begin{matrix}\frac{1}{3}(z+2s_1+s_2 \\ +2b_1+b_2)\end{matrix} & 0 \\ 0 & 0 & \begin{matrix}\frac{1}{3}(z-2s_1-s_2 \\ +2b_1+b_2)\end{matrix} & 0 & 0 \end{pmatrix}, \tag{SM3.38}$$

$$T_3 = \begin{pmatrix} 0 & 0 & 0 & 0 & \frac{1}{3}(z+2b_1-2b_2) \\ 0 & 0 & 0 & \begin{matrix}\frac{1}{3}(z-s_1+s_2 \\ -b_1+b_2)\end{matrix} & 0 \\ 0 & 0 & \begin{matrix}\frac{1}{3}(z+s_1-s_2 \\ -b_1+b_2)\end{matrix} & 0 & 0 \end{pmatrix}. \tag{SM3.39}$$

Define

(SM3.40)
$$
\begin{aligned}
&w_i^T = (s_i, b_i, 0, 0, 0),\ i = 1, 2,\\
&W_1 = \mathrm{diag}\left(\frac{1}{3}(2s_1+1), \frac{1}{3}(1-s_1)+b_1, \frac{1}{3}(1-s_1)-b_1\right),\\
&W_2 = \mathrm{diag}\left(\frac{1}{3}(2s_2+1), \frac{1}{3}(1-s_2)+b_2, \frac{1}{3}(1-s_2)-b_2\right),\\
&W_3 = \mathrm{diag}\left(\frac{1}{3}(1-2s_1-2s_2), \frac{1}{3}(1+s_1+s_2)-b_1-b_2, \frac{1}{3}(1+s_1+s_2)+b_1+b_2\right).
\end{aligned}
$$

Then, the quasi-entropy Ξ_4 can be reduced to

$$
\begin{aligned}
\Xi_{4,\mathrm{Bi}} =& -\ln\det\begin{pmatrix}1 & & \\ & \Lambda & \\ & & \Lambda\end{pmatrix}\begin{pmatrix}1 & w_1^T & (2w_2+w_1)^T\\ w_1 & R_1 & S\\ 2w_2+w_1 & S^T & R_6\end{pmatrix}\begin{pmatrix}1 & & \\ & \Lambda & \\ & & \Lambda\end{pmatrix}\\
&-\ln\det\begin{pmatrix}1 & \\ & \Lambda\end{pmatrix}\begin{pmatrix}W_1 & T_1\\ T_1^T & R_3\end{pmatrix}\begin{pmatrix}1 & \\ & \Lambda\end{pmatrix}\\
&-\ln\det\begin{pmatrix}1 & \\ & \Lambda\end{pmatrix}\begin{pmatrix}W_2 & T_2\\ T_2^T & R_4\end{pmatrix}\begin{pmatrix}1 & \\ & \Lambda\end{pmatrix}\\
&-\ln\det\begin{pmatrix}1 & \\ & \Lambda\end{pmatrix}\begin{pmatrix}W_3 & T_3\\ T_3^T & R_5\end{pmatrix}\begin{pmatrix}1 & \\ & \Lambda\end{pmatrix}\\
=& -\ln\det\begin{pmatrix}1 & w_1^T & (2w_2+w_1)^T\\ w_1 & R_1 & S\\ 2w_2+w_1 & S^T & R_6\end{pmatrix} - \ln\det\begin{pmatrix}W_1 & T_1\\ T_1^T & R_3\end{pmatrix}
\end{aligned}
$$

(SM3.41)
$$
-\ln\det\begin{pmatrix}W_2 & T_2\\ T_2^T & R_4\end{pmatrix} - \ln\det\begin{pmatrix}W_3 & T_3\\ T_3^T & R_5\end{pmatrix} - 10\ln\det\Lambda.
$$

The expressions of R_i, S, T_i can all be found above.

SM4. The uniaxial case: Theorem 5.1. Assume that Q_i are uniaxial, i.e. $b_i = 0$ so that

$$
Q_i = s_i\left(\mathbf{n}_1^2 - \frac{\mathfrak{i}}{3}\right),\ i = 1, 2.
$$

By (3.20), we require that the two scalars s_i satisfy

$$
-\frac{1}{2} < s_1,\ s_2,\ -s_1-s_2 < 1. \tag{SM4.1}
$$

For the original entropy, the discussion is similar to the biaxial case.

LEMMA SM4.1. *If s_i satisfy* (SM4.1), *then there exists a unique density function*

$$\rho = \frac{1}{Z}\exp\left(\sum_{i=1,2}\lambda_i(\mathbf{m}_i\cdot\mathbf{n}_1)^2\right)$$

such that $\langle(\mathbf{m}_i^2)_0\rangle = s_i(\mathbf{n}_1^2)_0$.

