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Statistical foundations of liquid-crystal theory:

I. Discrete systems of rod-like molecules

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Abstract

We develop a mechanical theory for systems of rod-like particles. Central to our approach is the assumption that the external power expenditure for any subsystem of rods is independent of the underlying frame of reference. This assumption is used to derive the basic balance laws for forces and torques. By considering inertial forces on par with other forces, these laws hold relative to any frame of reference, inertial or noninertial. Finally, we introduce a simple set of constitutive relations to govern the interactions between rods and find restrictions necessary and sufficient for these laws to be consistent with thermodynamics. Our framework provides a foundation for a statistical mechanical derivation of the macroscopic balance laws governing liquid crystals.

Keywords

Newtonian mechanics; power; frame-indifference; rod-rod interactions; constitutive theory

1 Introduction

The continuum theory of liquid crystals is based on the idea that, at some microscopic scale, each material point consists of a collection of rigid, rod-like molecules. The orientations of these molecules, when averaged, gives rise to a kinematical descriptor, often referred to as an order parameter, not present in traditional continuum theories.

In the simplest continuum theories of liquid crystals, the order parameter is a vector field with unit magnitude. Initiated by Oseen [1], this approach was taken up by Ericksen [2], who formulated general laws of balance, and Leslie [3], who derived general constitutive relations. The books of de Gennes & Prost [4], Chandrasekhar [5], and Virga [6] and the review articles of Stephen & Straley [7], Ericksen [8], Jenkins [9], and Leslie [10] demonstrate that the Ericksen–Leslie theory captures and explains many facets of the behavior of nematic liquid crystals. To describe transformations between the isotropic and uniaxial phases of a nematic liquid crystal de Gennes [11] invoked ideas of Landau [12,13] to yield a phenomenological continuum theory based on a symmetric and traceless tensor-valued order parameter. Building upon Ericksen’s [14] general theory for anisotropic fluids, MacMillan [15] provided a dynamical generalization that includes as special cases not only the Ericksen–Leslie theory but also Ericksen’s [16] theory for liquid crystals with variable degree of orientation. Further developments in this vein are described by Sonnet, Maffettone & Virga [17], who employed a variational principle to obtain equations of motion and

carefully applied invariance and symmetry considerations to arrive at constitutive relations. The presence of an order parameter, whether unit-vector- or tensor-valued, leads to alterations of the fundamental balance laws familiar from treatments of more conventional media. Although the mass balance and momentum balance are unchanged, the moment of momentum balance contains additional terms: aside from an inertial term associated with the rotation of the order parameter, there are terms associated with surface and body couples. The energy balance has a non-standard kinetic energy term linked with rotary inertia, as well as terms accounting for additional power expenditures associated with the surface and body couples. There is also an additional balance law, originally proposed by Oseen [1], associated with the order parameter, which we shall call the orientation balance. Ideally, it should be possible to derive the balance laws, including all the non-standard terms and the orientation balance, using statistical mechanics in much the same way that Irving & Kirkwood [18] and Noll [19] derived the conventional continuum laws of balance.

Connections between various features of the discrete and continuous descriptions of liquid crystals have appeared in the literature. Lubensky [20] contributed a precise formula for the order parameter in terms of the orientations of the molecules. This was achieved by first modeling the molecules as rigid rods with orientations described by unit vectors. These unit vectors were then used to form a tensor order parameter that is symmetric and traceless and measures how far the state of the medium deviates from isotropic—that is, a state in which the rods are randomly oriented. Importantly, it transpires that the unit vector associated with the largest eigenvalue of the tensor order parameter corresponds to the order parameter used in unit-vector-based theories. Lubensky [20] also provided a formula for the additional inertial term appearing in the moment of momentum balance in terms of the rotation of the microscopic rods. However, he gave no formulas for the additional terms appearing in the moment of momentum and the energy balances. Despite Oseen's [1] proposal, Lubensky [20] did not introduce an additional balance law for the order parameter. Instead, he argued for a supplemental compatibility condition involving the skew part of the Cauchy stress. In combination with the moment of momentum balance, that compatibility condition gives rise to an evolution equation for the order parameter.

Beginning with a careful inspection of the moment of momentum balance for a single rigid rod, Müller [21] furnished some motivation for the additional terms in the macroscopic moment of momentum balance. Recognizing that the orientation of a rigid rod is completely determined by the position of its center of mass and a unit vector describing its orientation, Müller [21] decomposed each term in the moment of momentum balance into components associated with the center of mass and orientation of the rod. He then used these terms for guidance in formulating a macroscopic balance for the moment of momentum of a liquid crystal. In a similar fashion, Müller [21] motivated the additional terms in the energy balance. Like Lubensky [20], Müller [21] stipulated a compatibility condition which, in combination with the moment of momentum balance, gives rise to an evolution equation for the order parameter.

A rigorous statistical derivation of the macroscopic balance laws for liquid crystals, following the approach pioneered by Irving & Kirkwood [18] and enhanced by Noll [19] for conventional continua, remains absent from the literature. To carry out such a derivation requires a discrete theory for systems of rigid rods that encompasses both the interactions between rods and how rods are affected by the environment. In their derivations of the balance laws of conventional continua, Irving & Kirkwood [18] and Noll [19] dealt with the interactions between particles and the momentum balance of a particle. For liquid crystals consisting of collections of long molecules that can be modeled as rigid rods, it seems likely that a derivation of the macroscopic balance laws would require knowledge of the interactions between rods and the momentum balance for a rod. Moreover, due to the extra

structure of a rod, the moment of momentum balance of a rod is also likely to play an important role. Thus, once the interactions between rods and the balances of momentum and moment of momentum for discrete systems of rods are understood, statistical mechanics can be used to clarify the microscopic basis for the non-classical terms that enter the moment of momentum balance, energy balance, and, perhaps most importantly, the orientation balance.

The orientation balance merits some extra discussion. As mentioned above, there are two distinct approaches to arriving at an equation governing the evolution of the order parameter. Some workers postulate this balance independently, while others, under the presumption that a compatibility condition holds, derive it from the moment of momentum balance. Although these two points of view appear to conflict, they both carry elements of truth. When considering systems of rigid rods, we show that it is possible to derive a balance from the moment of momentum balance that is a discrete precursor of the orientation balance for liquid crystals. However, when obtaining the balance laws for liquid crystals via statistics, the orientation balance arises from considerations independent of those used to arrive at the other balance laws. This is analogous to the role of the moment of momentum balance in classical particle mechanics. In this case, granted that particle-particle interactions are governed by a potential that depends only on the distance between the particles and the orientation of the line connecting the particles, the forces between particles are equal and opposite and are directed along the line connecting the particles. Using this, the moment of momentum balance for systems of particles can be derived from the momentum balance. Nevertheless, the macroscopic moment of momentum balance ensues using statistics independent of from those leading to the macroscopic momentum balance.

Here, we develop a discrete foundation for a statistical derivation of the balance laws for liquid crystals. This idea is not without precedent. For instance, to provide motivation for their theory for continuous bodies with affine microstructure, Capriz & Podio Guidugli [22] fashioned a discrete theory in which the particles were constrained to affine motions. Our formulation follows Fried's [23] approach to the mechanics of classical particle systems. We begin by describing a system of rigid rods and synopsizing the kinematics of such a system. Forces and couples are then introduced as basic concepts and the induced power expenditures are discussed. To obtain the balance laws, we capitalize on the approach put forward by Noll [24] in the context of continuum mechanics. This approach assumes that surface tractions and external body forces, inertial contributions included, are frame-indifferent. It also assumes that the external power expended on any part of a body does not change when viewed in different frames of reference. These two assumptions are sufficient to obtain the two main balance laws. Beatty [25] extended Noll's [24] approach to account for torques not generated by forces—that is, for couples. With an application of this method, we obtain the expected balance laws for systems of rigid rods along with other salient results. Noll's [24] approach is advantageous because it allows the balance laws for momentum and moment of momentum to be obtained without prior knowledge of their exact forms. All that is required in advance is an expression for the external power expenditure.

The paper is organized as follows. In Section 2, we introduce essential notation. In Section 3, motivation for later developments is provided via the consideration of a single one-dimensional rod, which we use to model a rod-like particle. The material in Sections 4 and 5 concerns the mathematical description of systems of rod-like particles and their kinematics, respectively. The notions of force, torque, and power are discussed in Sections 6–8. In Section 9, we define what it means for an object to be frame-indifferent. The implications of assuming that the external power is frame-indifferent are explored in Section 10. In Section 11, it is shown how the law of power balance follows from the balance of forces and balance of torques. In Section 13, we specialize our results to an inertial frame of reference. In

Section 14, we describe the principle of interaction-energy imbalance and in Section 15 we discuss constitutive relations and how they are impacted by that principle. In Section 16, we describe the form the balance laws for systems of rigid rods take when these constitutive relations are used. Finally, in Section 17, we summarize our results.

2 Notation

Here we collect some notation for later use.

Let $\mathbb{R}$ denote the set of real numbers. Further, let $\mathbb{P}^\times$ denote the set of strictly positive real numbers and $\mathbb{P}$ denote the set of positive numbers, zero included.

Given a finite-dimensional inner-product space $\mathcal{V}$ the set of all unit vectors in $\mathcal{V}$ is denoted by $\text{Usph}(\mathcal{V})$. The set of all linear mappings from $\mathcal{V}$ to itself is denoted by $\text{Lin}(\mathcal{V})$. Given vectors $\mathbf{a}$ and $\mathbf{b}$ in $\mathcal{V}$ the element of $\text{Lin}(\mathcal{V})$ denoted by $\mathbf{a} \otimes \mathbf{b}$, called the tensor product, is defined by

$$(\mathbf{a} \otimes \mathbf{b})\mathbf{v} := (\mathbf{b} \cdot \mathbf{v})\mathbf{a} \quad \text{for all } \mathbf{v} \in \mathcal{V}. \quad (1)$$

The set of all orthogonal linear mappings on $\mathcal{V}$ is denoted by $\text{Orth}(\mathcal{V})$. Recall that an orthogonal mapping $\mathbf{Q}$ satisfies

$$\mathbf{Q}\mathbf{Q}^\top = \mathbf{Q}^\top\mathbf{Q} = \mathbf{1}, \quad (2)$$

where $\mathbf{Q}^\top$ is the transpose of $\mathbf{Q}$. The subset of $\text{Orth}^+(\mathcal{V})$ consisting of all orthogonal linear mappings with positive determinant, that is of all rotations, is denoted by $\text{Orth}^+(\mathcal{V})$. A linear mapping $\mathbf{W}$ is said to be skew if

$$\mathbf{W}^\top = -\mathbf{W}. \quad (3)$$

The set of all skew linear mappings is denoted by $\text{Skew}(\mathcal{V})$. The wedge product $\mathbf{a} \wedge \mathbf{b}$ of $\mathbf{a}$ and $\mathbf{b}$ in $\mathcal{V}$ is the linear mapping defined by¹

$$\mathbf{a} \wedge \mathbf{b} := \frac{1}{\sqrt{2}}(\mathbf{a} \otimes \mathbf{b} - \mathbf{b} \otimes \mathbf{a}). \quad (4)$$

It is not difficult to see that $\mathbf{a} \wedge \mathbf{b}$ is skew. The circle product $\mathbf{a} \odot \mathbf{b}$ of $\mathbf{a}$ and $\mathbf{b}$ is the linear mapping defined by²

$$\mathbf{a} \odot \mathbf{b} := \frac{1}{\sqrt{2}}(\mathbf{a} \otimes \mathbf{b} + \mathbf{b} \otimes \mathbf{a}). \quad (5)$$

¹More often, the wedge product of $\mathbf{a}$ and $\mathbf{b}$ is defined by

$$\mathbf{a} \wedge \mathbf{b} := \mathbf{a} \otimes \mathbf{b} - \mathbf{b} \otimes \mathbf{a} \quad \text{or} \quad \mathbf{a} \wedge \mathbf{b} := \frac{1}{2}(\mathbf{a} \otimes \mathbf{b} - \mathbf{b} \otimes \mathbf{a}).$$

The factor of $1/\sqrt{2}$ appearing in (4) ensures that the magnitude of $\mathbf{a} \wedge \mathbf{b}$ is equal to that of the corresponding axial vector. This choice is common in the field of mathematical physics. See, for example, Reed & Simon [26].

²The factor of $1/\sqrt{2}$ appearing in (5) ensures consistency with (4).

Let an open subset $\mathcal{D}$ of $\mathbb{R}^4$ and a smooth function $\psi : \mathcal{D} \rightarrow \mathbb{R}$ be given. For any i in $\{1, 2, 3, 4\}$, we denote by

$$\psi_{,i} : \mathcal{D} \rightarrow \mathbb{R} \quad (6)$$

the partial derivative of ψ with respect to its i -th argument; in particular, for $i = 1$, we have

$$\psi_{,1}(a_1, a_2, a_3, a_4) = \lim_{h \rightarrow 0} \frac{\psi(a_1 + h, a_2, a_3, a_4) - \psi(a_1, a_2, a_3, a_4)}{h}, \quad (7)$$

for all (a_1, a_2, a_3, a_4) in $\mathcal{D}$

3 One-dimensional rigid rods

To motivate various concepts used to treat systems of rod-like particles it is advantageous to consider a single rod-like particle. Following Müller [21], we model such a particle as a one-dimensional rigid rod.

