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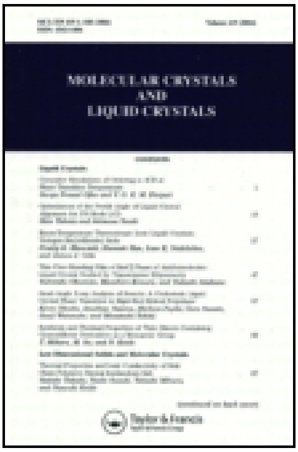

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The Connection Between Ericksen-Leslie Equations and the Balances of Mesoscopic Theory of Liquid Crystals

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THE CONNECTION BETWEEN ERICKSEN-LESLIE EQUATIONS AND THE BALANCES OF MESOSCOPIC THEORY OF LIQUID CRYSTALS

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Abstract Ericksen-Leslie equations can be derived, if the mesoscopic local balance equations are exploited by use of the orientation distribution function for total alignment.

INTRODUCTION

Describing liquid crystals on the mesoscopic level all fields depend not only on position and time, but also on the orientation of the particles described by the microscopic director. Defined on this so-called nematic space balance equations of the mesoscopic fields of mass, momentum, spin and internal energy can be derived. The macroscopic quantities are averages of mesoscopic ones weighted by the orientation distribution function (ODF) which describes the orientation of all molecules in a volume element.

In contrast to the mesoscopic concept Ericksen-Leslie theory uses a macroscopic director field for describing the mean orientation of a liquid crystal. There are only two cases in which a macroscopic director field can be defined mesoscopically: If the ODF is uniaxial (symmetric with respect to rotation) or delta-shaped (locally total alignment of the molecules). The Ericksen-Leslie equations can be recovered only for total alignment by averaging the mesoscopic balances of spin and internal energy.

MESOSCOPIC CONCEPT

A liquid crystal is composed of differently orientated particles for which we presuppose, that their orientation can be described individually by the direction of their microscopic directors. Thus the microscopic director $\boldsymbol{n}$ is defined as a unit vector pointing into the temporary direction of a needle-shaped rigid particle, or, if the

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particle is of plane shape, the microscopic director is perpendicular to the particle. Because the microscopic director is normalized

$$\boldsymbol{n}^2 = 1, \quad \boldsymbol{n} \in \mathrm{S}^2, \tag{1}$$

the microscopic alignment has two degrees of freedom. Since the particles may rotate, the microscopic director changes in time, and we define the microscopic *orientation change velocity* by

$$\boldsymbol{u}(\boldsymbol{n}, \boldsymbol{x}, t) := \frac{\mathrm{d}}{\mathrm{dt}} \boldsymbol{n}, \quad \text{with} \quad \boldsymbol{u}(\boldsymbol{n}, \boldsymbol{x}, t) \cdot \boldsymbol{n} = 0, \tag{2}$$

as an independent mesoscopic field having the symmetry property

$$\boldsymbol{u}(-\boldsymbol{n}, \boldsymbol{x}, t) = -\boldsymbol{u}(\boldsymbol{n}, \boldsymbol{x}, t). \tag{3}$$

If we consider molecules of a volume element the alignment of their axes is specified by a normalized distribution function f on the unit sphere, called *orientation distribution function* (ODF). The ODF describes the density generated by intersection points on the unit sphere S^2 between the molecular axes and the sphere. Because in general the alignment of the molecules is a function of position and time the ODF is defined on a six-dimensional space $\mathrm{S}^2 \times \mathrm{I\!R}^3 \times \mathrm{I\!R}^1$

$$f(\boldsymbol{n}, \boldsymbol{x}, t) \equiv f(\cdot), \quad (\cdot) \equiv (\boldsymbol{n}, \boldsymbol{x}, t) \in \mathrm{S}^2 \times \mathrm{I\!R}^3 \times \mathrm{I\!R}^1. \tag{4}$$

The 5-dimensional subspace $\mathrm{S}^2 \times \mathrm{I\!R}^3$ consisting of the orientation- and of the position-part is called *nematic space.* Because there are always two points of intersection opposite to each other on the S^2 the ODF shows the so-called head-tail symmetry

$$f(-\boldsymbol{n}, \boldsymbol{x}, t) = f(\boldsymbol{n}, \boldsymbol{x}, t). \tag{5}$$

By the ODF a mesoscopic classification of different types of orientation, so-called *phases*, becomes possible.

