UNIVERSITY OF
OXFORD
Mathematical
Institute

From Polyatomic Gas to Liquid Crystals: A Kinetic Approach

P. E. Farrell*, G. Russo†, U. Zerbinati*

* *Mathematical Institute*
University of Oxford

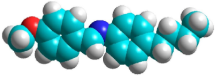
† *Dipartimento di Matematica ed Informatica*
Università di Catania

SciCADE 2024, 15th of July, Singapor

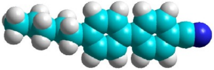
Oxford
Mathematics

The molecules

Our ultimate goal is to understand properties of special molecules such as MBBA and 5CB, which are well known to establish a liquid crystal mesophase under appropriate conditions.



MBBA

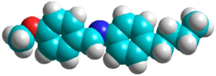


5CB

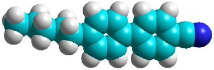
The molecules

Our ultimate goal is to understand properties of special molecules such as MBBA and 5CB, which are well known to establish a liquid crystal mesophase under appropriate conditions.

- Molecules can be regarded as **slender bodies**.



MBBA

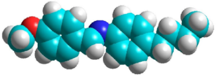


5CB

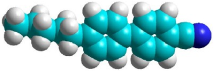
The molecules

Our ultimate goal is to understand properties of special molecules such as MBBA and 5CB, which are well known to establish a liquid crystal mesophase under appropriate conditions.

- Molecules can be regarded as **slender bodies**.
- Molecules are **achiral**, i.e. they can be superimposed with their mirror images.



MBBA

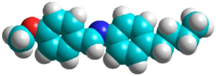


5CB

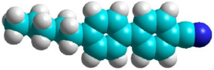
The molecules

Our ultimate goal is to understand properties of special molecules such as MBBA and 5CB, which are well known to establish a liquid crystal mesophase under appropriate conditions.

- Molecules can be regarded as **slender bodies**.
- Molecules are **achiral**, i.e. they can be superimposed with their mirror images.
- Molecules are **neutrally charged**.



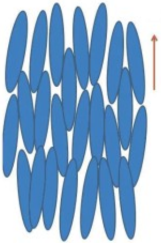
MBBA



5CB

The nematic ordering

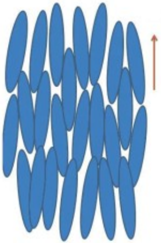
Onsager first related the ability of certain colloidal particles to have a partial ordering before they freeze (hence retaining the ability to flow) to the particle geometry. The greater the elongation of the molecule, the more likely the colloidal will form a nematic ordering.



The nemetic ordering

Onsager first related the ability of certain colloidal particles to have a partial ordering before they freeze (hence retaining the ability to flow) to the particle geometry. The greater the elongation of the molecule, the more likely the colloidal will form a nematic ordering.

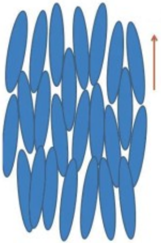
- There is an **enthalpic drive**, i.e. the van der Waals forces favor alignment.



The nematic ordering

Onsager first related the ability of certain colloidal particles to have a partial ordering before they freeze (hence retaining the ability to flow) to the particle geometry. The greater the elongation of the molecule, the more likely the colloidal will form a nematic ordering.

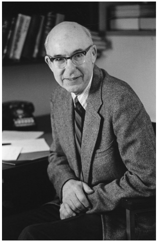
- There is an **enthalpic drive**, i.e. the van der Waals forces favor alignment.
- There is an **entropic drive**, i.e. aligned elongated molecules are more loosely packed, i.e. we have fewer constraints on the velocity and position.



Kinetic Theory

Kinetic Theory of Non-Spherical Molecules

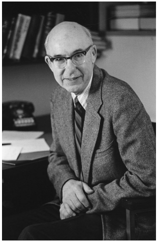
- In 1956 derived the first kinetic theory for **non-spherical** molecules.



Charles Francis Curtiss, 1921–2007

Kinetic Theory of Non-Spherical Molecules

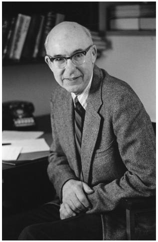
- In 1956 derived the first kinetic theory for **non-spherical** molecules.
- In 1963 together with J.S. Dahler, used the **BBGKY** formalism to derive a kinetic theory for **non-spherical** molecules.