3.1 Mathematical model

Let a frame of reference in the form of a three-dimensional Euclidean point space $\mathcal{E}$, with associated vector space $\mathcal{V}$ and a scalar L in $\mathbb{P}^\times$ be given. Put $R := [-L/2, L/2]$. A mapping $\kappa : R \rightarrow \mathcal{E}$ is called an isometry if it preserves distances, that is, if

$$|r_1 - r_2| = d_{\mathcal{E}}(\kappa(r_1), \kappa(r_2)) \quad \text{for all } r_1, r_2 \in R, \quad (8)$$

where $d_{\mathcal{E}}$ is the distance function associated with $\mathcal{E}$. The set R together with all isometries from R to $\mathcal{E}$ can be seen to model a one-dimensional rigid rod of length L . Each isometry κ describes a possible position of the rod. The range $\text{Rng } \kappa$ of an isometry κ gives the points in $\mathcal{E}$ that the rod occupies and is called a placement of the rod R . The elements r of R are called material points.

Every placement κ of R is completely determined by a point $x_c := \kappa(0)$, called the center of R in the placement κ , and a unit vector

$$\mathbf{d} := \frac{\kappa(L/2) - \kappa(-L/2)}{L}, \quad (9)$$

called the director of R in the placement κ . Using the fact that κ is an isometry, we have that

$$\kappa(r) = x_c + r\mathbf{d} \quad \text{for all } r \in R. \quad (10)$$

3.2 Motion of a one-dimensional rigid rod

Let $\mathcal{Q}$ be a time-interval, that is an open, connected subset of $\mathbb{R}$. A motion of a rod R is a mapping μ of the form

$$\mu : R \times \mathcal{I} \rightarrow \mathcal{E} \quad (11)$$

such that, for all t in $\mathcal{Q}$ the mapping $\mu_t := \mu(\cdot, t) : R \rightarrow \mathcal{E}$ is a placement of R . Since, during a motion, R may at different times occupy different placements, its center and director may vary with time. We denote by

$$x_c : \mathcal{I} \rightarrow \mathcal{E} \quad \text{and} \quad \mathbf{d} : \mathcal{I} \rightarrow \text{Usph}(\mathcal{V}) \quad (12)$$

the mappings that, at each time during a motion, give the center and the director of R , respectively.

As is customary in mechanics, we use a superposed dot to denote differentiation with respect to time. If a motion μ is smooth, we then write

$$\mathbf{v} := \dot{\mu} \quad \text{and} \quad \mathbf{a} := \dot{\mathbf{v}} = \ddot{\mu} \quad (13)$$

for the velocity and acceleration of R , both of which are mappings from $R \times \mathcal{Q}$ to $\mathcal{V}$. In an analogous way we write

$$\mathbf{v}_c := \dot{x}_c \quad \text{and} \quad \mathbf{a}_c := \dot{\mathbf{v}}_c = \ddot{x}_c \quad (14)$$

for the velocity and acceleration of the center of the rod, which are both mappings from $\mathcal{Q}$ to $\mathcal{V}$. Further, we write

$$\mathbf{s} := \dot{\mathbf{d}} \quad (15)$$

for the spin of R . Since $|\mathbf{d}|^2 = 1$, we have

$$\mathbf{d} \cdot \mathbf{s} = 0. \quad (16)$$

Given $r \in R$, it follows from (10), (13), and (14) that

$$\left. \begin{aligned} \mu(r, t) &= x_c(t) + r\mathbf{d}(t), \\ \mathbf{v}(r, t) &= \mathbf{v}_c(t) + r\mathbf{s}(t), \\ \mathbf{a}(r, t) &= \mathbf{a}_c(t) + r\dot{\mathbf{s}}(t), \end{aligned} \right\} \quad \text{for all } (r, t) \in R \times \mathcal{I}. \quad (17)$$

3.3 Change of frame

A change of frame is specified by three ingredients: two mappings

$$z: \mathcal{I} \rightarrow \mathcal{E} \quad \text{and} \quad \mathbf{Q}: \mathcal{I} \rightarrow \text{Orth}^+(\mathcal{V}) \quad (18)$$

and a point y in $\mathcal{E}$ so that any point x in $\mathcal{E}$, when viewed in the new frame at time t , is given by

$$x^*(t) = z(t) + \mathbf{Q}(t)(x - y). \quad (19)$$

Since the values of $\mathbf{Q}$ are orthogonal, we have $\mathbf{Q}\mathbf{Q}^\top = \mathbf{1}$. Differentiating this relation, we find that

$$\dot{\mathbf{Q}}\mathbf{Q}^\top \quad \text{has skew values.} \quad (20)$$

It follows from (9) and (19) that if $\mathbf{d}^*$ is the director of the rod R viewed in the new frame, then

$$\mathbf{d}^* = \mathbf{Q}\mathbf{d} \quad \text{and} \quad \mathbf{s}^* = \dot{\mathbf{d}}^* = \dot{\mathbf{Q}}\mathbf{d} + \mathbf{Q}\mathbf{s}. \quad (21)$$

Let $\mathbf{v}_c^* = \dot{x}_c^*$ denote the velocity of the center of R in the new frame. By taking $x = x_c$ and differentiating (19), we obtain

$$\mathbf{v}_c^* = \dot{\mathbf{z}} + \dot{\mathbf{Q}}(x_c - y) + \mathbf{Q}\mathbf{v}_c = \dot{\mathbf{z}} + \dot{\mathbf{Q}}\mathbf{Q}^\top(x_c - y)^* + \mathbf{Q}\mathbf{v}_c. \quad (22)$$

3.4 Forces, moments, and power for a rod

We assume that all forces acting on the rod R are continuously distributed, so that, given a motion μ of R , there is a function

$$\mathbf{f}: R \times \mathcal{J} \rightarrow \mathcal{V} \quad (23)$$

such that $\mathbf{f}(r, t)$ gives the force per unit length acting on R at the point $\mu(r, t)$ at time t .

The resultant force $\mathbf{f}_{\text{res}}: \mathcal{Q} \rightarrow \mathcal{V}$ defined by

$$\mathbf{f}_{\text{res}}(t) := \int_R \mathbf{f}(r, t) dr \quad \text{for all } t \in \mathcal{J}, \quad (24)$$

gives the net force acting on R at each time t . Let a point y in $\mathcal{E}$ be given. Analogously, the torque $\mathbf{R}: \mathcal{Q} \rightarrow \text{Skew}(\mathcal{V})$ acting on R about y generated by $\mathbf{f}$ is defined by

$$\mathbf{R}(t) := \int_R (\mu(r, t) - y) \wedge \mathbf{f}(r, t) dr \quad \text{for all } t \in \mathcal{J}. \quad (25)$$

Using (17)₁ and (24), we have

$$\mathbf{R}(t) = \int_R (x_c(t) + r\mathbf{d}(t) - y) \wedge \mathbf{f}(r, t) dr = (x_c(t) - y) \wedge \int_R \mathbf{f}(r, t) dr + \mathbf{d}(t) \wedge \int_R r\mathbf{f}(r, t) dr = (x_c(t) - y) \wedge \mathbf{f}_{\text{res}}(t) + \mathbf{d}(t) \wedge \int_R r\mathbf{f}(r, t) dr.$$

Motivated by this calculation, we define the resultant couple $\mathbf{c}: \mathcal{Q} \rightarrow \mathcal{V}$ by

$$\mathbf{c}(t) := \int_R r\mathbf{f}(r, t) dr \quad \text{for all } t \in \mathcal{J} \quad (26)$$

so that the net torque on R is given by

$$\mathbf{R} = (x_c - y) \wedge \mathbf{f}_{\text{res}} + \mathbf{d} \wedge \mathbf{c}. \quad (27)$$

Notice that although it has the dimensions of a torque, $\mathbf{c}$ is not a torque; indeed, $\mathbf{c}$ only gives a torque once it is wedged with a director.

We refer to

$$P(t) = \int_R \mathbf{f}(r, t) \cdot \mathbf{v}(r, t) dr \quad (28)$$

as the power expended on R at time t . Notice that, on using (17)₂, (24), and (26), we have

$$P = \mathbf{v}_c \cdot \mathbf{f}_{\text{res}} + \mathbf{s} \cdot \mathbf{c}. \quad (29)$$

On the right-hand side of (29), the first term is the power expenditure associated with the velocity of the center of the rod and the second term is the power expenditure associated with the rate of change of the orientation of R .

3.5 Mass, inertia, and inertial forces

The force $\mathbf{f}$ acting on the rod R is assumed to admit an additive decomposition including both an inertial contribution $\mathbf{f}^{\text{in}}$ and a noninertial contribution $\mathbf{f}^{\text{ni}}$ and, thus, to have the form

$$\mathbf{f} = \mathbf{f}^{\text{in}} + \mathbf{f}^{\text{ni}}. \quad (30)$$

We also assume that R has a mass m with uniformly distributed density ρ in $\mathbb{P}^\times$.

If the frame of reference $\mathcal{E}$ under consideration is inertial, then $\mathbf{f}^{\text{in}}$ has the form

$$\mathbf{f}^{\text{in}}(r, t) := -\rho \mathbf{a}(r, t) = -\rho(\mathbf{a}_c(t) + r\dot{\mathbf{s}}(t)) \quad \text{for all } (r, t) \in R \times \mathcal{I}. \quad (31)$$

The resultant force $\mathbf{f}_{\text{res}}^{\text{in}}$ due to inertial forces can be computed using (24), giving

$$\mathbf{f}_{\text{res}}^{\text{in}}(t) = \int_R \mathbf{f}^{\text{in}}(r, t) dr = -m \mathbf{a}_c(t) \quad \text{for all } t \in \mathcal{I} \quad (32)$$

and the couple force $\mathbf{c}^{\text{in}}$ due to inertial forces can be computed using (26), giving

$$\mathbf{c}^{\text{in}}(t) = \int_R r \mathbf{f}^{\text{in}}(r, t) dr = -\frac{mL^2}{12} \dot{\mathbf{s}}(t) \quad \text{for all } t \in \mathcal{I}. \quad (33)$$

The linear momentum $\mathbf{p}$ of R is defined by

$$\mathbf{p}(t) := \int_R \rho \mathbf{v}(r, t) dr \quad \text{for all } t \in \mathcal{I}. \quad (34)$$

Using (17)₂, we have

$$\mathbf{p} = m \mathbf{v}_c. \quad (35)$$

Similarly, the angular momentum $\mathbf{L}(\cdot; y)$ of R relative to a point y in $\mathcal{E}$ is defined by

$$\mathbf{L}(t; y) := \int_R \rho(\mu(r, t) - y) \wedge \mathbf{v}(r, t) dr \quad \text{for all } t \in \mathcal{I}. \quad (36)$$

Using (17)₂, we have

$$\mathbf{L}(\cdot; y) = m(x_c - y) \wedge \mathbf{v}_c + I \mathbf{d} \wedge \mathbf{s}, \quad (37)$$

where

$$I := \frac{mL^2}{12} \quad (38)$$

is the scalar moment of inertia.

Finally, the moment of inertia tensor $\mathbf{Y}$ of R at time t is

$$\mathbf{Y}(t) := \int_R \rho(|\mu(r, t)|^2 \mathbf{1} - (\mu(r, t) - x_c(t)) \otimes (\mu(r, t) - x_c(t))) dr \quad (39)$$

$$=I(\mathbf{1} - \mathbf{d}(t) \otimes \mathbf{d}(t)). \quad (40)$$

Notice that $\mathbf{Y}$ is positive semidefinite. Ordinarily, the moment of inertia tensor of a rigid body is positive definite. The degeneracy here arises because the rigid body under consideration is one-dimensional.

3.6 Summary

We have seen that a placement of a one-dimensional rigid-rod is completely characterized by the position of its center of mass and its director. Also, to give expressions for the forces on the rod, the moments on the rod, and the power expended on the rigid rod, only the resultant force and the resultant couple come into play.

When considering placements for a system of such rods, we therefore deal only with the positions of the centers and the directors of the rods. When we consider forces acting on the rods, we need only consider the resultant force and resultant couple on each rod. Furthermore, when dealing with mass and inertia, only two constants come up: the mass m and the scalar moment of inertia I . The tensor moment of inertia is not needed here; however, it is needed when deriving the macroscopic balance laws for liquid crystals.

4 Systems of rigid rods

Motivated by the developments presented in the last section, we define a system of rigid rods to be a finite set $\mathcal{B}$ consisting of at least two elements together with a set of mappings, called configurations, of the form

$$\kappa: \mathcal{B} \rightarrow \mathcal{E} \times \text{Usph}(\mathcal{V}). \quad (41)$$

Elements of $\mathcal{B}$, usually denoted by p, q , and so on, are called rods. Given a rod p in $\mathcal{B}$, we call $\kappa(p) = (x_p, \mathbf{d}_p)$ its configuration. The point x_p represents the position of the center of p and the unit vector $\mathbf{d}_p$ represents the director of p in the placement κ . We assume that the configurations of the rods are such that no overlap occurs in any placement.

A subset $\mathcal{P}$ of $\mathcal{B}$ represents a subsystem of rigid rods. Given a subsystem $\mathcal{P}$ the complementary subsystem $\mathcal{B} \setminus \mathcal{P}$ of all rods that are not in $\mathcal{P}$ is denoted by $\mathcal{P}^c$. Given a rod p in $\mathcal{B}$, we denote by $\mathcal{P}_p$ all rods in $\mathcal{P}$ that are not p : $\mathcal{P}_p := \mathcal{P} \setminus \{p\}$. A given subsystem $\mathcal{P}$ has the structure of a system of rigid rods whose placements are restrictions of placements of $\mathcal{B}$.