We omit the rest of the derivation since it is the same as the biaxial case.

We turn to the quasi-entropy. Here, we need to notice that

$$2X_6 + X_4 = \begin{pmatrix} 0 & \frac{3}{14} & & & \\ \frac{3}{14} & 0 & & & \\ & & \frac{4}{7} & & \\ & & & -\frac{4}{7} & \\ & & & & 0 \end{pmatrix} \overset{\text{def}}{=} X_6', \tag{SM4.2}$$

$$8X_6 + 8X_5 + X_4 = \begin{pmatrix} 0 & 0 & & & \\ 0 & 1 & & & \\ & & 0 & & \\ & & & 0 & \\ & & & & -4 \end{pmatrix} \overset{\text{def}}{=} X_5'. \tag{SM4.3}$$

Let us define

$$\begin{aligned} a_1' &= a_1 - \frac{1}{2}a_3 + \frac{3}{8}a_2, \quad a_2' = \frac{1}{8}a_2, \quad a_3 = \frac{1}{2}(a_3 - a_2),\\ \tilde{a}_1' &= \tilde{a}_1 - \frac{1}{2}\tilde{a}_3 + \frac{3}{8}\tilde{a}_2, \quad \tilde{a}_2' = \frac{1}{8}\tilde{a}_2, \quad \tilde{a}_3 = \frac{1}{2}(\tilde{a}_3 - \tilde{a}_2),\\ \bar{a}_1' &= \bar{a}_1 - \frac{1}{2}\bar{a}_3 + \frac{3}{8}\bar{a}_2, \quad \bar{a}_2' = \frac{1}{8}\bar{a}_2, \quad \bar{a}_3 = \frac{1}{2}(\bar{a}_3 - \bar{a}_2). \end{aligned}$$

It can be verified that

$$a_1X_4 + a_2X_5 + a_3X_6 = a_1'X_4 + a_2'X_5' + a_3'X_6'.$$

In what follows, we show that when Q_i are uniaxial, $\Xi_{4,\mathrm{Bi}}$ reaches its minimum only when $a_2' = a_3' = \tilde{a}_2' = \tilde{a}_3' = \bar{a}_2' = \bar{a}_3' = z = 0$.

Let us discuss each of the log-determinant in (SM3.41). We could rearrange the indices to arriave at

$$\begin{aligned} &-\ln\det\begin{pmatrix} 1 & w_1^T & (2w_2+w_1)^T \\ w_1 & R_1 & S \\ 2w_2+w_1 & S^T & R_6 \end{pmatrix}\\ &= -\ln\det\begin{pmatrix} 1 & (s_1, 2s_1+s_2) & 0_{1\times 2} \\ (s_1, 2s_1+s_2)^T & \Upsilon_1 & \frac{3}{14}\Theta_3 - z\Pi_1 \\ 0_{2\times 1} & \frac{3}{14}\Theta_3 + z\Pi_1 & \Upsilon_2 + \Theta_2 \end{pmatrix}\\ &\quad -\ln\det(\Upsilon_3 + \frac{4}{7}\Theta_3) - \ln\det(\Upsilon_3 - \frac{4}{7}\Theta_3) - \ln\det(4\Upsilon_2 - 4\Theta_2), \end{aligned} \tag{SM4.4}$$