Charles Francis Curtiss, 1921–2007

Kinetic Theory of Non-Spherical Molecules

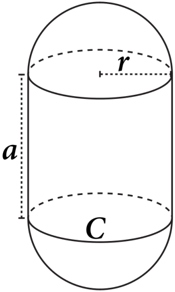
- In 1956 derived the first kinetic theory for **non-spherical** molecules.
- In 1963 together with J.S. Dahler, used the **BBGKY** formalism to derive a kinetic theory for **non-spherical** molecules.
- Fostered a kinetic theory "school" who was very active in development of a theory for **hard convex body fluids**.



Charles Francis Curtiss, 1921–2007

Curtiss collision operator

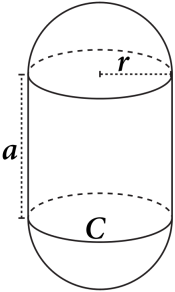
In his seminal paper, Curtiss proposed a kinetic theory for spherocylindrical molecules as an idealisation of a polyatomic gas.



Curtiss collision operator

In his seminal paper, Curtiss proposed a kinetic theory for spherocylindrical molecules as an idealisation of a polyatomic gas.

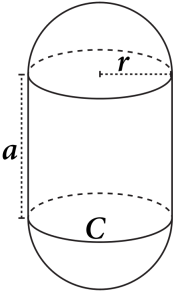
- He considered a larger configuration space made by **position**, **velocity**, the **Euler angles** for describing the orientation of each molecule, and the **angular velocity** with respect to a fixed coordinate system.



Curtiss collision operator

In his seminal paper, Curtiss proposed a kinetic theory for spherocylindrical molecules as an idealisation of a polyatomic gas.

- He considered a larger configuration space made by **position**, **velocity**, the **Euler angles** for describing the orientation of each molecule, and the **angular velocity** with respect to a fixed coordinate system.
- Molecules would interact by **excluded volume**, which give rise to **short range interactions**, hence the **nematic ordering**.



This led Curtiss to formulate the following **Boltzmann** type equation,

$$\partial_t f + \nabla_{\boldsymbol{r}} \cdot (\boldsymbol{v} f) + \nabla_{\boldsymbol{\alpha}} \cdot (\dot{\boldsymbol{\alpha}} f) = C[f, f] \tag{1}$$

where $f(\boldsymbol{r}, \boldsymbol{v}, \boldsymbol{\alpha}, \varsigma)$ is the probability of having a particle in the $(\boldsymbol{r}, \boldsymbol{v}, \boldsymbol{\alpha}, \varsigma)$ spot of the configuration space, normalised by $\frac{1}{n}$.

This led Curtiss to formulate the following **Boltzmann** type equation,

$$\partial_t f + \nabla_{\boldsymbol{r}} \cdot (\boldsymbol{v} f) + \nabla_{\boldsymbol{\alpha}} \cdot (\dot{\boldsymbol{\alpha}} f) = C[f, f]$$

where $f(\boldsymbol{r}, \boldsymbol{v}, \boldsymbol{\alpha}, \varsigma)$ is the probability of having a particle in the $(\boldsymbol{r}, \boldsymbol{v}, \boldsymbol{\alpha}, \varsigma)$ spot of the configuration space, normalised by $\frac{1}{n}$.

$$C[f, f] = \iiiint (f_1^{'} f^{'} - f_1 f)(\boldsymbol{k} \cdot \boldsymbol{g}) S(\boldsymbol{k}) d\boldsymbol{k} d\boldsymbol{v}_1 d\boldsymbol{\alpha}_1 d\varsigma_1$$

with $S(\boldsymbol{k}) d\boldsymbol{k}$ being the surface element of the excluded volume and $\boldsymbol{g} = \boldsymbol{v}_1 - \boldsymbol{v} + \boldsymbol{\omega}_1 \times \boldsymbol{r}_1 - \boldsymbol{\omega} \times \boldsymbol{r}$. Here without loss of generality the equation is stated in **absence of external force** and **torque**.

Collision invariants

It is possible to prove that the following quantities are **collision invariants** for $C[f,f]$, i.e.

$$\iiint \psi^{(i)} C[f,f] d\boldsymbol{v}_1 d\varsigma_1 d\boldsymbol{\alpha}_1 = 0.$$

---

[1] The inertia tensor for the spherocylinder we are considering.