We say that two subsystems $\mathcal{P}$ and $\mathcal{Q}$ are disjoint if $\mathcal{P} \cap \mathcal{Q} = \emptyset$. We denote the set of all subsystems of $\mathcal{B}$ by $\text{Sub } \mathcal{B}$ and the set of all pairs of subsystems of $\mathcal{B}$ that are disjoint by $(\text{Sub } \mathcal{B})_{\text{dis}}^2$.

Let $\mathcal{W}$ be a linear space. A mapping $\mathbf{h} : \text{Sub } \mathcal{B} \rightarrow \mathcal{W}$ is said to be additive if

$$\mathbf{h}(\mathcal{P} \cup \mathcal{Q}) = \mathbf{h}(\mathcal{P}) + \mathbf{h}(\mathcal{Q}) \quad \text{for all } (\mathcal{P}, \mathcal{Q}) \in (\text{Sub } \mathcal{B})_{\text{dis}}^2. \quad (42)$$

A mapping $\mathbf{I} : (\text{Sub } \mathcal{B})_{\text{dis}}^2 \rightarrow \mathcal{W}$ is said to be an interaction if for all subsystems $\mathcal{P}$ both

$$\mathbf{I}(\cdot, \mathcal{P}') : (\text{Sub } \mathcal{P})_{\text{dis}}^2 \rightarrow \mathcal{W} \quad \text{and} \quad \mathbf{I}(\mathcal{P}', \cdot) : (\text{Sub } \mathcal{P})_{\text{dis}}^2 \rightarrow \mathcal{W} \quad (43)$$

are additive.

For the rest of this paper, let a system of rigid rods $\mathcal{B}$ be given.

5 Motion of a system of rigid rods

Let $\mathcal{Q}$ be a time-interval. A motion of a system of rigid rods $\mathcal{B}$ is a mapping

$$\mu: \mathcal{B} \times \mathcal{I} \rightarrow \mathcal{E} \times \text{Usph}(\mathcal{V}) \quad (44)$$

such that for all t in $\mathcal{Q}$, $\mu_t := \mu(\cdot, t)$ is a configuration of $\mathcal{B}$. Given a rod p in $\mathcal{B}$, we denote by $x_p: \mathcal{Q} \rightarrow \mathcal{E}$ the mapping that gives the center of p at each time and we denote by $\mathbf{d}_p: \mathcal{Q} \rightarrow \text{Usph}(\mathcal{V})$ the mapping that gives the director of p at each time, so that

$$\mu(p, t) = (x_p(t), \mathbf{d}_p(t)) \quad \text{for all } (p, t) \in \mathcal{B} \times \mathcal{I}. \quad (45)$$

We assume that x_p and $\mathbf{d}_p$ are of class C^2 for all p in $\mathcal{B}$.

The velocity and acceleration of a rod p are given by

$$\mathbf{v}_p := \dot{x}_p \quad \text{and} \quad \mathbf{a}_p := \dot{\mathbf{v}}_p = \ddot{x}_p. \quad (46)$$

The spin, or rate-of-change of the director, of a rod p is denoted by

$$\mathbf{s}_p := \dot{\mathbf{d}}_p. \quad (47)$$

Differentiating the relation $|\mathbf{d}_p|^2 = 1$, we obtain

$$\mathbf{s}_p \cdot \mathbf{d}_p = 0. \quad (48)$$

Given rods p and q , we use

$$\mathbf{r}_{pq} := x_p - x_q \quad (49)$$

to denote the vector going from the center of q to that of p . Furthermore, we write

$$\mathbf{v}_{pq} := \mathbf{v}_p - \mathbf{v}_q \quad (50)$$

for the velocity of rod p relative to rod q .

6 Forces

Consider a configuration of the system $\mathcal{B}$ and a rod p in $\mathcal{B}$. We assume that all influences acting on p are due either to interactions with other rods in $\mathcal{B}$ or to interactions with the environment external to $\mathcal{B}$. Motivated by the developments appearing in Section 3.4, we introduce resultant forces and couples. The resultant force of a rod q acting on rod p is denoted by $\mathbf{f}_{pq}$ and the resultant environmental force acting on rod p is denoted by $\mathbf{f}_p^{\text{ext}}$.

Similarly, $\mathbf{c}_{pq}$ and $\mathbf{c}_p^{\text{ext}}$ denote, respectively, the resultant couple of q on p and the resultant environmental couple on p . We assume that the resultant environmental force and couple admit additive decompositions,

$$\mathbf{f}_p^{\text{ext}} = \mathbf{f}_p^{\text{in}} + \mathbf{f}_p^{\text{ni}} \quad \text{and} \quad \mathbf{c}_p^{\text{ext}} = \mathbf{c}_p^{\text{in}} + \mathbf{c}_p^{\text{ni}}, \quad (51)$$

involving inertial contributions $\mathbf{f}_p^{\text{in}}$ and $\mathbf{c}_p^{\text{in}}$ and noninertial contributions $\mathbf{f}_p^{\text{ni}}$ and $\mathbf{c}_p^{\text{ni}}$.

Given disjoint subsystems $\mathcal{P}$ and $\mathcal{Q}$ of $\mathcal{B}$, let

$$\mathbf{f}(\mathcal{P}, \mathcal{Q}) := \sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{Q}} \mathbf{f}_{pq} \quad (52)$$

denote the total resultant force of subsystem $\mathcal{Q}$ on subsystem $\mathcal{P}$. Similarly, let

$$\mathbf{f}^{\text{ext}}(\mathcal{P}) := \sum_{p \in \mathcal{P}} \mathbf{f}_p^{\text{ext}} \quad \text{and} \quad \mathbf{c}^{\text{ext}}(\mathcal{P}) := \sum_{p \in \mathcal{P}} \mathbf{c}_p^{\text{ext}} \quad (53)$$

denote the total resultant environmental force and the total resultant environmental couple acting on subsystem $\mathcal{P}$ respectively. As is customary, the sum over the empty set is defined to be zero:

$$\mathbf{f}(\mathcal{P}, \emptyset) = \mathbf{f}(\emptyset, \mathcal{P}) = \mathbf{0}. \quad (54)$$

Physically, (54) means that the subsystem consisting of no rods does not exert any forces on any other subsystem. Using the above definitions it is not hard to show that $\mathbf{f}^{\text{ext}}$ and $\mathbf{c}^{\text{ext}}$ are additive and that $\mathbf{f}$ is an interaction, as defined in (42) and (43).

If the system is in motion, then all of the forces introduced above also depend on time. For notational brevity, we do not make dependence on time explicit.

7 Torques

Consider a placement of the system $\mathcal{B}$ and rods p and q in $\mathcal{B}$. Once again we are motivated by developments appearing in Section 3.4. Let a point y in $\mathcal{E}$ be given. The torque about y from rod q acting on rod p is given by

$$\mathbf{R}_{pq}(y) := (x_p - y) \wedge \mathbf{f}_{pq} + \mathbf{d}_p \wedge \mathbf{c}_{pq} \quad (55)$$

and the torque about y from the environment acting on p is given by

$$\mathbf{R}_p^{\text{ext}}(y) := (x_p - y) \wedge \mathbf{f}_p^{\text{ext}} + \mathbf{d}_p \wedge \mathbf{c}_p^{\text{ext}}. \quad (56)$$

Given disjoint subsystems $\mathcal{P}$ and $\mathcal{Q}$ of $\mathcal{B}$

$$\mathbf{R}(\mathcal{P}, \mathcal{Q}; y) := \sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{Q}} ((x_p - y) \wedge \mathbf{f}_{pq} + \mathbf{d}_p \wedge \mathbf{c}_{pq}) \quad (57)$$

denotes the net torque about y of subsystem $\mathcal{Q}$ acting on subsystem $\mathcal{P}$. Similarly,

$$\mathbf{R}^{\text{ext}}(\mathcal{P}; y) := \sum_{p \in \mathcal{P}} ((x_p - y) \wedge \mathbf{f}_p^{\text{ext}} + \mathbf{d}_p \wedge \mathbf{c}_p^{\text{ext}}) \quad (58)$$

denotes the net torque about y on subsystem $\mathcal{P}$. Using these definitions, one can easily show that $\mathbf{R}^{\text{ext}}(\cdot; y)$ is additive and that $\mathbf{R}(\cdot, \cdot; y)$ is an interaction, as defined in (42) and (43).

As in the discussion of forces, if the system is in motion, then all of the torques introduced above also depend on time. We do not make the dependence on time explicit.

8 Power

Let p and q be distinct rods belonging to the system $\mathcal{B}$ of rods and assume that $\mathcal{B}$ is undergoing some motion μ . The expression

$$\mathbf{f}_{pq} \cdot \mathbf{v}_p + \mathbf{c}_{pq} \cdot \mathbf{s}_p \quad (59)$$

gives the power expenditure associated with rod p moving with velocity $\mathbf{v}_p$ under the action of the resultant force $\mathbf{f}_{pq}$ and whose director is changing at a rate $\mathbf{s}_p$ under the action of the resultant couple $\mathbf{c}_{pq}$. Similarly,

$$\mathbf{f}_p^{\text{ext}} \cdot \mathbf{v}_p + \mathbf{c}_p^{\text{ext}} \cdot \mathbf{s}_p \quad (60)$$

gives the power expenditure associated with rod p moving with velocity $\mathbf{v}_p$ under the action of the resultant force $\mathbf{f}_p^{\text{ext}}$ and whose director is changing at a rate $\mathbf{s}_p$ under the action of the resultant couple $\mathbf{c}_p^{\text{ext}}$.

Given a subsystem $\mathcal{P}$ and a rod p in $\mathcal{P}$ we see from (59) that the sum

$$\sum_{q \in \mathcal{P}_p} (\mathbf{f}_{pq} \cdot \mathbf{v}_p + \mathbf{c}_{pq} \cdot \mathbf{s}_p) \quad (61)$$

encompasses the net power expended on p by all the other rods in $\mathcal{P}$. Summing (61) over all p in $\mathcal{P}$ we obtain the net internal power $P_{\text{int}}(\mathcal{P})$ expended on $\mathcal{P}$

$$P_{\text{int}}(\mathcal{P}) = \sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{P}_p} (\mathbf{f}_{pq} \cdot \mathbf{v}_p + \mathbf{c}_{pq} \cdot \mathbf{s}_p). \quad (62)$$

Similarly, the net power expended on p from the exterior of the subsystem $\mathcal{P}$ is given by

$$\sum_{q \in \mathcal{P}'} (\mathbf{f}_{pq} \cdot \mathbf{v}_p + \mathbf{c}_{pq} \cdot \mathbf{s}_p) + \mathbf{f}_p^{\text{ext}} \cdot \mathbf{v}_p + \mathbf{c}_p^{\text{ext}} \cdot \mathbf{s}_p. \quad (63)$$

Summing (63) over all p in $\mathcal{P}$ gives the external power $P_{\text{ext}}(\mathcal{P})$ expended on $\mathcal{P}$

$$P_{\text{ext}}(\mathcal{P}) := \sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{P}'} (\mathbf{f}_{pq} \cdot \mathbf{v}_p + \mathbf{c}_{pq} \cdot \mathbf{s}_p) + \sum_{p \in \mathcal{P}} (\mathbf{f}_p^{\text{ext}} \cdot \mathbf{v}_p + \mathbf{c}_p^{\text{ext}} \cdot \mathbf{s}_p). \quad (64)$$

Notice that neither the internal power P_{int} nor the external power P_{ext} is additive. Other nonadditive mappings have been considered in the literature. For example, Gurtin & Williams [27] considered a general form of an energy balance in which the rate of change of the internal energy is not additive.

9 Frame-indifferent objects and assumptions

Recall the discussion in Section 3.3. A scalar ϕ , vector $\mathbf{w}$, and a linear mapping $\mathbf{L}$ are said to be frame-indifferent if the transformation rules

$$\phi^* = \phi, \mathbf{w}^* = \mathbf{Q}\mathbf{w}, \text{ and } \mathbf{L}^* = \mathbf{Q}\mathbf{L}\mathbf{Q}^\top \quad (65)$$

hold for any change of frame.

Let p and q be rods in $\mathcal{B}$. By (19), we have

$$\mathbf{r}_{pq}^* = \mathbf{x}_p^* - \mathbf{x}_q^* = \mathbf{Q}(\mathbf{x}_p - \mathbf{x}_q) = \mathbf{Q}\mathbf{r}_{pq}, \quad (66)$$

whereby $\mathbf{r}_{pq}$ is frame-indifferent. Also,

$$r_{pq}^* = |\mathbf{r}_{pq}^*| = |\mathbf{Q}\mathbf{r}_{pq}| = |\mathbf{r}_{pq}| = r_{pq}, \quad (67)$$

whereby r_{pq} is frame-indifferent. However,

$$\mathbf{v}_{pq}^* = \mathbf{v}_p^* - \mathbf{v}_q^* = \dot{\mathbf{Q}}\mathbf{Q}^\top \mathbf{r}_{pq}^* + \mathbf{Q}(\mathbf{v}_p - \mathbf{v}_q) = \dot{\mathbf{Q}}\mathbf{Q}^\top \mathbf{r}_{pq}^* + \mathbf{Q}\mathbf{v}_{pq}, \quad (68)$$

whereby the relative velocity between rods is not frame-indifferent. From (21), we see that the director of each rod is frame-indifferent but that the spin is not.