where the blocks Υ_i, Θ_i and Π_1 are given by

$$
\begin{aligned}
\Upsilon_1 &= \begin{pmatrix} \frac{1}{5}+\frac{2}{7}s_1+\frac{18}{35}a_1' & -\frac{2}{7}(s_1+2s_2)+\frac{18}{35}(a_1'+2\bar{a}_1') \\ -\frac{2}{7}(s_1+2s_2)+\frac{18}{35}(a_1'+2\bar{a}_1') & \frac{3}{5}-\frac{6}{7}s_1+\frac{18}{35}(a_1'+4\tilde{a}_1'+4\bar{a}_1') \end{pmatrix}, \\
\Upsilon_2 &= \begin{pmatrix} \frac{1}{15}-\frac{2}{21}s_1+\frac{1}{35}a_1' & \frac{2}{21}(s_1+2s_2)+\frac{1}{35}(a_1'+2\bar{a}_1') \\ \frac{2}{21}(s_1+2s_2)+\frac{1}{35}(a_1'+2\bar{a}_1') & \frac{1}{5}+\frac{2}{7}s_1+\frac{1}{35}(a_1'+4\tilde{a}_1'+4\bar{a}_1') \end{pmatrix}, \\
\Upsilon_3 &= \begin{pmatrix} \frac{4}{15}+\frac{4}{21}s_1-\frac{16}{35}a_1' & -\frac{4}{21}(s_1+2s_2)-\frac{16}{35}(a_1'+2\bar{a}_1') \\ -\frac{4}{21}(s_1+2s_2)-\frac{16}{35}(a_1'+2\bar{a}_1') & \frac{4}{5}-\frac{4}{7}s_1-\frac{16}{35}(a_1'+4\tilde{a}_1'+4\bar{a}_1') \end{pmatrix}, \\
\Theta_2 &= \begin{pmatrix} a_2' & a_2'+2\bar{a}_2' \\ a_2'+2\bar{a}_2' & a_2'+4\tilde{a}_2'+4\bar{a}_2' \end{pmatrix}, \\
\Theta_3 &= \begin{pmatrix} a_3' & a_3'+2\bar{a}_3' \\ a_3'+2\bar{a}_3' & a_3'+4\tilde{a}_3'+4\bar{a}_3' \end{pmatrix}, \\
\Pi_1 &= \begin{pmatrix} 0 & \frac{3}{2} \\ -\frac{3}{2} & 0 \end{pmatrix}.
\end{aligned}
$$

Notice that Υ_i does not depend on $a_i', \tilde{a}_i', \bar{a}_i'$ for $i = 2, 3$, and Θ_2, Θ_3 only depend on them.

By Lemma SM2.2, we deduce that

$$
\begin{aligned}
&-\ln\det \begin{pmatrix} 1 & (s_1, 2s_1+s_2) & 0_{1\times 2} \\ (s_1, 2s_1+s_2)^T & \Upsilon_1 & \frac{3}{14}\Theta_3 - z\Pi_1 \\ 0_{2\times 1} & \frac{3}{14}\Theta_3 + z\Pi_1 & \Upsilon_2+\Theta_2 \end{pmatrix} \\
&\geq -\ln\det \begin{pmatrix} 1 & (s_1, 2s_1+s_2) \\ (s_1, 2s_1+s_2)^T & \Upsilon_1 \end{pmatrix} - \ln\det(\Upsilon_2+\Theta_2). \qquad \text{(SM4.5)}
\end{aligned}
$$

The equality holds if and only if $z = 0$ and $\Theta_3 = 0$. In addition, it shall be noticed that $-\ln\det A$ is strictly convex about A (see, for example, Lemma 4.5 in [SM3] for a proof). Therefore, we obtain

$$
\begin{aligned}
&-\ln\det(\Upsilon_2+\Theta_2) - \ln\det(4\Upsilon_2 - 4\Theta_2) \geq -2\ln\det\Upsilon_2 - 2\ln 4, \\
&-\ln\det(\Upsilon_3 + \frac{4}{7}\Theta_3) - \ln\det(\Upsilon_3 - \frac{4}{7}\Theta_3) \geq -2\ln\det\Upsilon_3. \qquad \text{(SM4.6)}
\end{aligned}
$$

The equalities hold if and only if $\Theta_2 = \Theta_3 = 0$.

Let us look into another log-determinant in (SM3.41). It follows that

$$
\begin{aligned}
&-\ln\det \begin{pmatrix} W_1 & T_1 \\ T_1^T & R_3 \end{pmatrix} = \\
&-\ln\det \begin{pmatrix}
\xi_1 & & & & & & & \frac{1}{3}z \\
& \xi_2 & & & & & -\xi_3+\frac{1}{3}z & \\
& & \xi_2 & & & \xi_3+\frac{1}{3}z & & \\
& & & \xi_4 & \frac{3}{14}\bar{a}_2' & & & \\
& & & \frac{3}{14}\bar{a}_2' & \xi_5+\bar{a}_3' & & & \\
& & \xi_3+\frac{1}{3}z & & & \xi_6+\frac{4}{7}\bar{a}_2' & & \\
& -\xi_3+\frac{1}{3}z & & & & & \xi_6-\frac{4}{7}\bar{a}_2' & \\
\frac{1}{3}z & & & & & & & 4\xi_5-4\bar{a}_3'
\end{pmatrix}.
\end{aligned}
$$

In the above, those ξ_i are given by

$$\begin{aligned}
\xi_1 &= \frac{1}{3}(2s_1+1), \quad \xi_2 = \frac{1}{3}(1-s_1), \quad \xi_3 = \frac{1}{3}(s_1+2s_2),\\
\xi_4 &= \frac{3}{5}+\frac{6}{7}(s_1+s_2)+\frac{72}{35}\bar{a}_1',\\
\xi_5 &= \frac{1}{5}-\frac{2}{7}(s_1+s_2)+\frac{4}{35}\bar{a}_1',\\
\xi_6 &= \frac{4}{5}+\frac{4}{7}(s_1+s_2)-\frac{64}{35}\bar{a}_1'.
\end{aligned}$$