LOCAL ORIENTATIONAL BALANCES

Presupposing global balances of mass, of momentum, of angular momentum, and of internal energy we can derive the following four local balance equations which are defined on the nematic space and which are therefore denoted as *local orientational balances* [1]:

Mass

$$\frac{\partial}{\partial t}\rho(\cdot) + \nabla_x \cdot [\rho(\cdot)\, \boldsymbol{v}(\cdot)] + \nabla_n \cdot [\rho(\cdot)\, \boldsymbol{u}(\cdot)] = 0. \tag{6}$$

Here the orientational mass density $\rho(\cdot)$ is defined by

$$\rho(\cdot) := \rho(\boldsymbol{x}, t) f(\cdot), \qquad \rho(-\boldsymbol{n}, \boldsymbol{x}, t) = \rho(\boldsymbol{n}, \boldsymbol{x}, t). \tag{7}$$

Thus the macroscopic mass density $\rho(\boldsymbol{x}, t)$ results from (7) by integration over the orientation

$$\int_{S^2} \rho(\cdot)\, d^2n = \rho(\boldsymbol{x}, t) \int_{S^2} f(\cdot)\, d^2n = \rho(\boldsymbol{x}, t). \tag{8}$$

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Here $\boldsymbol{v}(\cdot)$ in (6) is the orientational material velocity (barycentric velocity field of all molecules of microscopic director $\boldsymbol{n}$ at position $\boldsymbol{x}$ at time t) which has the symmetry

$$\boldsymbol{v}(-\boldsymbol{n},\ \boldsymbol{x},t) = \boldsymbol{v}(\boldsymbol{n},\ \boldsymbol{x},t). \tag{9}$$

From (6) we see that the flux in the orientational sub-space $\nabla_n\cdot[\rho(\cdot)\ \boldsymbol{u}(\cdot)]$ is analogous to the time rate of mass caused by chemical reactions in a mixture. Consequently the mesoscopic description of liquid crystals has the structure of a formal mixture theory: The "components" of this mixture are composed of all molecules in a volume element which have the same alignment [2].

Momentum

The orientational balance of momentum reads

$$\frac{\partial}{\partial t}[\rho(\cdot)\ \boldsymbol{v}(\cdot)] + \nabla_x\cdot[\ \boldsymbol{v}(\cdot)\ \boldsymbol{v}(\cdot)\rho(\cdot) - \boldsymbol{T}^T(\cdot)] + \nabla_n\cdot[\rho(\cdot)\ \boldsymbol{u}(\cdot)\ \boldsymbol{v}(\cdot)] = \\ = \rho(\cdot)\ \boldsymbol{k}(\cdot). \tag{10}$$

Here $\boldsymbol{T}^T(\cdot)$ is the transposed orientational stress tensor, and $\boldsymbol{k}(\cdot)$ the external orientational field of acceleration which have the symmetry properties

$$\boldsymbol{T}(-\boldsymbol{n},\ \boldsymbol{x},t) = \boldsymbol{T}(\boldsymbol{n},\ \boldsymbol{x},t), \qquad \boldsymbol{k}(-\boldsymbol{n},\ \boldsymbol{x},t) = \boldsymbol{k}(\boldsymbol{n},\ \boldsymbol{x},t). \tag{11}$$

The divergence of the flux $\nabla_n\cdot[\rho(\cdot)\ \boldsymbol{u}(\cdot)\ \boldsymbol{v}(\cdot)]$ acts as an additional force density on the nematic space.

Spin

If the orientational spin is defined by

$$\boldsymbol{s}(\cdot) := I\ \boldsymbol{n}\times\ \boldsymbol{u}(\cdot) \tag{12}$$

(I is the microscopic moment of inertia belonging to a single needle-shaped molecule) we obtain the local spin balance [3]:

$$\frac{\partial}{\partial t}[\rho(\cdot)\ \boldsymbol{s}(\cdot)] + \nabla_x\cdot[\rho(\cdot)\ \boldsymbol{v}(\cdot)\ \boldsymbol{s}(\cdot) - (\ \boldsymbol{n}\times\ \boldsymbol{\pi}(\cdot))^T] + \\ +\nabla_n\cdot[\rho(\cdot)\ \boldsymbol{u}(\cdot)\ \boldsymbol{s}(\cdot)] = \ \boldsymbol{\varepsilon} :\ \boldsymbol{T}(\cdot) + \rho(\cdot)\ \boldsymbol{n}\times\ \boldsymbol{g}(\cdot). \tag{13}$$

Here $\boldsymbol{\varepsilon}$ is the Levi-Civita tensor, $\boldsymbol{\pi}(\cdot)$ the couple stress tensor, and $\boldsymbol{g}(\cdot)$ the couple force density which both have the symmetry properties

$$\boldsymbol{\pi}(-\boldsymbol{n},\ \boldsymbol{x},t) = -\ \boldsymbol{\pi}(\boldsymbol{n},\ \boldsymbol{x},t), \qquad \boldsymbol{g}(-\boldsymbol{n},\ \boldsymbol{x},t) = -\ \boldsymbol{g}(\boldsymbol{n},\ \boldsymbol{x},t). \tag{14}$$

The right-hand side of (13) indicates that one part of the spin supply is caused by the antisymmetric part of the stress tensor.