We now make two assumptions involving frame-indifference:

Assumption 1 For all rods p and q in $\mathcal{B}$, $\mathbf{f}_{pq}$ and $\mathbf{c}_{pq}$ are frame-indifferent:

$$\mathbf{f}_{pq}^* = \mathbf{Q}\mathbf{f}_{pq} \quad \text{and} \quad \mathbf{c}_{pq}^* = \mathbf{Q}\mathbf{c}_{pq}. \quad (69)$$

Assumption 2 For all subsystems $\mathcal{P}$ of $\mathcal{B}$, the external power expended on $\mathcal{P}$ is frame-indifferent:

$$P_{\text{ext}}^*(\mathcal{P}) = P_{\text{ext}}(\mathcal{P}). \quad (70)$$

10 Consequences of frame-indifference

Let us investigate the implications of Assumptions 1 and 2. Note that

$$P_{\text{ext}}^*(\mathcal{P}) = \sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{P}'} (\mathbf{f}_{pq}^* \cdot \mathbf{v}_p^* + \mathbf{c}_{pq}^* \cdot \mathbf{s}_p^*) + \sum_{p \in \mathcal{P}} ((\mathbf{f}_p^{\text{ext}})^* \cdot \mathbf{v}_p^* + (\mathbf{c}_p^{\text{ext}})^* \cdot \mathbf{s}_p^*) \quad (71)$$

is the external power expended on $\mathcal{P}$ in the new frame. Using (21)₂, (22), and Assumption 2, we find that the external power is frame-indifferent if and only if

$$\begin{aligned} 0 &= P_{\text{ext}}^*(\mathcal{P}) - P_{\text{ext}}(\mathcal{P}) \\ &= \left(\sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{P}'} \mathbf{f}_{pq}^* \right. \\ &\quad \left. + \sum_{p \in \mathcal{P}} (\mathbf{f}_p^{\text{ext}})^* \right) \\ &\quad \cdot \dot{\mathbf{z}} + \sum_{p \in \mathcal{P}} ((\mathbf{f}_p^{\text{ext}})^* - \mathbf{Q}\mathbf{f}_p^{\text{ext}}) \cdot \mathbf{Q}\mathbf{v}_p + \sum_{p \in \mathcal{P}} ((\mathbf{c}_p^{\text{ext}})^* - \mathbf{Q}\mathbf{c}_p^{\text{ext}}) \cdot \mathbf{Q}\mathbf{s}_p + \sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{P}'} (\mathbf{f}_{pq}^* \cdot \dot{\mathbf{Q}}\mathbf{Q}^\top (\mathbf{x}_p - \mathbf{x}_q)^* + \mathbf{c}_{pq}^* \cdot \dot{\mathbf{Q}}\mathbf{Q}^\top \mathbf{d}_p^*) \\ &\quad + \sum_{p \in \mathcal{P}} ((\mathbf{f}_p^{\text{ext}})^* \cdot \dot{\mathbf{Q}}\mathbf{Q}^\top (\mathbf{x}_p - \mathbf{y})^* + (\mathbf{c}_p^{\text{ext}})^* \cdot \dot{\mathbf{Q}}\mathbf{Q}^\top \mathbf{d}_p^*) \end{aligned} \quad (72)$$

for all changes of frame and all subsystems $\mathcal{P}$ of $\mathcal{B}$.

10.1 Force and torque balance

If we consider a change of frame for which $\mathbf{v} = \mathbf{0}$ and $\dot{\mathbf{Q}} = \mathbf{0}$, then (72) becomes

$$\sum_{p \in \mathcal{P}} ((\mathbf{f}_p^{\text{ext}})^* - Q \mathbf{f}_p^{\text{ext}}) \cdot Q \mathbf{v}_p + \sum_{p \in \mathcal{P}} ((\mathbf{c}_p^{\text{ext}})^* - Q \mathbf{c}_p^{\text{ext}}) \cdot Q \mathbf{s}_p = 0. \quad (73)$$

Now consider a change of frame for which just $\dot{\mathbf{Q}} = \mathbf{0}$ and use (73) with (72) to find that

$$\left(\sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{P}'} \mathbf{f}_{pq}^* + \sum_{p \in \mathcal{P}} (\mathbf{f}_p^{\text{ext}})^* \right) \cdot \dot{\mathbf{z}} = 0. \quad (74)$$

Since we can consider any change of frame, $\dot{\mathbf{z}}$ can be chosen arbitrarily and we conclude that

$$\sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{P}'} \mathbf{f}_{pq}^* + \sum_{p \in \mathcal{P}} (\mathbf{f}_p^{\text{ext}})^* = \mathbf{0}. \quad (75)$$

Since it must hold for any new frame, the stars can be dropped from the foregoing equation. On using (52), (53)₁, and (75), it follows that

$$\mathbf{f}(\mathcal{P}, \mathcal{P}') + \mathbf{f}^{\text{ext}}(\mathcal{P}) = \mathbf{0}, \quad (76)$$

which is referred to as the balance of forces for the subsystem $\mathcal{P}$

Looking back at (72) and using (73) and (75), we find that

$$\begin{aligned} 0 = & \sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{P}'} (\mathbf{f}_{pq}^* \cdot \dot{\mathbf{Q}} \mathbf{Q}^\top (x_p - y)^* + \mathbf{c}_{pq}^* \cdot \dot{\mathbf{Q}} \mathbf{Q}^\top \mathbf{d}_p^*) + \sum_{p \in \mathcal{P}} ((\mathbf{f}_p^{\text{ext}})^* \cdot \dot{\mathbf{Q}} \mathbf{Q}^\top (x_p - y)^* \\ & + (\mathbf{c}_p^{\text{ext}})^* \cdot \dot{\mathbf{Q}} \mathbf{Q}^\top \mathbf{d}_p^*) = \left(\sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{P}'} (\mathbf{f}_{pq}^* \otimes (x_p - y)^* + \mathbf{c}_{pq}^* \otimes \mathbf{d}_p^*) + \sum_{p \in \mathcal{P}} ((\mathbf{f}_p^{\text{ext}})^* \otimes (x_p - y)^* + (\mathbf{c}_p^{\text{ext}})^* \otimes \mathbf{d}_p^*) \right) \cdot \dot{\mathbf{Q}} \mathbf{Q}^\top. \end{aligned} \quad (77)$$

Recall that for a linear mapping $\mathbf{A}$, if $\mathbf{A} \cdot \mathbf{W} = 0$ for all skew linear mappings $\mathbf{W}$, then the skew part of $\mathbf{A}$ must be zero (or, equivalently, $\mathbf{A}$ must be symmetric). Using this fact and recalling that $\dot{\mathbf{Q}} \mathbf{Q}^\top$ can have arbitrary skew values, we may conclude that the skew part of the parenthetical term in (77) must be zero. This can be written as

$$\mathbf{0} = \sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{P}'} (\mathbf{f}_{pq}^* \wedge (x_p - y)^* + \mathbf{c}_{pq}^* \wedge \mathbf{d}_p^*) + \sum_{p \in \mathcal{P}} ((\mathbf{f}_p^{\text{ext}})^* \wedge (x_p - y)^* + (\mathbf{c}_p^{\text{ext}})^* \wedge \mathbf{d}_p^*). \quad (78)$$

As with (75), the stars can be removed from this equation and on using (57) and (58), (78) can be written as

$$\mathbf{R}(\mathcal{P}, \mathcal{P}'; y) + \mathbf{R}^{\text{ext}}(\mathcal{P}; y) = \mathbf{0}, \quad (79)$$

which is referred to as the balance of torques for the subsystem $\mathcal{P}$ of $\mathcal{B}$.

10.2 Laws of mutual action

Applying the balance of forces (76) to the entire system $\mathcal{B}$ yields

$$\mathbf{f}^{\text{ext}}(\mathcal{B}) = \mathbf{0}. \quad (80)$$

Let $\mathcal{P}$ be a subsystem of $\mathcal{B}$. On considering the force balance of both $\mathcal{P}$ and its complementary subsystem $\mathcal{P}'$ and adds these two balances, one obtains, with the help of the additivity of $\mathbf{f}^{\text{ext}}$ and (80),

$$\mathbf{f}(\mathcal{P}, \mathcal{P}') + \mathbf{f}(\mathcal{P}', \mathcal{P}) = \mathbf{0}. \quad (81)$$

Let $\mathcal{Q}$ be subsystem of $\mathcal{B}$ that is disjoint from $\mathcal{P}$ so that $(\mathcal{P}, \mathcal{Q}) \in (\text{Sub } \mathcal{B})_{\text{dis}}^2$. Notice that

$$(\mathcal{P} \cup \mathcal{Q})' \cup \mathcal{P} = \mathcal{Q}' \quad \text{and} \quad (\mathcal{P} \cup \mathcal{Q})' \cup \mathcal{Q} = \mathcal{P}'; \quad (82)$$

then, bearing in mind that $\mathbf{f}$ is an interaction, we have

$$\begin{aligned} & \mathbf{f}(\mathcal{P}, \mathcal{P}') + \mathbf{f}(\mathcal{Q}, \mathcal{Q}') \\ &= \mathbf{f}(\mathcal{P}, (\mathcal{P} \cup \mathcal{Q})' \cup \mathcal{Q}) + \mathbf{f}(\mathcal{Q}, (\mathcal{P} \cup \mathcal{Q})' \cup \mathcal{P}) = \mathbf{f}(\mathcal{P}, (\mathcal{P} \cup \mathcal{Q})') + \mathbf{f}(\mathcal{P}, \mathcal{Q}) \\ &+ \mathbf{f}(\mathcal{Q}, (\mathcal{P} \cup \mathcal{Q})') \\ &+ \mathbf{f}(\mathcal{Q}, \mathcal{P}) \\ &= \mathbf{f}(\mathcal{P} \cup \mathcal{Q}, (\mathcal{P} \cup \mathcal{Q})') \\ &+ \mathbf{f}(\mathcal{P}, \mathcal{Q}) + \mathbf{f}(\mathcal{Q}, \mathcal{P}). \end{aligned}$$

Thus, using (76) and the additivity of $\mathbf{f}^{\text{ext}}$, we have

$$\mathbf{f}(\mathcal{P}, \mathcal{Q}) + \mathbf{f}(\mathcal{Q}, \mathcal{P}) = \mathbf{f}(\mathcal{P}, \mathcal{P}') + \mathbf{f}(\mathcal{Q}, \mathcal{Q}') - \mathbf{f}(\mathcal{P} \cup \mathcal{Q}, (\mathcal{P} \cup \mathcal{Q})') = -\mathbf{f}^{\text{ext}}(\mathcal{P}) - \mathbf{f}^{\text{ext}}(\mathcal{Q}) + \mathbf{f}^{\text{ext}}(\mathcal{P} \cup \mathcal{Q}) = \mathbf{0}. \quad (83)$$

Since $(\mathcal{P}, \mathcal{Q})$ is an arbitrary element of $(\text{Sub } \mathcal{B})_{\text{dis}}^2$, we have the result

$$\mathbf{f}(\mathcal{P}, \mathcal{Q}) = -\mathbf{f}(\mathcal{Q}, \mathcal{P}) \quad \text{for all } (\mathcal{P}, \mathcal{Q}) \in (\text{Sub } \mathcal{B})_{\text{dis}}^2. \quad (84)$$

This is called the law of mutual action, also known as Newton's third law. When $\mathcal{P}$ consists of the single rod p and $\mathcal{Q}$ consists of the single rod q , then (84) reduces to

$$\mathbf{f}_{pq} = -\mathbf{f}_{qp}, \quad (85)$$

which says that the force of rod q on rod p is opposite to that of the force of rod p on rod q .

An analogous argument using the torque balance (79) shows that

$$\mathbf{R}(\mathcal{P}, \mathcal{Q}; y) = -\mathbf{R}(\mathcal{Q}, \mathcal{P}; y) \quad \text{for all } (\mathcal{P}, \mathcal{Q}) \in (\text{Sub } \mathcal{B})_{\text{dis}}^2 \quad (86)$$

and we have as a special case that

$$\mathbf{R}_{pq}(y) = -\mathbf{R}_{qp}(y) \quad (87)$$

for all p and q in $\mathcal{B}$. This says that the torque of rod q on rod p is opposite to that of the torque of rod p on rod q .

10.3 External forces and torques are frame-indifferent

Since, by Assumption 1, resultant forces between rods are frame-indifferent, we have

$$\sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{P}'} \mathbf{f}_{pq}^* = \sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{P}'} Q \mathbf{f}_{pq} = Q \mathbf{f}(\mathcal{P}, \mathcal{P}'), \quad (88)$$

which, with the help of (75) and (76), implies that

$$\sum_{p \in \mathcal{P}} (\mathbf{f}_p^{\text{ext}})^* = Q \mathbf{f}^{\text{ext}}(\mathcal{P}). \quad (89)$$

Taking $\mathcal{P}$ to consist of a single rod p , we find that

$$(\mathbf{f}_p^{\text{ext}})^* = Q \mathbf{f}_p^{\text{ext}}, \quad (90)$$

whereby we find that external resultant forces are frame-indifferent.