Since the function $-\ln x$ is monotonely decreasing and strictly convex, we have the inequality

$$\begin{aligned}
&-\ln\left(\xi_1\left(4\xi_5-4\bar{a}_3'\right)-\frac{1}{9}z^2\right)-\ln\left(\xi_2\left(\xi_6-\frac{4}{7}\bar{a}_2'\right)-\left(\xi_3-\frac{1}{3}z\right)^2\right)\\
&-\ln\left(\xi_2\left(\xi_6+\frac{4}{7}\bar{a}_2'\right)-\left(\xi_3+\frac{1}{3}z\right)^2\right)-\ln\left(\xi_4\left(\xi_5+\bar{a}_3'\right)-\left(\frac{3}{14}\bar{a}_2'\right)^2\right)\\
\geq&-\ln\left(\xi_1\left(4\xi_5-4\bar{a}_3'\right)\right)-\ln\left(\xi_2\left(\xi_6-\frac{4}{7}\bar{a}_2'\right)-\xi_3^2+\frac{2}{3}\xi_3 z\right)\\
&-\ln\left(\xi_2\left(\xi_6+\frac{4}{7}\bar{a}_2'\right)-\xi_3^2-\frac{2}{3}\xi_3 z\right)-\ln\left(\xi_1\left(\xi_5+\bar{a}_3'\right)\right)\\
=&-\ln\xi_1-\ln\xi_4-\ln 4\\
&-\ln\left(\xi_5-\bar{a}_3'\right)-\ln\left(\xi_5+\bar{a}_3'\right)\\
&-\ln\left(\xi_2\left(\xi_6-\frac{4}{7}\bar{a}_2'\right)-\xi_3^2+\frac{2}{3}\xi_3 z\right)-\ln\left(\xi_2\left(\xi_6+\frac{4}{7}\bar{a}_2'\right)\right)\\
\geq&-\ln\xi_1-\ln\xi_4-\ln 4-2\ln\xi_5-2\ln\left(\xi_2\xi_6-\xi_3^2\right). \qquad \text{(SM4.7)}
\end{aligned}$$

The equalities hold if and only if $\bar{a}_2' = \bar{a}_3' = z = 0$.

Similarly, we could deal with the other two log-determinants in (SM3.41). Summarizing (SM4.5), (SM4.6) and (SM4.7), we conclude that when Q_i are uniaxial, at the minimizer we must have $a_2' = a_3' = \tilde{a}_2' = \tilde{a}_3' = \bar{a}_2' = \bar{a}_3' = z = 0$.

SM5. The orientational elasticity. For the readers' convenience, we present the orientational elasticity for the biaxial nematic phases that can be found in [SM5], where the elasitic constants expressed the coefficients in the molecular-theory-based static Q-tensor model. In addition, the variational derivatives with respect to the orthonomal frame $\mathfrak{p} = (\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3)$ are derived.

We first write down an equivalent formulation of (4.44). Using the following relations

$$\begin{aligned}
&\nabla\cdot\mathbf{n}_2 = -D_{31}+D_{13}, \qquad \mathbf{n}_2\cdot\nabla\times\mathbf{n}_2 = D_{33}+D_{11},\\
&\mathbf{n}_3\cdot\nabla\times\mathbf{n}_2 = -D_{23}, \qquad \mathbf{n}_1\cdot\nabla\times\mathbf{n}_2 = -D_{21},\\
&|\mathbf{n}_2\times\nabla\times\mathbf{n}_2|^2 = (\mathbf{n}_1\cdot\nabla\times\mathbf{n}_2)^2+(\mathbf{n}_3\cdot\nabla\times\mathbf{n}_2)^2,
\end{aligned}$$

together with (4.44) yields that the equivalent expression analogous to the Oseen-Frank energy can be given by

$$\frac{\mathcal{F}_{Bi}(\mathfrak{p})}{ck_BT} = \int \mathrm{d}\boldsymbol{x}\ \frac{1}{2}\Big(K_1(\nabla\cdot\mathbf{n}_1)^2+K_2(\mathbf{n}_1\cdot\nabla\times\mathbf{n}_1)^2+K_3(\mathbf{n}_1\times\nabla\times\mathbf{n}_1)^2$$