Internal Energy

The balance of internal energy reads [3]

$$\begin{aligned}\frac{\partial}{\partial t}[\rho(\cdot)\varepsilon(\cdot)] &+ \nabla_x\cdot[\rho(\cdot)\ \boldsymbol{v}(\cdot)\varepsilon(\cdot)] + \nabla_n\cdot[\rho(\cdot)\ \boldsymbol{u}(\cdot)\varepsilon(\cdot)] = \\ = \rho(\cdot)r(\cdot) &+ [\nabla_x\ \boldsymbol{v}(\cdot)] :\ \boldsymbol{T}(\cdot) + [\nabla_x\ \boldsymbol{u}(\cdot)] :\ \boldsymbol{\pi}(\cdot) - \\ &- \nabla_x\cdot\ \boldsymbol{q}(\cdot) - [\ \boldsymbol{n}\times\ \boldsymbol{u}(\cdot)]\cdot\ \boldsymbol{\varepsilon} :\ \boldsymbol{T}(\cdot).\end{aligned} \tag{15}$$

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Here $\varepsilon(\cdot)$ is the orientational internal energy, $r(\cdot)$ the orientational radiation supply, and $\boldsymbol{q}(\cdot)$ the orientational heat flux density which have the properties

$$\varepsilon(-\boldsymbol{n},\ \boldsymbol{x},t)=\varepsilon(\boldsymbol{n},\ \boldsymbol{x},t), \qquad r(-\boldsymbol{n},\ \boldsymbol{x},t)=r(\boldsymbol{n},\ \boldsymbol{x},t), \tag{16}$$

$$\boldsymbol{q}(-\boldsymbol{n},\ \boldsymbol{x},t) = \boldsymbol{q}(\boldsymbol{n},\ \boldsymbol{x},t). \tag{17}$$

According to the right-hand side of (15) the spin supply in (13) induces one part of the supply of the internal energy.

TOTAL ALIGNMENT

Integration of orientational balance equations over the unit sphere results in balance equations of micropolar media [3]. Here we are not interested in the general shape of these balances, but we write them down in the special case of total alignment of all molecules which is described at a particular position by a δ-shaped ODF. Because of the head-tail symmetry (5) the ODF has a double δ-peak whose connecting line determines the macroscopic director field $\boldsymbol{d}(\boldsymbol{x},t)$. Thus the ODF reads as follows

$$f(\cdot)=(1/2)[\delta(\boldsymbol{n}-\boldsymbol{d}(\boldsymbol{x},t))+\delta(\boldsymbol{n}+\boldsymbol{d}(\boldsymbol{x},t))]\equiv\Delta_{\boldsymbol{d}}(\cdot). \tag{18}$$

We now integrate the orientational balances of mass (6), of momentum (10), of spin (13), and of internal energy (15) over all orientations. Then the particular ODF (18) describing total alignment is inserted into these balances being integrated over the unit sphere. Taking into consideration the proposition [2]

$$\int_{S^2}\nabla_n\cdot[\boldsymbol{u}(\cdot)\Phi(\cdot)]d^2n=0 \tag{19}$$

we obtain the following balances of micropolar media:

Macroscopic mass balance

$$\frac{\partial}{\partial t}\rho(\boldsymbol{x},t)+\nabla_x\cdot[\boldsymbol{v}(\boldsymbol{x},t)\rho(\boldsymbol{x},t)]=0. \tag{20}$$

Here the macroscopic mass density is defined by (8) and the macroscopic material velocity on $\mathbb{R}^3$ by

$$\boldsymbol{v}(\boldsymbol{x},t):=\int_{S^2}\Delta_{\boldsymbol{d}}(\cdot)\,\boldsymbol{v}(\cdot)d^2n\ . \tag{21}$$

Macroscopic momentum balance

$$\frac{\partial}{\partial t}[\rho(\boldsymbol{x},t)\,\boldsymbol{v}(\boldsymbol{x},t)]+\nabla_x\cdot[\boldsymbol{v}(\boldsymbol{x},t)\,\boldsymbol{v}(\boldsymbol{x},t)\rho(\boldsymbol{x},t)-\boldsymbol{T}^T(\boldsymbol{x},t)]= \\ =\rho(\boldsymbol{x},t)\,\boldsymbol{k}(\boldsymbol{x},t). \tag{22}$$