To obtain the analogous result for external torques, first notice that, by Assumption 1, we have for any two rods p and q in $\mathcal{B}$ and point y in $\mathcal{E}$,

$$(\mathbf{R}_{pq}(y))^* = (x_p - y)^* \wedge \mathbf{f}_{pq}^* + \mathbf{d}_p^* \wedge \mathbf{c}_{pq}^* = Q(x_p - y) \wedge Q \mathbf{f}_{pq} + Q \mathbf{d}_p \wedge Q \mathbf{c}_{pq} = Q \mathbf{R}_{pq}(y) Q^\top,$$

whereby we find that torques between rods are frame-indifferent. It follows that

$$\sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{P}'} (\mathbf{R}_{pq}(y))^* = \sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{P}'} Q \mathbf{R}_{pq}(y) Q^\top = Q \mathbf{R}(\mathcal{P}, \mathcal{P}'; \mathbf{y}) Q^\top. \quad (91)$$

With the help of (79), when $\mathcal{P}$ consists of a single rod p , we find that

$$(\mathbf{R}_p^{\text{ext}}(y))^* = Q \mathbf{R}_p^{\text{ext}} Q^\top, \quad (92)$$

whereby we find that external torques are frame-indifferent. Notice that since

$(x_p - y)^* \wedge (\mathbf{f}_p^{\text{ext}})^* = Q((x_p - y) \wedge \mathbf{f}_p^{\text{ext}}) Q^\top$ and $\mathbf{d}_p^* = Q \mathbf{d}_p$, we can use (56) and (92) to obtain

$$Q \mathbf{d}_p \wedge ((\mathbf{c}_p^{\text{ext}})^* - Q \mathbf{c}_p^{\text{ext}}) = \mathbf{0}. \quad (93)$$

This is possible if and only if $(\mathbf{c}_p^{\text{ext}})^* - Q \mathbf{c}_p^{\text{ext}}$ is parallel to $Q \mathbf{d}_p$ —that is, if and only if there is a $\lambda \in \mathbb{R}$ such that

$$\lambda Q \mathbf{d}_p = (\mathbf{c}_p^{\text{ext}})^* - Q \mathbf{c}_p^{\text{ext}} \quad (94)$$

and, thus, external couple forces are in general not frame-indifferent.

10.4 Balance Laws for a Single Rod

We now specialize the balance of forces and the balance of torques to the situation where the subsystem $\mathcal{P}$ consists of a single rod p .

When $\mathcal{P}$ consists of a single rod, (76) becomes

$$\sum_{q \in \mathcal{B}_p} \mathbf{f}_{pq} + \mathbf{f}_p^{\text{ext}} = \mathbf{0} \quad (95)$$

and (79) becomes

$$\sum_{q \in \mathcal{B}_p} ((x_p - y) \wedge \mathbf{f}_{pq} + \mathbf{d}_p \wedge \mathbf{c}_{pq}) + (x_p - y) \wedge \mathbf{f}_p^{\text{ext}} + \mathbf{d}_p \wedge \mathbf{c}_p^{\text{ext}} = \mathbf{0}. \quad (96)$$

Note that if one assumes that (95) and (96) hold for all rods p in $\mathcal{B}$, then one can prove that (76) and (79) hold.

However, (95) cannot be used to obtain (96). This illustrates a remark appearing in Footnote 8 of Fried [23]. Even for systems of point-like particles, the balance of torques is not a general consequence of the balance of forces. However, if the forces between the particles are central, meaning that $\mathbf{f}_{pq}$ is parallel to $\mathbf{r}_{pq}$, then the balance of torques does follow from the balance of forces. For a discussion of this see, for example, Chapter 4 of Rao [28].

Since (96) must hold for all points y in $\mathcal{E}$, we may choose $y := x_p$ to find that

$$\mathbf{d}_p \wedge \left(\sum_{q \in \mathcal{B}_p} \mathbf{c}_{pq} + \mathbf{c}_p^{\text{ext}} \right) = \mathbf{0}. \quad (97)$$

This is possible if and only if $\sum_{q \in \mathcal{B}_p} \mathbf{c}_{pq} + \mathbf{c}_p^{\text{ext}}$ is parallel to $\mathbf{d}_p$, or, equivalently, if and only if there is a λ_p in $\mathbb{R}$ such that

$$\lambda_p \mathbf{d}_p = \sum_{q \in \mathcal{B}_p} \mathbf{c}_{pq} + \mathbf{c}_p^{\text{ext}}. \quad (98)$$

11 Law of Power Balance

Let p be a rod in some subsystem $\mathcal{P}$ of $\mathcal{B}$. We then have

$$\mathcal{B}_p = (\mathcal{P} \cup \mathcal{P}') \setminus \{p\} = \mathcal{P}_p \cup \mathcal{P}'. \quad (99)$$

Using this, (62), (95), and (98), we find that

$$\begin{aligned} P_{\text{int}}(\mathcal{P}) &= \sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{P}_p} (\mathbf{f}_{pq} \cdot \mathbf{v}_p + \mathbf{c}_{pq} \cdot \mathbf{s}_p) = - \sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{P}'} (\mathbf{f}_{pq} \cdot \mathbf{v}_p + \mathbf{c}_{pq} \cdot \mathbf{s}_p) + \sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{B}_p} (\mathbf{f}_{pq} \cdot \mathbf{v}_p + \mathbf{c}_{pq} \cdot \mathbf{s}_p) \\ &= - \sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{P}'} (\mathbf{f}_{pq} \cdot \mathbf{v}_p + \mathbf{c}_{pq} \cdot \mathbf{s}_p) - \sum_{p \in \mathcal{P}} (\mathbf{f}_p^{\text{ext}} \cdot \mathbf{v}_p + (\mathbf{c}_p^{\text{ext}} - \lambda_p \mathbf{d}_p) \cdot \mathbf{s}_p). \end{aligned} \quad (100)$$

Furthermore, using (48), (64), and (100), we obtain

$$P_{\text{int}}(\mathcal{P}) = -P_{\text{ext}}(\mathcal{P}). \quad (101)$$

Identity (101) is known as the balance of power for the subsystem $\mathcal{P}$ and says that the external power expended on any subsystem $\mathcal{P}$ is equal to the opposite of the internal power expended on $\mathcal{P}$.

By taking the inner-product of (95) with $\mathbf{v}_p$ and summing over all p in some subsystem $\mathcal{P}$ we deduce the relation

$$\sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{B}_p} \mathbf{f}_{pq} \cdot \mathbf{v}_p + \sum_{p \in \mathcal{P}} \mathbf{f}_p^{\text{ext}} \cdot \mathbf{v}_p = 0, \quad (102)$$

which is a power balance that only consists of a power expenditures associated with forces. In a similar fashion, using (96), we arrive at

$$\sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{B}_p} \mathbf{c}_{pq} \cdot \mathbf{s}_p + \sum_{p \in \mathcal{P}} \mathbf{c}_p^{\text{ext}} \cdot \mathbf{s}_p = 0, \quad (103)$$

which is a power balance consisting of power expenditures associated with couples. Adding (102) and (103) yields (101).

12 An alternative approach

At approximately the same time that Noll [24] advanced his approach to obtaining the basic balance laws employed above, Green & Rivlin [29] proposed an alternative approach based on stipulating that, under superposed rigid motions, the forces must satisfy a certain transformation rule and the energy balance must be invariant. Since a superposed rigid motion is in practice, though not conceptually, equivalent to a change of frame and since in a purely mechanical setting energy balance is replaced by power balance, when applied in the present setting, the approach of Green & Rivlin [29] leads to the following assumptions:

Assumption 3 For all rods p and q in $\mathcal{B}$, $\mathbf{f}_{pq}$, $\mathbf{c}_{pq}$, $\mathbf{f}_p^{\text{ext}}$, and $\mathbf{c}_p^{\text{ext}}$ are frame-indifferent:

$$\mathbf{f}_{pq}^* = \mathbf{Q} \mathbf{f}_{pq}, \quad \mathbf{c}_{pq}^* = \mathbf{Q} \mathbf{c}_{pq}, \quad (\mathbf{f}_p^{\text{ext}})^* = \mathbf{Q} \mathbf{f}_p^{\text{ext}}, \quad \text{and} \quad (\mathbf{c}_p^{\text{ext}})^* = \mathbf{Q} \mathbf{c}_p^{\text{ext}}.$$

Assumption 4 For all subsystems $\mathcal{P}$ of $\mathcal{B}$, the balance of power is frame-indifferent:

$$\text{If } P_{\text{int}}(\mathcal{P}) + P_{\text{ext}}(\mathcal{P}) = 0 \text{ then } P_{\text{int}}^*(\mathcal{P}) + P_{\text{ext}}^*(\mathcal{P}) = 0 \text{ for any change of frame.}$$

Notice that Assumptions 3 and 4 are weaker than Assumptions 1 and 2. In lieu of Assumption 4, one might impose the weaker requirement that the total power

$$P_{\text{tot}}(\mathcal{P}) := P_{\text{int}}(\mathcal{P}) + P_{\text{ext}}(\mathcal{P})$$

of any subsystem $\mathcal{P}$ of $\mathcal{B}$ be frame-indifferent. There are two reasons for this. First, the total power P_{tot} is additive, like many other quantities of interest, such as the net force and couple acting on a subsystem, and second, this weaker alternative to Assumption 4 more closely resembles Assumption 2.

Granted that Assumptions 3 and 4 hold and bearing in mind the transformation rules stated in Section 9, an argument similar to that in Section 10 leads to a force balance

$$\frac{1}{2} \sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{P}_p} (\mathbf{f}_{pq} + \mathbf{f}_{qp}) + \mathbf{f}(\mathcal{P}, \mathcal{P}') + \mathbf{f}^{\text{ext}}(\mathcal{P}) = 0 \quad \text{for all } \mathcal{P} \in \text{Sub } \mathcal{B} \quad (104)$$

and a torque balance

$$\frac{1}{2} \sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{P}_p} (\mathbf{R}_{pq} + \mathbf{R}_{qp}) + \mathbf{R}(\mathcal{P}, \mathcal{P}'; y) + \mathbf{R}^{\text{ext}}(\mathcal{P}; y) = 0 \quad \text{for all } \mathcal{P} \in \text{Sub } \mathcal{B}. \quad (105)$$

Unless the laws of mutual action hold, in which case $\mathbf{f}_{pq} = -\mathbf{f}_{qp}$ and $\mathbf{R}_{pq} = -\mathbf{R}_{qp}$ for all rods p and q in $\mathcal{B}$, the balances (104) and (105), differ from (76) and (79).³ To deduce force and torque balances consistent with our using the approach of Green & Rivlin [29], it is therefore necessary to augment Assumptions 3 and 4 with an additional assumption imposing the laws of mutual action. Of course, this is consistent with the previously stated observation that Assumptions 1 and 2 are stronger than Assumptions 3 and 4. Moreover, it is noteworthy that only by imposing (the stronger) Assumptions 1 and 2 is it possible to derive the laws of mutual action, as was done in Subsection 10.2. To our knowledge, this is the only known example in which the approaches of Noll [24] and Green & Rivlin [29] yield different results. Beatty [25] noted that the method of Green & Rivlin [29] “would yield the same mechanics even with a false energy equation” and for this reasons we elected to follow Noll [24].

13 Digression on inertia

So far, the frame of reference $\mathcal{E}$ has been arbitrary. However, there are certain frames, called *inertial frames*, that are of particular interest. We now specialize our results to the case where $\mathcal{E}$ is an inertial frame.

13.1 Mass, moment of inertia, momenta, and inertial forces

Many of the concepts introduced in this subsection are based on the discussion in Subsection 3.5.

Given a system $\mathcal{B}$ of rods, we assume that each rod p has a mass m and a moment of inertia I , both of which are elements of the set $\mathbb{P}^\times$ of strictly positive numbers. We define the linear momentum $\mathbf{p}_p$ and the moment of momentum $\mathbf{L}_p(y)$ relative to a point y in $\mathcal{E}$ of the rod p by

$$\mathbf{p}_p := m\mathbf{v}_p \quad \text{and} \quad \mathbf{L}_p(y) := m(x_p - y) \wedge \mathbf{v}_p + I\mathbf{d}_p \wedge \mathbf{s}_p, \quad (106)$$

respectively.

Recall the decompositions of the environmental force and couple introduced in (51). In an inertial frame of reference, the inertial resultant force on a rod p has the form

$$\mathbf{f}_p^{\text{in}} = -m\mathbf{a}_p \quad (107)$$

and the inertial resultant couple on p has the form

³Moreover, (104) and (105) are respectively equivalent to (76) and (79) if and only if $\mathbf{f}_{pq} = -\mathbf{f}_{qp}$ and $\mathbf{R}_{pq} = -\mathbf{R}_{qp}$ for all choices of p and q .

$$\mathbf{c}_p^{\text{in}} = -I\dot{\mathbf{s}}_p. \quad (108)$$

We define the total linear momentum $\mathbf{p}(\mathcal{P})$ and the total moment of momentum $\mathbf{L}(\mathcal{P}; y)$ about a point y in $\mathcal{E}$ of a subsystem $\mathcal{P}$ by

$$\mathbf{p}(\mathcal{P}) := \sum_{p \in \mathcal{P}} \mathbf{p}_p \quad \text{and} \quad \mathbf{L}(\mathcal{P}; y) := \sum_{p \in \mathcal{P}} \mathbf{L}_p(y), \quad (109)$$

respectively. It is an easy consequence of these definitions that $\mathbf{p}$ and $\mathbf{L}(\cdot; y)$, when considered as mappings on Sub $\mathcal{B}$, are additive as defined in (42).