$$
\begin{aligned}
&+K_4(\nabla\cdot\mathbf{n}_2)^2+K_5(\mathbf{n}_2\cdot\nabla\times\mathbf{n}_2)^2+K_6(\mathbf{n}_2\times\nabla\times\mathbf{n}_2)^2\\
&+K_7(\nabla\cdot\mathbf{n}_3)^2+K_8(\mathbf{n}_3\cdot\nabla\times\mathbf{n}_3)^2+K_9(\mathbf{n}_3\times\nabla\times\mathbf{n}_3)^2\\
&+K_{10}(\mathbf{n}_1\cdot\nabla\times\mathbf{n}_3)^2+K_{11}(\mathbf{n}_2\cdot\nabla\times\mathbf{n}_1)^2+K_{12}(\mathbf{n}_3\cdot\nabla\times\mathbf{n}_2)^2\Big),
\end{aligned}
\tag{SM5.1}
$$

where the elastic coefficients $K_i(i=1,\cdots,12)$ can be expressed by $K_{ijkl}(i,j,k,l=1,2,3)$ (see [SM1] for details). In the above, we also neglect the surface terms (4.45).

The next task is to provide the biaxial elastic energy with the form (4.44) derived from the molecular-theory-based static tensor model (3.2), where the elastic coefficients K_{ijkl} are expressed by molecular parameters. We refer to [SM5] for more detailed discussion.

Assume that the minimizers of the bulk energy in (3.2) has the following biaxial form:

$$
Q_\alpha=(s_\alpha+b_\alpha)\mathbf{n}_1^2+2b_\alpha\mathbf{n}_2^2-\Big(\frac{1}{3}s_\alpha+b_\alpha\Big)\mathbf{i},\quad \alpha=1,2.
$$

Then the corresponding derivative terms are calculated as

$$
\begin{aligned}
|\nabla Q_\alpha|^2=&\,2(s_\alpha+b_\alpha)^2(\partial_k n_{1i})^2+8b_\alpha^2(\partial_k n_{2i})^2+8b_\alpha(s_\alpha+b_\alpha)n_{1i}n_{2j}\partial_k n_{1j}\partial_k n_{2i},\\
\partial_i Q_{1jk}\partial_i Q_{2jk}=&\,2(s_1+b_1)(s_2+b_2)(\partial_i n_{1j})^2+8b_1b_2(\partial_i n_{2j})^2\\
&+4[b_1(s_2+b_2)+b_2(s_1+b_1)]n_{1j}n_{2k}\partial_i n_{1k}\partial_i n_{2j},\\
\partial_i Q_{\alpha ik}\partial_j Q_{\beta jk}=&\,(s_\alpha+b_\alpha)(s_\beta+b_\beta)\big(|\nabla\cdot\mathbf{n}_1|^2+n_{1i}n_{1j}\partial_i n_{1k}\partial_j n_{1k}\big)\\
&+2\big[b_\alpha(s_\beta+b_\beta)+b_\beta(s_\alpha+b_\alpha)\big]\big((\nabla\cdot\mathbf{n}_1)n_{1k}n_{2j}\partial_j n_{2k}\\
&+(\nabla\cdot\mathbf{n}_2)n_{1i}n_{2k}\partial_i n_{1k}+n_{1i}n_{2j}\partial_i n_{1k}\partial_j n_{2k}\big)\\
&+4b_\alpha b_\beta\big(|\nabla\cdot\mathbf{n}_2|^2+n_{2i}n_{2j}\partial_i n_{2k}\partial_j n_{2k}\big).
\end{aligned}
$$

From which and the elastic energy in (3.2) implies that

$$
\begin{aligned}
\frac{\mathcal{F}_{Bi}(\mathfrak{p})}{ck_BT}=&\int \mathrm{d}\mathbf{x}\frac{1}{2}\Big[J_1(\partial_i n_{1j})^2+J_2(\partial_i n_{2j})^2+J_3n_{1i}n_{2j}\partial_k n_{1j}\partial_k n_{2i}\\
&+J_4\big(|\nabla\cdot\mathbf{n}_1|^2+n_{1i}n_{1j}\partial_i n_{1k}\partial_j n_{1k}\big)+J_5\big(|\nabla\cdot\mathbf{n}_2|^2+n_{2i}n_{2j}\partial_i n_{2k}\partial_j n_{2k}\big)\\
&+J_6\big((\nabla\cdot\mathbf{n}_1)n_{1k}n_{2j}\partial_j n_{2k}+(\nabla\cdot\mathbf{n}_2)n_{1i}n_{2k}\partial_i n_{1k}+n_{1i}n_{2j}\partial_i n_{1k}\partial_j n_{2k}\big)\Big],
\end{aligned}
\tag{SM5.2}
$$

where the coefficients $J_i(i=1,\cdots,6)$ are given by (4.47).