The macroscopic acceleration field and the macroscopic stress tensor are defined by

$$\boldsymbol{k}(\boldsymbol{x},t):=\int_{S^2}\Delta_{\boldsymbol{d}}(\cdot)\,\boldsymbol{k}(\cdot)d^2n\ , \tag{23}$$

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and

$$\boldsymbol{T}(\boldsymbol{x},t) := \int_{S^2} \boldsymbol{T}(\cdot) d^2 n. \tag{24}$$

From (20) and (22) follows that the macroscopic balances of mass and momentum *remain unchanged for liquid crystals. According to* (24) *the macroscopic stress* tensor is in case of total alignment the sum of the orientational ones, a statement which is not valid in general [2].

Macroscopic spin balance

$$\begin{aligned}\frac{\partial}{\partial t}[\rho(\boldsymbol{x},t)\ \boldsymbol{s}(\boldsymbol{x},t)] + \nabla_x\cdot[\rho(\boldsymbol{x},t)\ \boldsymbol{v}(\boldsymbol{x},t)\ \boldsymbol{s}(\boldsymbol{x},t)] &= \\ = \boldsymbol{\varepsilon} :\ \boldsymbol{T}(\boldsymbol{x},t) + \rho(\boldsymbol{x},t)\ \boldsymbol{\ell}(\boldsymbol{x},t) + \nabla_x\cdot\ \boldsymbol{m}^T(\boldsymbol{x},t).\end{aligned} \tag{25}$$

Here the macroscopic spin is defined by

$$\begin{aligned}\boldsymbol{s}(\boldsymbol{x},t) := \int_{S^2} I\Delta_{\boldsymbol{d}}(\cdot)\ \boldsymbol{n} \times \ \boldsymbol{u}(\cdot) d^2 n = \\ = I\ \boldsymbol{d}(\boldsymbol{x},t) \times \ \boldsymbol{u}(\ \boldsymbol{d}(\boldsymbol{x},t),\ \boldsymbol{x},t) = I\ \boldsymbol{d}(\boldsymbol{x},t) \times \ \dot{\boldsymbol{d}}(\boldsymbol{x},t).\end{aligned} \tag{26}$$

The last equal sign follows according to (2) and (18). The volume torque is

$$\boldsymbol{\ell}(\boldsymbol{x},t) := \int_{S^2} \Delta_{\boldsymbol{d}}(\cdot)\ \boldsymbol{n} \times \ \boldsymbol{g}(\cdot) d^2 n = \ \boldsymbol{d}(\boldsymbol{x},t) \times \ \boldsymbol{g}(\boldsymbol{x},t), \tag{27}$$

and the surface torque is defined by

$$\boldsymbol{m}(\boldsymbol{x},t) := \int_{S^2} \boldsymbol{n} \times \ \boldsymbol{\pi}(\cdot) d^2 n, \tag{28}$$

a relation which - as (24) - is not valid in general. The macroscopic spin (26) in case of total alignment is in accordance with the definition of spin used by Ericksen [4] and Leslie [5].

Macroscopic balance of internal energy

$$\begin{aligned}\frac{\partial}{\partial t}[\rho(\boldsymbol{x},t)\varepsilon(\boldsymbol{x},t)] + \nabla_x\cdot[\rho(\boldsymbol{x},t)\ \boldsymbol{v}(\boldsymbol{x},t)\varepsilon(\boldsymbol{x},t)] = \\ = \rho(\boldsymbol{x},t) r(\boldsymbol{x},t) - \nabla_x\cdot\ \boldsymbol{q}(\boldsymbol{x},t) + [\nabla_x\ \boldsymbol{v}(\boldsymbol{x},t)] :\ \boldsymbol{T}(\boldsymbol{x},t) + \\ + \frac{1}{I}[\nabla_x\ \boldsymbol{s}(\boldsymbol{x},t)] :\ \boldsymbol{m}(\boldsymbol{x},t) - \frac{1}{I}\ \boldsymbol{s}(\boldsymbol{x},t)\cdot\ \boldsymbol{\varepsilon} :\ \boldsymbol{T}(\boldsymbol{x},t).\end{aligned} \tag{29}$$