13.2 Laws of linear and moment of momentum balance

Let $\mathcal{P}$ again be a subsystem of rods. Since $\mathcal{E}$ is assumed to be an inertial frame, it follows from (51)₁, (53)₁, (106)₁, (107), and (109)₁ that

$$\mathbf{f}^{\text{ext}}(\mathcal{P}) = \sum_{p \in \mathcal{P}} \mathbf{f}_p^{\text{ni}} + \sum_{p \in \mathcal{P}} \mathbf{f}_p^{\text{in}} = \mathbf{f}^{\text{ni}}(\mathcal{P}) - \dot{\mathbf{p}}(\mathcal{P}), \quad (110)$$

where $\mathbf{f}^{\text{ni}}(\mathcal{P}) := \sum_{p \in \mathcal{P}} \mathbf{f}_p^{\text{ni}}$. Similarly, using (51)₂, (53)₂, (106)₂, (108), and (109)₂, we find that

$$\mathbf{R}^{\text{ext}}(\mathcal{P}; y) = \mathbf{R}^{\text{ni}}(\mathcal{P}; y) - \dot{\mathbf{L}}(\mathcal{P}; y), \quad (111)$$

where $\mathbf{R}^{\text{ni}}(\mathcal{P}; y) := \sum_{p \in \mathcal{P}} ((x_p - y) \wedge \mathbf{f}_p^{\text{ni}} + \mathbf{d}_p \wedge \mathbf{c}_p^{\text{ni}})$. Plugging (110) and (111) into (76) and (79), we obtain

$$\mathbf{f}(\mathcal{P}, \mathcal{P}') + \mathbf{f}^{\text{ni}}(\mathcal{P}) = \dot{\mathbf{p}}(\mathcal{P}) \quad (112)$$

and

$$\mathbf{R}(\mathcal{P}, \mathcal{P}'; y) + \mathbf{R}^{\text{ni}}(\mathcal{P}; y) = \dot{\mathbf{L}}(\mathcal{P}; y). \quad (113)$$

These are called the balance of momentum and the balance of moment of momentum for $\mathcal{P}$ (in an inertial frame).

Remark 1 One should be careful not to confuse the balance of forces (76) and the balance of momentum (112)₁. While the balance of forces holds in any frame of reference, the balance of momentum only holds in inertial frames of reference. A similar distinction holds for the balance of torques (79) and the balance of moment of momentum (113).

Specializing these results to the case where $\mathcal{P}$ consists of a single rod p (see Section 10.4), we find that (112) becomes

$$\sum_{q \in \mathcal{B}'_p} \mathbf{f}_{pq} + \mathbf{f}_p^{\text{ni}} = m \mathbf{a}_p \quad (114)$$

and (113) becomes

$$\sum_{q \in \mathcal{B}'_p} \mathbf{c}_{pq} + \mathbf{c}_p^{\text{ni}} = I \dot{\mathbf{s}}_p + \lambda_p \mathbf{d}_p. \quad (115)$$

Equation (114) is consistent with (10.19)₃ of Müller [21]. However, Müller [21] includes an extra term due to surface interactions. Since such interactions are neglected here, no such term appears in (115).

One can write (115) in a different form. Taking the inner-product of (115) with $\mathbf{d}_p$ one finds that

$$\lambda_p = \sum_{q \in \mathcal{B}_p} \mathbf{d}_p \cdot \mathbf{c}_{pq} + \mathbf{d}_p \cdot \mathbf{c}_p^{\text{ni}} + I |\mathbf{s}_p|^2. \quad (116)$$

Here we have used the fact that $|\mathbf{s}_p|^2 = -\mathbf{d}_p \cdot \dot{\mathbf{s}}_p$, which follows from differentiating the relation $|\mathbf{d}_p|^2 = 0$ with respect to time twice. Plugging this into (115), taking the circle product with $\mathbf{d}_p$ summing over all p in some subsystem $\mathcal{P}$ and using the notation

$$\mathbf{P}_p := \mathbf{1} - \mathbf{d}_p \otimes \mathbf{d}_p, \quad (117)$$

we deduce that

$$\sum_{p \in \mathcal{P}} \frac{1}{2} I \ddot{\mathbf{d}}_p \odot \mathbf{d}_p + \sum_{p \in \mathcal{P}} I |\mathbf{s}_p|^2 \mathbf{d}_p \odot \mathbf{d}_p - \sum_{p \in \mathcal{P}} I \mathbf{s}_p \odot \mathbf{s}_p = \sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{B}_p} \mathbf{d}_p \odot \mathbf{P}_p \mathbf{c}_{pq} + \sum_{p \in \mathcal{P}} \mathbf{d}_p \odot \mathbf{P}_p \mathbf{c}_p^{\text{ni}}. \quad (118)$$

This formulation of the moment of momentum balance foreshadows the macroscopic orientation balance for liquid crystals. In a similar way, plugging (116) into (115), but this time taking the circle product with $\mathbf{s}_p$ and then summing over all p in some subsystem $\mathcal{P}$ we obtain

$$\sum_{p \in \mathcal{P}} I \ddot{\mathbf{s}}_p \odot \mathbf{s}_p + \sum_{p \in \mathcal{P}} 2I |\mathbf{s}_p|^2 \mathbf{d}_p \odot \mathbf{s}_p = \sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{B}_p} 2\mathbf{s}_p \odot \mathbf{P}_p \mathbf{c}_{pq} + \sum_{p \in \mathcal{P}} 2\mathbf{s}_p \odot \mathbf{P}_p \mathbf{c}_p^{\text{ni}}. \quad (119)$$

This formulation of the moment of moment balance foreshadows the macroscopic mesofluctuation balance for liquid crystals. Both (118) and (119) resemble the classical virial theorem (see, for example, Landau & Lifchitz [30]).

Remark 2 When working with the equations (114) and (115), we must remember the stipulation that rods cannot overlap. Since our goal is not to solve the discrete equations, but instead to provide a basis for deriving macroscopic balance laws, we do not make this constraint explicit here.

13.3 Kinetic energy

Let p be a rod in system $\mathcal{B}$. The kinetic energy k_p of the rod p is defined by

$$k_p := \frac{1}{2} m |\mathbf{v}_p|^2 + \frac{1}{2} I |\mathbf{s}_p|^2. \quad (120)$$

Given a subsystem $\mathcal{P}$ of $\mathcal{B}$, the total kinetic energy of $\mathcal{P}$ is given by

$$k(\mathcal{P}) = \sum_{p \in \mathcal{P}} k_p. \quad (121)$$

It is easy to see that k is additive in the sense described in (42). The derivative of the total kinetic energy of $\mathcal{P}$ with respect to time is given by

$$\dot{\overline{k(\mathcal{P})}} = \sum_{p \in \mathcal{P}} (m \mathbf{v}_p \cdot \mathbf{a}_p + I \mathbf{s}_p \cdot \dot{\mathbf{s}}_p). \quad (122)$$

By (51), (64), (107), and (108), we have

$$P_{\text{ext}}(\mathcal{P}) = \sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{P}'} (\mathbf{f}_{pq} \cdot \mathbf{v}_p + \mathbf{c}_{pq} \cdot \mathbf{s}_p) + \sum_{p \in \mathcal{P}} (\mathbf{f}_p^{\text{ext}} \cdot \mathbf{v}_p + \mathbf{c}_p^{\text{ext}} \cdot \mathbf{s}_p) = \sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{P}'} (\mathbf{f}_{pq} \cdot \mathbf{v}_p + \mathbf{c}_{pq} \cdot \mathbf{s}_p) + \sum_{p \in \mathcal{P}} (\mathbf{f}_p^{\text{ni}} \cdot \mathbf{v}_p + \mathbf{c}_p^{\text{ni}} \cdot \mathbf{s}_p) - \sum_{p \in \mathcal{P}} (m \mathbf{a}_p \cdot \mathbf{v}_p + I \dot{\mathbf{s}}_p \cdot \mathbf{s}_p).$$

with

$$P_{\text{ext}}^{\text{ni}}(\mathcal{P}) := \sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{P}'} (\mathbf{f}_{pq} \cdot \mathbf{v}_p + \mathbf{c}_{pq} \cdot \mathbf{s}_p) + \sum_{p \in \mathcal{P}} (\mathbf{f}_p^{\text{ni}} \cdot \mathbf{v}_p + \mathbf{c}_p^{\text{ni}} \cdot \mathbf{s}_p). \quad (124)$$

Using (101), (123) becomes

$$\dot{\overline{k(\mathcal{P})}} = P_{\text{ext}}^{\text{ni}}(\mathcal{P}) + P_{\text{int}}(\mathcal{P})$$

and is known as the kinetic energy balance for $\mathcal{P}$

It should be stressed that (124) does not hold if the frame $\mathcal{E}$ is not inertial. In fact, if $\mathcal{E}$ is not an inertial frame of reference then the concept of kinetic energy is not useful.

14 Principle of interaction-energy imbalance

Consider the system $\mathcal{B}$ in some motion μ . Assume that each pair of rods p and q has an associated interaction-energy ψ_{pq} at each time throughout the motion. The interaction-energy between p and q is required to be the same as that between q and p , so that

$$\psi_{pq} = \psi_{qp}. \quad (125)$$

Remark 3 Recall that the placements of the rods are restricted so that no two rods overlap. It may be possible to ensure that this constraint is met by choosing appropriate interaction-energy functions. This would likely involve the introduction of indicator functions.

We also assume that the interaction-energy of a rod with itself is zero:

$$\psi_{pp} = 0 \quad \text{for all } p \in \mathcal{B}. \quad (126)$$

Given a subsystem $\mathcal{P}$ we denote the total interaction-energy of the system with itself by

$$\dot{\psi}(\mathcal{P}) := \frac{1}{2} \sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{P}} \dot{\psi}_{pq}. \quad (127)$$

The principle of interaction-energy imbalance states that, for any motion of any subsystem $\mathcal{P}$ the rate of change of the interaction-energy of the system is always less than or equal to the power expended on the subsystem by external influences:

$$\overline{\dot{\psi}(\mathcal{P})} \leq P_{\text{ext}}(\mathcal{P}). \quad (128)$$

This principle can be interpreted as the manifestation of the first two laws of thermodynamics in a purely mechanical setting. On using the balance of power (101), the inequality (128) can be written as

$$\overline{\dot{\psi}(\mathcal{P})} + P_{\text{int}}(\mathcal{P}) \leq 0. \quad (129)$$

On taking $\mathcal{P}$ to consist of just two rods p and q , (129) yields

$$\dot{\psi}_{pq} + \mathbf{f}_{pq} \cdot \mathbf{v}_{pq} + \mathbf{c}_{pq} \cdot \mathbf{s}_p + \mathbf{c}_{qp} \cdot \mathbf{s}_q \leq 0. \quad (130)$$

15 Constitutive relations

So far, everything that has been said holds true for general systems of rods. However, it is to be expected that interactions between different kinds of rods generally differ. To characterize how rods comprising a given system interact with each other and with the environment, particular constitutive relations must be specified.

15.1 Motivating the constitutive relations

Our motivation for the generic constitutive relation governing the interaction-energy between two rod-like particles is based on two ideas, the first being that the rod-like particles are modeled by one-dimensional rigid rods, as described in Section 3, and the second being the principle of material frame-indifference. The principle of material frame-indifference states that the constitutive relations governing the internal interactions between the parts of a system should not depend on whatever external frame of reference is used to describe them. This principle restricts the form of constitutive relations.

Let R_p and R_q denote two one-dimensional rigid rods. Here, we use the notation of Section 3—with subscripts p and q to distinguish between the one-dimensional rigid rods. Consider a placement κ_p for R_p and a placement κ_q for R_q such that

$$\text{Rng } \kappa_p \cap \text{Rng } \kappa_q = \emptyset, \quad (131)$$

so that the rods do not intersect. Let r_p be a material point in R_p and r_q be a material point in R_q . We assume that the interaction-energy between the material points r_p and r_q depends only on the position of these material points in their respective placements—that is, the points

$$\kappa_p(r_p) = x_p + r_p \mathbf{d}_p \quad \text{and} \quad \kappa_q(r_q) = x_q + r_q \mathbf{d}_q, \quad (132)$$

where the representations for κ_p and κ_q given in (10) have been employed. Using the principle of material frame-indifference, it can be shown that the interaction-energy only depends on the magnitude of the relative position vector (see Part 2 of Noll [31]) or, equivalently, its square

$$\left| (x_p + r_p \mathbf{d}_p) - (x_q + r_q \mathbf{d}_q) \right|^2 = \left| \mathbf{r}_{pq} \right|^2 + 2r_p \mathbf{r}_{pq} \cdot \mathbf{d}_p - 2r_q \mathbf{r}_{pq} \cdot \mathbf{d}_q - 2r_p r_q \mathbf{d}_p \cdot \mathbf{d}_q + r_p^2 + r_q^2. \quad (133)$$

Let $\widehat{\psi}_{r_p, r_q}$ denote the function that takes in the value in (133) and gives the interaction-energy between the material points r_p and r_q when the rods are in the placements under consideration. By integrating the interaction-energy between material points over both rods, we obtain

$$\int_{R_p} \int_{R_q} \widehat{\psi}_{r_p, r_q} \left(\left| \kappa_p(r_p) - \kappa_q(r_q) \right|^2 \right) \mathbf{d}r_q \mathbf{d}r_p, \quad (134)$$

which is the total interaction-energy between the rods R_p and R_q . It follows from (133) and (134) that with knowledge of the four numbers

$$\left| \mathbf{r}_{pq} \right|^2, \quad \mathbf{r}_{pq} \cdot \mathbf{d}_p, \quad \mathbf{r}_{pq} \cdot \mathbf{d}_q, \quad \text{and} \quad \mathbf{d}_p \cdot \mathbf{d}_q, \quad (135)$$

and of the functions $\widehat{\psi}_{r_p, r_q}$, r_p in R_p and r_q in R_q , one may compute the interaction-energy between rods R_p and R_q . Thus, there is function

$$\widehat{\psi}: \mathbb{P}^x \times \mathbb{R}^3 \rightarrow \mathbb{R} \quad (136)$$

such that

$$\widehat{\psi}_{pq} = \widehat{\psi} \left(\left| \mathbf{r}_{pq} \right|^2, \mathbf{r}_{pq} \cdot \mathbf{d}_p, \mathbf{r}_{pq} \cdot \mathbf{d}_q, \mathbf{d}_p \cdot \mathbf{d}_q \right) \quad (137)$$

gives the interaction-energy between rods R_p and R_q when they are in a placement in which their centers are at x_p and x_q and their directors are given by $\mathbf{d}_p$ and $\mathbf{d}_q$. This interaction energy includes, as a special case, the particular expression

$$\psi_{pq} = \frac{1}{2} a \left(\left| \mathbf{r}_{pq} \right| \right) (3(\mathbf{d}_p \cdot \mathbf{d}_q)^2 - 1) \quad (138)$$

used in the Maier–Saupe theory [32]. In (138), a is some function of the distance between the rods.