We need to express the derivative terms in (SM5.2) by the nine invariant $D_{\lambda\delta}(\lambda,\delta=1,2,3)$. For example, the following four terms can be respectively expressed as

$$
\begin{aligned}
(\partial_i n_{1j})^2=&\,\delta_{jl}\delta_{ik}\partial_k n_{1l}\partial_i n_{1j}\\
=&\,(n_{2j}n_{2l}+n_{3j}n_{3l})(n_{1i}n_{1k}+n_{2i}n_{2k}+n_{3i}n_{3k})\partial_k n_{1l}\partial_i n_{1j}\\
=&\,\big(n_{1i}n_{2j}n_{1k}n_{2l}+n_{2i}n_{2j}n_{2k}n_{2l}+n_{3i}n_{2j}n_{3k}n_{2l}+n_{1i}n_{3j}n_{1k}n_{3l}\\
&+n_{2i}n_{3j}n_{2k}n_{3l}+n_{3i}n_{3j}n_{3k}n_{3l}\big)\partial_k n_{1l}\partial_i n_{1j}\\
=&\,D_{13}^2+D_{23}^2+D_{33}^2+D_{12}^2+D_{22}^2+D_{32}^2,\\
\partial_j n_{1j}=&\,\delta_{ij}\partial_i n_{1j}=(n_{2i}n_{2j}+n_{3i}n_{3j})\partial_i n_{1j}\\
=&\,D_{32}-D_{23},\\
n_{1i}n_{2j}\partial_k n_{1j}\partial_k n_{2i}=&\,\delta_{jl}\delta_{ks}n_{1i}n_{2l}\partial_k n_{1j}\partial_s n_{2i}\\
=&\,n_{2j}n_{2l}(n_{1k}n_{1s}+n_{2k}n_{2s}+n_{3k}n_{3s})n_{1i}n_{2l}\partial_k n_{1j}\partial_s n_{2i}
\end{aligned}
$$

$$
\begin{aligned}
&= (n_{1k}n_{2j}n_{1s}n_{1i} + n_{2k}n_{2j}n_{2s}n_{1i} + n_{3k}n_{2j}n_{3s}n_{1i})\partial_k n_{1j}\partial_s n_{2i} \\
&= -(D_{13}^2 + D_{23}^2 + D_{33}^2), \\
n_{1i}n_{1j}\partial_i n_{1k}\partial_j n_{1k} &= \delta_{kl}n_{1i}n_{1j}\partial_i n_{1l}\partial_j n_{1k} \\
&= (n_{2k}n_{2l} + n_{3k}n_{3l})n_{1i}n_{1j}\partial_i n_{1l}\partial_j n_{1k} \\
&= D_{12}^2 + D_{13}^2.
\end{aligned}
$$

While the remaining four terms can be similarly expressed as follows:

$$
\begin{aligned}
(\partial_i n_{2j})^2 &= D_{13}^2 + D_{23}^2 + D_{33}^2 + D_{11}^2 + D_{21}^2 + D_{31}^2, \\
\partial_j n_{2j} &= D_{13} - D_{31}, \\
n_{2i}n_{2j}\partial_i n_{2k}\partial_j n_{2k} &= D_{21}^2 + D_{23}^2, \\
n_{1i}n_{2j}\partial_i n_{1k}\partial_j n_{2k} &= -D_{12}D_{21}.
\end{aligned}
$$

Plugging the above eight relations into (SM5.2), we immediately obtain the biaxial elastic energy (4.44), where the elastic coefficients $K_{ijkl}(i,j,k,l = 1,2,3)$, completely determined by the molecular parameters, are given by (4.46).

Then, we calculate the variational derivative about the frame $\mathfrak{p}$, and derive the variational derivative along the infinitesimal rotation round $\mathbf{n}_i (i = 1,2,3)$. For instance, the variational derivative along the infinitesimal rotation round $\mathbf{n}_1$ is given by

$$
n_{2\alpha}\frac{\delta}{\delta n_{3\alpha}} - n_{3\alpha}\frac{\delta}{\delta n_{2\alpha}},
$$

where the operator $\frac{\delta}{\delta n_{3\alpha}}$ represents the variational derivative about $\mathbf{n}_3$ assuming that $\mathbf{n}_3$ is an independent vector (ignoring the constraints that $\mathbf{n}_3 \cdot \mathbf{n}_3 = 1$ and $\mathbf{n}_3 \cdot \mathbf{n}_1 = \mathbf{n}_3 \cdot \mathbf{n}_2 = 0$).