Here the macroscopic internal energy is defined by

$$\varepsilon(\boldsymbol{x},t) := \int_{S^2} \Delta_{\boldsymbol{d}}(\cdot)\varepsilon(\cdot) d^2 n = \varepsilon(\ \boldsymbol{d}(\boldsymbol{x},t),\ \boldsymbol{x},t) \tag{30}$$

the macroscopic radiation supply is

$$r(\boldsymbol{x},t) := \int_{S^2} \Delta_{\boldsymbol{d}}(\cdot) r(\cdot) d^2 n, \tag{31}$$

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and the macroscopic heat flux density is defined by

$$\begin{aligned} \boldsymbol{q}(\boldsymbol{x},t) := \int_{S^2} [\,\boldsymbol{q}(\cdot) + \boldsymbol{v}(\cdot)\cdot \boldsymbol{T}(\cdot) + \boldsymbol{u}(\cdot)\cdot \boldsymbol{\pi}(\cdot)]d^2n - \\ - \boldsymbol{v}(\boldsymbol{x},t)\cdot \boldsymbol{T}(\boldsymbol{x},t) - \frac{1}{\theta}\,\boldsymbol{s}(\boldsymbol{x},t)\cdot \boldsymbol{m}(\boldsymbol{x},t). \end{aligned} \tag{32}$$

Again we should emphasize that the definitions (24), (28), (30) - (32) are only valid, if the molecules are totally aligned [2]. The derived macroscopic balance of internal energy (29) is in accordance with that used by Ericksen [6] and Leslie [7]. Consequently we derived the spin balance (25) and the balance of internal energy (29) by mesoscopic concepts in case of presupposed totally aligned molecules. Now the question arises, if the shape of these balances are also valid for other types of alignment. This is not the case, as a proposition verifies [8]. But also without of a strict proof it can be perceived that Ericksen-Leslie equations are only valid for total alignment: The general expressions for (26) and (30) are [3]

$$\boldsymbol{s}(\boldsymbol{x},t) := \int_{S^2} If(\cdot)\,\boldsymbol{n}\times \boldsymbol{u}(\cdot)d^2n, \tag{33}$$

and

$$\begin{aligned} \varepsilon(\boldsymbol{x},t) := \int_{S^2} f(\cdot)\left\{\frac{1}{2}[\,\boldsymbol{v}(\cdot)]^2 + \frac{1}{2}I[\,\boldsymbol{n}\times \boldsymbol{u}(\cdot)]^2 + \epsilon(\cdot)\right\} d^2n - \\ - \left\{\frac{1}{2}[\,\boldsymbol{v}(\boldsymbol{x},t)]^2 + \frac{1}{2I}[\,\boldsymbol{s}(\boldsymbol{x},t)]^2\right\}. \end{aligned} \tag{34}$$

Both expressions can be treated generally using the mean value theorem. By this we obtain

$$\boldsymbol{s}(\boldsymbol{x},t) = I\,\boldsymbol{N}(\boldsymbol{x},t)\times \boldsymbol{u}(\boldsymbol{N}(\boldsymbol{x},t),\,\boldsymbol{x},t), \tag{35}$$

and

$$\begin{aligned} \varepsilon(\boldsymbol{x},t) &= \frac{1}{2}[\,\boldsymbol{v}(\boldsymbol{M}(\boldsymbol{x},t),\,\boldsymbol{x},t)]^2 + \\ &+ \frac{1}{2}I[\,\boldsymbol{M}(\boldsymbol{x},t)\times \boldsymbol{u}(\boldsymbol{M}(\boldsymbol{x},t),\,\boldsymbol{x},t)]^2 + \\ &+ \varepsilon(\boldsymbol{M}(\boldsymbol{x},t),\,\boldsymbol{x},t) + \\ &+ \left\{\frac{1}{2}[\,\boldsymbol{v}(\boldsymbol{x},t)]^2 + \frac{1}{2I}[\,\boldsymbol{s}(\boldsymbol{x},t)]^2\right\}. \end{aligned} \tag{36}$$

Here $\boldsymbol{N}$ and $\boldsymbol{M}$ are mean values on S^2. Of course in general $\boldsymbol{N}$ and $\boldsymbol{M}$ are different from each other because they are mean values obtained from different equations. Therefore $\boldsymbol{N}$ is the "spin-director", whereas $\boldsymbol{M}$ is the "internal-energy-director". Consequently there exists no common macroscopic director in the general case.

RESULTS

The Ericksen-Leslie theory of liquid crystals is characterized by the definition of the macroscopic spin (26) which appears in the macroscopic balances of spin (25) and internal energy (29). The mesoscopic foundation of these macroscopic balances verifies that the Ericksen-Leslie theory is only valid for locally total alignment of the molecules. Possible introductions of the macroscopic director without total alignment do not lead to Ericksen-Leslie balances of liquid crystals.

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