Motivated by this, we assume that the constitutive relations for the resultant force and resultant couple have a similar dependence:

$$\mathbf{f}_{pq} = \widehat{\mathbf{f}} \left(\left| \mathbf{r}_{pq} \right|^2, \mathbf{r}_{pq} \cdot \mathbf{d}_p, \mathbf{r}_{pq} \cdot \mathbf{d}_q, \mathbf{d}_p \cdot \mathbf{d}_q \right), \quad (139)$$

$$\mathbf{c}_{pq} = \widehat{\mathbf{c}} \left(\left| \mathbf{r}_{pq} \right|^2, \mathbf{r}_{pq} \cdot \mathbf{d}_p, \mathbf{r}_{pq} \cdot \mathbf{d}_q, \mathbf{d}_p \cdot \mathbf{d}_q \right). \quad (140)$$

It can be readily verified that the constitutive relations (139)–(140) satisfy the principle of material frame-indifference.

The noninertial resultant environmental forces $\mathbf{f}_p^{\text{in}}$ and coulees $\mathbf{c}_p^{\text{in}}$ are also determined by constitutive relations—more precisely referred to as external constitutive relations. Put

$$\mathcal{U}_\perp^2 := \{(\mathbf{u}, \mathbf{v}) \in \mathcal{V}^2 \mid \|\mathbf{u}\| = 1 \text{ and } \mathbf{u} \cdot \mathbf{v} = 0\}. \quad (141)$$

The noninertial resultant environmental force on a rod p is assumed to depend only on the position of the rod, its director, the rate of change of these objects, and time. Thus, there is a mapping $\widehat{\mathbf{f}}^{\text{ni}}: \mathcal{E} \times \mathcal{V} \times \mathcal{U}_\perp^2 \times \mathcal{I} \rightarrow \mathcal{V}$ such that

$$\mathbf{f}_p^{\text{ni}} = \widehat{\mathbf{f}}^{\text{ni}}(x_p, \mathbf{v}_p, \mathbf{d}_p, \mathbf{s}_p, t) \quad (142)$$

gives the noninertial resultant environmental force on rod p when it is located at x_p has velocity $\mathbf{v}_p$, director $\mathbf{d}_p$, spin $\mathbf{s}_p$ and time t . Similarly, we assume there is a mapping $\widehat{\mathbf{c}}^{\text{ni}}: \mathcal{E} \times \mathcal{V} \times \mathcal{U}_\perp^2 \times \mathcal{I} \rightarrow \mathcal{V}$ such that

$$\mathbf{c}_p^{\text{ni}} = \widehat{\mathbf{c}}^{\text{ni}}(x_p, \mathbf{v}_p, \mathbf{d}_p, \mathbf{s}_p, t) \quad (143)$$

gives the noninertial resultant environmental couple on rod p when it is located at x_p has velocity $\mathbf{v}_p$, director $\mathbf{d}_p$, spin $\mathbf{s}_p$ and time t . These external constitutive relations are general enough to model forces and couples from the environment due to time-dependent gravitational, electrical, or magnetic fields. Arguments similar to those leading to (137) can be used to motivate the constitutive relations (142)–(143).

Remark 4 The particular form of the relations (137) and (139)–(140) depends heavily on the assumption that the constitutive relations governing interactions between a pair of rods depend only on instantaneous information regarding the placement of those rods. To subsume rate- or some more complicated history-dependence, it would be necessary to replace (137) and (139)–(140) with correspondingly more complicated laws. It transpires that constitutive relations of the form (137) and (139)–(140) are sufficiently general to allow for a statistical derivation for the continuum-level balance laws for liquid crystals.

15.2 Consequences of the principle of interaction-energy imbalance

The constitutive relations specified in (137) and (139)–(140) cannot be arbitrary and still be compatible with the principle of interaction-energy imbalance. We now investigate the restrictions that this principle places on the constitutive relations. This is achieved by employing the Coleman–Noll procedure, introduced by Coleman & Noll [33], in the purely mechanical setting considered here. It suffices to carry out this procedure for subsystems $\mathcal{P} := \{p, q\}$ consisting of only two rods p and q of $\mathcal{B}$.

Given a motion $\mu: \mathcal{P} \times \mathcal{Q} \rightarrow \mathcal{E}$ of the subsystem $\{p, q\}$, we define the mapping

$$\bar{C}_{pq}: \mathcal{I} \rightarrow \mathbb{P}^x \times \mathbb{R}^3 \quad (144)$$

by

$$\bar{C}_{pq}(t) := (|r_{pq}(t)|^2, r_{pq}(t) \cdot \mathbf{d}_p(t), r_{pq}(t) \cdot \mathbf{d}_q(t), \mathbf{d}_p(t) \cdot \mathbf{d}_q(t)) \quad \text{for all } t \in \mathcal{I}. \quad (145)$$

An analogous mapping $\bar{C}_{qp}$ is defined by interchanging the roles of p and q . Using the foregoing notation, (137), and the chain-rule, we obtain

$$\dot{\psi}_{pq} = 2(\widehat{\psi}_{,1} \circ \overline{C}_{pq}) \mathbf{r}_{pq} \cdot \mathbf{v}_{pq} + (\widehat{\psi}_{,2} \circ \overline{C}_{pq})(\mathbf{v}_{pq} \cdot \mathbf{d}_p + \mathbf{r}_{pq} \cdot \mathbf{s}_p) + (\widehat{\psi}_{,3} \circ \overline{C}_{pq})(\mathbf{v}_{pq} \cdot \mathbf{d}_q + \mathbf{r}_{pq} \cdot \mathbf{s}_q) + (\widehat{\psi}_{,4} \circ \overline{C}_{pq})(\mathbf{s}_p \cdot \mathbf{d}_q + \mathbf{d}_p \cdot \mathbf{s}_q).$$

Plugging this into (130) and using (139)–(140), we obtain

$$\begin{aligned} 0 \geq & (\widehat{\mathbf{f}} \circ \overline{C}_{pq} \\ & + 2(\widehat{\psi}_{,1} \circ \overline{C}_{pq}) \mathbf{r}_{pq} \\ & + (\widehat{\psi}_{,2} \circ \overline{C}_{pq}) \mathbf{d}_p \\ & + (\widehat{\psi}_{,3} \circ \overline{C}_{pq}) \mathbf{d}_q) \\ & \cdot \mathbf{v}_{pq} + (\widehat{\mathbf{c}} \circ \overline{C}_{pq} \\ & + (\widehat{\psi}_{,2} \circ \overline{C}_{pq}) \mathbf{r}_{pq} \\ & + (\widehat{\psi}_{,4} \circ \overline{C}_{pq}) \mathbf{d}_q) \\ & \cdot \mathbf{s}_p + (\widehat{\mathbf{c}} \circ \overline{C}_{qp} \\ & + (\widehat{\psi}_{,3} \circ \overline{C}_{pq}) \mathbf{r}_{pq} \\ & + (\widehat{\psi}_{,4} \circ \overline{C}_{pq}) \mathbf{d}_p) \cdot \mathbf{s}_q. \end{aligned} \quad (146)$$

Recall that (146) must hold for all possible motions.

The following result is not difficult to prove.

Proposition 1 *Let*

$$\mathbf{r} \in \mathcal{V} \quad \text{and} \quad \mathbf{e}, \mathbf{f} \in \text{Usph}(\mathcal{V}) \quad (147)$$

be given. Also, let

$$\mathbf{v}, \mathbf{e}', \mathbf{f}' \in \mathcal{V} \quad \text{such that} \quad \mathbf{e}' \cdot \mathbf{e} = \mathbf{f}' \cdot \mathbf{f} = 0 \quad (148)$$

be given. There is a motion of the subsystem $\mathcal{P} = \{p, q\}$ such that for some time $t_0 \in \mathcal{Q}$ we have

$$\mathbf{r} = \mathbf{r}_{pq}(t_0), \quad \mathbf{v} = \mathbf{v}_{pq}(t_0), \quad \mathbf{e} = \mathbf{d}_p(t_0), \quad \mathbf{f} = \mathbf{d}_p(t_0), \quad \mathbf{e}' = \mathbf{s}_p(t_0) \quad \text{and} \quad \mathbf{f}' = \mathbf{s}_q(t_0). \quad (149)$$

Let $\mathbf{r}$ in $\mathcal{V}$ and $\mathbf{e}$ and $\mathbf{f}$ in $\text{Usph}(\mathcal{V})$ be given and put $C := (|\mathbf{r}|^2, \mathbf{r} \cdot \mathbf{e}, \mathbf{r} \cdot \mathbf{f}, \mathbf{e} \cdot \mathbf{f})$. Find a motion guaranteed by the above proposition with $\mathbf{e}' = \mathbf{f}' = \mathbf{0}$ and $\mathbf{v}$ arbitrary and consider (146) at time t_0 to find that

$$0 \geq (\widehat{\mathbf{f}}(C) + 2\widehat{\psi}_{,1}(C)\mathbf{r} + \widehat{\psi}_{,2}(C)\mathbf{e} + \widehat{\psi}_{,3}(C)\mathbf{f}) \cdot \mathbf{v}. \quad (150)$$

Since this inequality must hold for all $\mathbf{v}$ in $\mathcal{V}$ we must have

$$\widehat{\mathbf{f}}(C) = -2\widehat{\psi}_{,1}(C)\mathbf{r} - \widehat{\psi}_{,2}(C)\mathbf{e} - \widehat{\psi}_{,3}(C)\mathbf{f}. \quad (151)$$

Now find a motion guaranteed by Proposition 1 with $\mathbf{f}' = \mathbf{v} = \mathbf{0}$ and consider (146) at time t_0 to find that

$$0 \geq (\widehat{\mathbf{c}}(C) + \widehat{\psi}_{,2}(C)\mathbf{r} + \widehat{\psi}_{,4}(C)\mathbf{f}) \cdot \mathbf{e}' \quad (152)$$

Since this inequality must hold for all $\mathbf{e}'$ such that $\mathbf{e}' \cdot \mathbf{e} = 0$, we may conclude that there is a λ in $\mathbb{R}$ such that

$$\lambda \mathbf{e} = \widehat{\mathbf{c}}(C) + \widehat{\psi}_{,2}(C)\mathbf{r} + \widehat{\psi}_{,4}(C)\mathbf{f}. \quad (153)$$

Now consider a motion guaranteed by Proposition 1 with $\mathbf{e}' = \mathbf{v} = \mathbf{0}$ and consider (146) at time t_0 to find that

$$0 \geq (\widehat{\mathbf{c}}(\tilde{C}) + \widehat{\psi}_{,3}(C)\mathbf{r} + \widehat{\psi}_{,4}(C)\mathbf{e}) \cdot \mathbf{f}', \quad (154)$$

where $\tilde{C} := \tilde{C}_{qp}(t_0) = (|\mathbf{r}|^2, -\mathbf{r} \cdot \mathbf{f}, -\mathbf{r} \cdot \mathbf{e}, \mathbf{f} \cdot \mathbf{e})$. This condition is equivalent to (152) because if the roles of p and q in (152) are interchanged, (154) results. To see this, start with (125) and use (137) to find that

$$\widehat{\psi}(|\mathbf{r}|^2, \mathbf{r} \cdot \mathbf{e}, \mathbf{e} \cdot \mathbf{f}, \mathbf{e} \cdot \mathbf{f}) = \widehat{\psi}(|\mathbf{r}|^2, -\mathbf{r} \cdot \mathbf{f}, -\mathbf{r} \cdot \mathbf{e}, \mathbf{f} \cdot \mathbf{e}), \quad (155)$$

where the minus signs arise because $\mathbf{r} = \mathbf{r}_{pq} = -\mathbf{r}_{qp}$. Take the gradient of (155) with respect to $\mathbf{f}$ to obtain

$$\widehat{\psi}_{,3}(C)\mathbf{r} + \widehat{\psi}_{,4}(C)\mathbf{e} = -\widehat{\psi}_{,2}(\tilde{C})\mathbf{r} + \widehat{\psi}_{,4}(\tilde{C})\mathbf{e}. \quad (156)$$

Substituting (156) this into (154) yields (152), but with the roles of p and q interchanged, including replacing the roles of $\mathbf{e}$ and $\mathbf{f}$, as defined in (149). Thus, the restrictions resulting from (154) do not carry any new information.