Therefore, the variational derivatives of the elastic energy (4.44) with respect to the frame $\mathfrak{p}$ can be respectively calculated as follows:

(SM5.3)

$$
\begin{aligned}
\frac{\delta \mathcal{F}_{Bi}}{\delta n_{1\alpha}} =& K_{1111}D_{11}n_{2k}\partial_\alpha n_{3k} - K_{2222}\partial_k(D_{22}n_{2k}n_{3\alpha}) + K_{3333}D_{33}n_{3k}\partial_k n_{2\alpha} \\
&+ K_{1212}\big(D_{12}n_{3k}\partial_\alpha n_{1k} - \partial_k(D_{12}n_{1k}n_{3\alpha})\big) + K_{2323}D_{23}n_{2k}\partial_k n_{2\alpha} \\
&- K_{3232}\partial_k(D_{32}n_{3k}n_{3\alpha}) + K_{1313}D_{13}n_{1k}(\partial_k n_{2\alpha} + \partial_\alpha n_{2k}) \\
&+ \frac{1}{2}K_{1221}\big(D_{21}n_{3k}\partial_\alpha n_{1k} - \partial_k(D_{21}n_{1k}n_{3\alpha})\big) \\
&+ \frac{1}{2}K_{2332}\big(D_{32}n_{2k}\partial_k n_{2\alpha} - \partial_k(D_{23}n_{3k}n_{3\alpha})\big) \\
&+ \frac{1}{2}K_{1331}D_{31}n_{1k}(\partial_k n_{2\alpha} + \partial_\alpha n_{2k}),
\end{aligned}
$$

(SM5.4)

$$
\begin{aligned}
\frac{\delta \mathcal{F}_{Bi}}{\delta n_{2\alpha}} =& K_{1111}D_{11}n_{1k}\partial_k n_{3\alpha} + K_{2222}D_{22}n_{3k}\partial_\alpha n_{1k} - K_{3333}\partial_k(D_{33}n_{3k}n_{1\alpha}) \\
&+ K_{2121}D_{21}n_{2k}(\partial_k n_{3\alpha} + \partial_\alpha n_{3k}) + K_{2323}\big(D_{23}n_{1k}\partial_\alpha n_{2k} - \partial_k(D_{23}n_{2k}n_{1\alpha})\big) \\
&+ K_{3131}D_{31}n_{3k}\partial_k n_{3\alpha} - K_{1313}\partial_k(D_{13}n_{1k}n_{1\alpha}) \\
&+ \frac{1}{2}K_{1221}D_{12}n_{2k}(\partial_k n_{3\alpha} + \partial_\alpha n_{3k})
\end{aligned}
$$

$$+\frac{1}{2}K_{2332}\big(D_{32}n_{1k}\partial_\alpha n_{2k}-\partial_k(D_{32}n_{2k}n_{1\alpha})\big)$$
$$+\frac{1}{2}K_{1331}\big(D_{13}n_{3k}\partial_k n_{3\alpha}-\partial_k(D_{31}n_{1k}n_{1\alpha})\big),$$

(SM5.5)
$$\begin{aligned}\frac{\delta\mathcal{F}_{Bi}}{\delta n_{3\alpha}}=&-K_{1111}\partial_k(D_{11}n_{1k}n_{2\alpha})+K_{2222}D_{22}n_{2k}\partial_k n_{1\alpha}+K_{3333}D_{33}n_{1k}\partial_\alpha n_{2k}\\&+K_{1212}D_{12}n_{1k}\partial_k n_{1\alpha}-K_{2121}\partial_k(D_{21}n_{2k}n_{2\alpha})+K_{3232}D_{32}n_{3k}(\partial_k n_{1\alpha}+\partial_\alpha n_{1k})\\&+K_{3131}\big(D_{31}n_{2k}\partial_\alpha n_{3k}-\partial_k(D_{31}n_{3k}n_{2\alpha})\big)\\&+\frac{1}{2}K_{1221}\big(D_{21}n_{1k}\partial_k n_{1\alpha}-\partial_k(D_{12}n_{2k}n_{2\alpha})\big)\\&+\frac{1}{2}K_{2332}D_{23}n_{3k}(\partial_k n_{1\alpha}+\partial_\alpha n_{1k})\\&+\frac{1}{2}K_{1331}\big(D_{13}n_{2k}\partial_\alpha n_{3k}-\partial_k(D_{13}n_{3k}n_{2\alpha})\big).\end{aligned}$$