Since $\mathbf{r}$ represents an arbitrary element of $\mathcal{V}$ and $\mathbf{e}$ and $\mathbf{f}$ represent arbitrary elements of $\text{Usph}(\mathcal{V})$, one direction of the theorem below has been established. The converse follows from a straightforward calculation.

Theorem 1 *The constitutive relations (137) and (139)–(140) satisfy the principle of interaction-energy imbalance if and only if there is a mapping*

$$\widehat{\lambda}: \mathbb{P}^\times \times \mathbb{R}^3 \rightarrow \mathbb{R} \quad (157)$$

such that

$$\widehat{\mathbf{f}}(C) = -2\widehat{\psi}_{,1}(C)\mathbf{r} - \widehat{\psi}_{,2}(C)\mathbf{e} - \widehat{\psi}_{,3}(C)\mathbf{f}, \quad (158)$$

$$\widehat{\mathbf{c}}(C) = \widehat{\lambda}(C)\mathbf{e} - \widehat{\psi}_{,2}(C)\mathbf{r} - \widehat{\psi}_{,4}(C)\mathbf{f}, \quad (159)$$

with $C = (|\mathbf{r}|^2, \mathbf{r} \cdot \mathbf{e}, \mathbf{r} \cdot \mathbf{f}, \mathbf{e} \cdot \mathbf{f})$, for all $\mathbf{r}$ in $\mathcal{V}$ and $\mathbf{e}$ and $\mathbf{f}$ in $\text{Usph}(\mathcal{V})$.

Notice that taking the inner-product of both sides of (159) with $\mathbf{e}$ delivers a formula for $\widehat{\lambda}(C)$.

16 Constitutively augmented balance laws

Recall the balances of momentum (114) and moment of momentum (115) for a single rod p . In light of the constitutive relations for the resultant forces and couples between rods that were introduced in the previous section, these balances can be written using the interaction-energy.

For convenience, we introduce the mapping

$$\tilde{\psi}: \mathcal{E} \times \text{Usph}(\mathcal{V}) \times \mathcal{E} \times \text{Usph}(\mathcal{V}) \rightarrow \mathbb{R} \quad (160)$$

defined by

$$\tilde{\psi}(x_p, \mathbf{d}_p, x_q, \mathbf{d}_q) := \widehat{\psi}(|\mathbf{r}_{pq}|^2, \mathbf{r}_{pq} \cdot \mathbf{d}_p, \mathbf{r}_{pq} \cdot \mathbf{d}_q, \mathbf{d}_p \cdot \mathbf{d}_q). \quad (161)$$

This mapping is useful because, by (139)–(140) and (158)–(159), we have

$$\nabla_{x_p} \tilde{\psi}(x_p, \mathbf{d}_p, x_q, \mathbf{d}_q) = -\widehat{\mathbf{f}}(C_{pq}), \quad (162)$$

$$\nabla_{\mathbf{d}_p} \tilde{\psi}(x_p, \mathbf{d}_p, x_q, \mathbf{d}_q) = -\widehat{\mathbf{c}}(C_{pq}) + \widehat{\lambda}(C_{pq}) \mathbf{d}_p, \quad (163)$$

where $C_{pq} = (|\mathbf{r}_{pq}|^2, \mathbf{r}_{pq} \cdot \mathbf{d}_p, \mathbf{r}_{pq} \cdot \mathbf{d}_q, \mathbf{d}_p \cdot \mathbf{d}_q)$. To ease the notational burden, from here on, when no confusion is likely to arise, we ignore the distinction between mappings and their values. With this convention, (162) and (163) can be written as

$$\nabla_{x_p} \psi_{pq} = -\mathbf{f}_{pq}, \quad (164)$$

$$\nabla_{\mathbf{d}_p} \psi_{pq} = -\mathbf{c}_{pq} + \lambda_{pq} \mathbf{d}_p. \quad (165)$$

We also define

$$\psi := \frac{1}{2} \sum_{p,q \in \mathcal{B}} \psi_{pq}. \quad (166)$$

Notice that, by (164) and (165), we have

$$\nabla_{x_p} \psi = - \sum_{q \in \mathcal{B}_p} \mathbf{f}_{pq}, \quad (167)$$

$$\nabla_{\mathbf{d}_p} \psi = - \sum_{q \in \mathcal{B}_p} (\mathbf{c}_{pq} - \lambda_{pq} \mathbf{d}_p), \quad (168)$$

and, thus, ψ can be used to write (114) as

$$-\nabla_{x_p} \psi + \mathbf{f}_p^{\text{ni}} = m \dot{\mathbf{v}}_p \quad (169)$$

and (115) as

$$-\nabla_{\mathbf{d}_p} \psi + \mathbf{c}_p^{\text{ni}} = I \dot{\mathbf{s}}_p + (\lambda_p - \sum_{q \in \mathcal{B}_p} \lambda_{pq}) \mathbf{d}_p. \quad (170)$$

Equations (169) and (115) are referred to as the constitutively augmented momentum and moment of momentum balance for rod p , respectively.

17 Summary

The formulation presented above is based on the following hypotheses:

H₁: Every rod p in a system $\mathcal{B}$ is subject to resultant forces $\mathbf{f}_{pq}$ exerted by other rods q in the system as well as a resultant environmental force $\mathbf{f}_p^{\text{ext}}$.

H₂: Every rod p in a system $\mathcal{B}$ is subject to resultant couples $\mathbf{c}_{pq}$ exerted by other rods q in the system p as well as a resultant environmental couple $\mathbf{c}_p^{\text{ext}}$.

H₃: The torques $\mathbf{R}_{pq}(y)$ and $\mathbf{R}_p^{\text{ext}}(y)$ exerted about a point y on a rod p are given by

$$\mathbf{R}_{pq}(y) = (x_p - y) \wedge \mathbf{f}_{pq} + \mathbf{d}_p \wedge \mathbf{c}_{pq} \quad \text{and} \quad \mathbf{R}_p(y) = (x_p - y) \wedge \mathbf{f}_p^{\text{ext}} + \mathbf{d}_p \wedge \mathbf{c}_p^{\text{ext}}.$$

H₄: The resultant forces and couples between rods are frame-indifferent.

H₅: For all subsystems $\mathcal{P}$ of $\mathcal{B}$, the net external power $P_{\text{ext}}(\mathcal{P})$ is frame-indifferent.

H₆: All pairs $\{p, q\}$ of rods have an interaction-energy Ψ_{pq} .

H₇: For all subsystems $\mathcal{P}$ of $\mathcal{B}$, the rate of change of the interaction-energy of the system $\mathcal{P}$ with itself is always less than or equal to the external power expended on $\mathcal{P}$.

The most important hypotheses are **H₄** and **H₅**. The consequences of these assumptions are:

C₁: The sum of all forces acting on all subsystems is zero:

$$\mathbf{f}(\mathcal{P}, \mathcal{P}') + \mathbf{f}^{\text{ext}}(\mathcal{P}) = \mathbf{0} \quad \text{for all} \quad \mathcal{P} \in \text{Sub } \mathcal{B}.$$

C₂: The sum of all torques acting on a subsystem about any point y is zero:

$$\mathbf{R}(\mathcal{P}, \mathcal{P}'; y) + \mathbf{R}^{\text{ext}}(\mathcal{P}; y) = \mathbf{0} \quad \text{for all} \quad \mathcal{P} \in \text{Sub } \mathcal{B}.$$

C₃: The resultant forces $\mathbf{f}_{pq}$ and $\mathbf{f}_{qp}$ between rods p and q satisfy

$$\mathbf{f}_{pq} = -\mathbf{f}_{qp}$$

and the torques $\mathbf{R}_{pq}(y)$ and $\mathbf{R}_{qp}(y)$ about a point y in $\mathcal{E}$ between rods p and q satisfy

$$\mathbf{R}_{pq}(y) = -\mathbf{R}_{qp}(y).$$

C₄: The resultant environmental force $\mathbf{f}_p^{\text{ext}}$ and torque $\mathbf{R}_p^{\text{ext}}(y)$, about any point y , acting on any rod p are frame-indifferent.

A major consequence of C₁ is the power balance

$$P_{\text{int}}(\mathcal{P}) = -P_{\text{ext}}(\mathcal{P}) \quad \text{for all } \mathcal{P} \in \text{Sub } \mathcal{B},$$

where P_{int} and P_{ext} represent the internal and external power expenditures. The balance laws stated in $\mathbf{C}_1$ and $\mathbf{C}_2$ hold in any frame of reference. However, if the frame of reference is inertial, then the force balance becomes the balance of linear momentum

$$\overline{\mathbf{p}(\mathcal{P})} = \mathbf{f}(\mathcal{P}, \mathcal{P}') + \mathbf{f}^{\text{ni}}(\mathcal{P}) \quad \text{for all } \mathcal{P} \in \text{Sub } \mathcal{B} \quad (171)$$

and the torque balance becomes the balance of moment of momentum

$$\overline{\mathbf{L}(\mathcal{P}; \mathbf{y})} = \mathbf{R}(\mathcal{P}, \mathcal{P}'; \mathbf{y}) + \mathbf{R}^{\text{ni}}(\mathcal{P}; \mathbf{y}) \quad \text{for all } \mathcal{P} \in \text{Sub } \mathcal{B}. \quad (172)$$

Two corollaries of (172) are

$$\sum_{p \in \mathcal{P}} \frac{1}{2} I \overline{\mathbf{d}_p \odot \mathbf{d}_p} + \sum_{p \in \mathcal{P}} I |\mathbf{s}_p|^2 \mathbf{d}_p \odot \mathbf{d}_p - \sum_{p \in \mathcal{P}} I \mathbf{s}_p \odot \mathbf{s}_p = \sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{B}_p} \mathbf{d}_p \odot \mathbf{P}_p \mathbf{c}_{pq} + \sum_{p \in \mathcal{P}} \mathbf{d}_p \odot \mathbf{P}_p \mathbf{c}_p^{\text{ni}} \quad (173)$$

and

$$\sum_{p \in \mathcal{P}} I \overline{\mathbf{s}_p \odot \mathbf{s}_p} + \sum_{p \in \mathcal{P}} 2I |\mathbf{s}_p|^2 \mathbf{d}_p \odot \mathbf{s}_p - \sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{B}_p} 2\mathbf{s}_p \odot \mathbf{P}_p \mathbf{c}_{pq} + \sum_{p \in \mathcal{P}} 2\mathbf{s}_p \odot \mathbf{P}_p \mathbf{c}_p^{\text{ni}}. \quad (174)$$

Equations (173) and (174) are, respectively, the microscopic precursors of the orientation balance and mesofluctuation balance in the continuum theory of liquid crystals. Although these microscopic balances can be derived from the microscopic moment of momentum balance, it transpires that the macroscopic versions of the orientation balance and mesofluctuation balance cannot be derived from the macroscopic moment of momentum balance.

Finally, proposed constitutive relations

$$\begin{aligned} \psi_{pq} &= \widehat{\psi}(|\mathbf{r}_{pq}|^2, \mathbf{r}_{pq} \cdot \mathbf{d}_p, \mathbf{r}_{pq} \cdot \mathbf{d}_q, \mathbf{d}_p \cdot \mathbf{d}_q), \\ \mathbf{f}_{pq} &= \widehat{\mathbf{f}}(|\mathbf{r}_{pq}|^2, \mathbf{r}_{pq} \cdot \mathbf{d}_p, \mathbf{r}_{pq} \cdot \mathbf{d}_q, \mathbf{d}_p \cdot \mathbf{d}_q), \\ \mathbf{c}_{pq} &= \widehat{\mathbf{c}}(|\mathbf{r}_{pq}|^2, \mathbf{r}_{pq} \cdot \mathbf{d}_p, \mathbf{r}_{pq} \cdot \mathbf{d}_q, \mathbf{d}_p \cdot \mathbf{d}_q), \end{aligned}$$

motivated by considering the interaction between two one-dimensional rigid rods and the principle of material frame-indifference, were considered. By hypothesis $\mathbf{H}_7$, these laws are restricted by the relations given in Theorem 1. Namely, the constitutive relation for the interaction-energy between rods determines the constitutive relation for the forces and the couple forces between rods. With the aforementioned restrictions, using these constitutive relations in the balances (171) and (172) and using the notation in Section 16 yield

$$-\sum_{p \in \mathcal{P}} \nabla_{x_p} \psi + \sum_{p \in \mathcal{P}} \mathbf{f}_p^{\text{ni}} = \sum_{p \in \mathcal{P}} m \dot{\mathbf{v}}_p \quad (175)$$

and

$$-\sum_{p \in \mathcal{P}} ((x_p - y) \wedge \nabla_{x_p} \psi + \mathbf{d}_p \wedge \nabla_{\mathbf{d}_p} \psi) + \sum_{p \in \mathcal{P}} ((x_p - y) \wedge \mathbf{f}_p^{\text{ni}} + \mathbf{d}_p \wedge \mathbf{c}_p^{\text{ni}}) = \sum_{p \in \mathcal{P}} (m(x_p - y) \wedge \mathbf{a}_p + I \mathbf{d}_p \wedge \dot{\mathbf{s}}_p) \quad (176)$$

for any subsystem $\mathcal{P}$

This work was motivated to provide a foundation upon which to develop the macroscopic balance laws for liquid crystals using statistical mechanics. Toward this, consequence C_3 combined with the specializations of (171) and (172) to the case when the subsystem $\mathcal{P}$ consists of a single rod play an essential role. The consequences (173) and (174) of (172) are also important inasmuch as they foreshadow the non-standard balances that arise in the continuum theory of liquid crystals.

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