Using the variational derivatives (SM5.5) and (SM5), we have

$$\begin{aligned}&n_{2\alpha}\frac{\delta\mathcal{F}_{Bi}}{\delta n_{3\alpha}}-n_{3\alpha}\frac{\delta\mathcal{F}_{Bi}}{\delta n_{2\alpha}}\\&=-K_{1111}n_{2\alpha}\partial_k(D_{11}n_{1k}n_{2\alpha})-K_{2222}D_{22}(D_{23}+D_{32})\\&\quad+K_{3333}\big(D_{33}D_{23}+n_{3\alpha}\partial_k(D_{33}n_{3k}n_{1\alpha})\big)-K_{1212}D_{12}D_{13}\\&\quad-K_{2121}\big(D_{21}D_{31}+n_{2\alpha}\partial_k(D_{21}n_{2k}n_{2\alpha})\big)+K_{3232}D_{32}(D_{22}-D_{33})\\&\quad-K_{2323}\big(D_{33}D_{23}-n_{3\alpha}\partial_k(D_{23}n_{2k}n_{1\alpha})\big)\\&\quad+K_{3131}\big(D_{31}D_{21}-n_{2\alpha}\partial_k(D_{31}n_{3k}n_{2\alpha})\big)+K_{1313}n_{3\alpha}\partial_k(D_{13}n_{1k}n_{1\alpha})\\&\quad-\frac{1}{2}K_{1221}\big(D_{21}D_{13}+D_{12}D_{31}+n_{2\alpha}\partial_k(D_{12}n_{2k}n_{2\alpha})\big)\\&\quad+\frac{1}{2}K_{2332}\big(D_{23}(D_{22}-D_{33})-D_{33}D_{32}+n_{3\alpha}\partial_k(D_{32}n_{2k}n_{1\alpha})\big)\\&\quad+\frac{1}{2}K_{1331}\big(D_{13}D_{21}-n_{2\alpha}\partial_k(D_{13}n_{3k}n_{2\alpha})+n_{3\alpha}\partial_k(D_{31}n_{1k}n_{1\alpha})\big).\end{aligned}\tag{SM5.6}$$

Similarly, we have

$$\begin{aligned}&n_{3\alpha}\frac{\delta\mathcal{F}_{Bi}}{\delta n_{1\alpha}}-n_{1\alpha}\frac{\delta\mathcal{F}_{Bi}}{\delta n_{3\alpha}}\\&=K_{1111}D_{11}(D_{13}+D_{31})-K_{2222}\partial_k(n_{2k}D_{22})-K_{3333}D_{33}(D_{13}+D_{31})\\&\quad+K_{1212}\big(D_{12}D_{32}-\partial_k(n_{1k}D_{12})\big)+(K_{2121}-K_{2323})D_{23}D_{21}\\&\quad-K_{3232}\big(D_{12}D_{32}+\partial_k(n_{3k}D_{32})\big)+K_{1313}D_{13}(D_{33}-D_{11})\\&\quad-K_{3131}D_{31}(D_{11}-D_{33})+\frac{1}{2}K_{1221}\big(D_{21}D_{32}+D_{12}D_{23}-\partial_k(n_{1k}D_{21})\big)\\&\quad-\frac{1}{2}K_{2332}\big(D_{32}D_{21}+D_{23}D_{12}+\partial_k(n_{3k}D_{23})\big)\\&\quad+\frac{1}{2}K_{1331}(D_{31}+D_{13})(D_{33}-D_{11}),\end{aligned}\tag{SM5.7}$$

and

$$n_{1\alpha}\frac{\delta\mathcal{F}_{Bi}}{\delta n_{2\alpha}}-n_{2\alpha}\frac{\delta\mathcal{F}_{Bi}}{\delta n_{1\alpha}}$$

$$
\begin{aligned}
&= -K_{1111}D_{11}(D_{12}+D_{21}) + K_{2222}D_{22}(D_{12}+D_{21}) - K_{3333}\partial_k(n_{3k}D_{33}) \\
&\quad + K_{2121}D_{21}(D_{11}-D_{22}) + K_{2323}\big(D_{23}D_{13} - \partial_k(n_{2k}D_{23})\big) \\
&\quad + (K_{3232}-K_{3131})D_{31}D_{32} - K_{1313}\big(D_{13}D_{23} + \partial_k(n_{1k}D_{13})\big) \\
&\quad - K_{1212}D_{12}(D_{22}-D_{11}) + \frac{1}{2}K_{1221}(D_{12}+D_{21})(D_{11}-D_{22}) \\
&\quad + \frac{1}{2}K_{2332}\big(D_{32}D_{13} + D_{23}D_{31} - \partial_k(n_{2k}D_{32})\big) \\
&\quad - \frac{1}{2}K_{1331}\big(D_{32}D_{13} + D_{23}D_{31} + \partial_k(n_{1k}D_{31})\big). \qquad \text{(SM5.8)}
\end{aligned}
$$

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