Collision invariants

It is possible to prove that the following quantities are **collision invariants** for $C[f,f]$, i.e.

$$\iiint \psi^{(i)} C[f,f] d\boldsymbol{v}_1 d\varsigma_1 d\boldsymbol{\alpha}_1 = 0.$$

- $\psi^{(1)} = 1$, the **number of particles** in the system;

---

[1] The inertia tensor for the spherocylinder we are considering.

Collision invariants

It is possible to prove that the following quantities are **collision invariants** for $C[f,f]$, i.e.

$$\iiint \psi^{(i)} C[f,f] d\boldsymbol{v}_1 d\varsigma_1 d\boldsymbol{\alpha}_1 = 0.$$

- $\psi^{(1)} = 1$, the **number of particles** in the system;
- $\psi^{(2)} = m\boldsymbol{v}$, the **linear momentum**;

---

[1] The inertia tensor for the spherocylinder we are considering.

Collision invariants

It is possible to prove that the following quantities are **collision invariants** for $C[f,f]$, i.e.

$$\iiint \psi^{(i)} C[f,f] d\boldsymbol{v}_1 d\varsigma_1 d\boldsymbol{\alpha}_1 = 0.$$

- $\psi^{(1)} = 1$, the **number of particles** in the system;
- $\psi^{(2)} = m\boldsymbol{v}$, the **linear momentum**;
- $\psi^{(3)} = \mathbb{I}^1 \cdot \omega + \boldsymbol{r} \times m\boldsymbol{v}$, the **angular momentum**;

---

[1] The inertia tensor for the spherocylinder we are considering.

Collision invariants

It is possible to prove that the following quantities are **collision invariants** for $C[f,f]$, i.e.

$$\iiint \psi^{(i)} C[f,f] d\boldsymbol{v}_1 d\varsigma_1 d\boldsymbol{\alpha}_1 = 0.$$

- $\psi^{(1)} = 1$, the **number of particles** in the system;
- $\psi^{(2)} = m\boldsymbol{v}$, the **linear momentum**;
- $\psi^{(3)} = \mathbb{I}$[1] $\cdot \omega + \boldsymbol{r} \times m\boldsymbol{v}$, the **angular momentum**;
- $\psi^{(4)} = \frac{1}{2} m\boldsymbol{v} \cdot \boldsymbol{v} + \frac{1}{2}\boldsymbol{\omega} \cdot \mathbb{I} \cdot \boldsymbol{\omega}$, the **kinetic energy of the system**.

---

[1] The inertia tensor for the spherocylinder we are considering.

The hydrodynamic equations – notation

We first introduce the **number density**, i.e.

$$n(\boldsymbol{r}) = \iiint f(\boldsymbol{r}, \boldsymbol{v}, \alpha, \varsigma) d\boldsymbol{v} d\alpha d\varsigma.$$

The hydrodynamic equations – notation

We first introduce the **number density**, i.e.

$$n(\boldsymbol{r}) = \iiint f(\boldsymbol{r}, \boldsymbol{v}, \alpha, \varsigma) d\boldsymbol{v} d\alpha d\varsigma.$$

Then we can give a meaning to the following *chevrons*, i.e.

$$\langle\!\langle \cdot \rangle\!\rangle(\boldsymbol{r}) := \frac{1}{n(\boldsymbol{r})} \iiint \cdot\, f(\boldsymbol{r}, \boldsymbol{v}, \alpha, \varsigma) d\boldsymbol{v} d\alpha d\varsigma.$$

The hydrodynamic equations – notation

We first introduce the **number density**, i.e.

$$n(\boldsymbol{r}) = \iiint f(\boldsymbol{r}, \boldsymbol{v}, \alpha, \varsigma) d\boldsymbol{v} d\alpha d\varsigma.$$

Then we can give a meaning to the following *chevrons*, i.e.

$$\langle\!\langle \cdot \rangle\!\rangle(\boldsymbol{r}) := \frac{1}{n(\boldsymbol{r})} \iiint \cdot \, f(\boldsymbol{r}, \boldsymbol{v}, \alpha, \varsigma) d\boldsymbol{v} d\alpha d\varsigma.$$

Using this notation we can define **macroscopic stream velocity** and **macroscopic stream angular velocity** respectively as:

$$\boldsymbol{v}_0 := \langle\!\langle \boldsymbol{v} \rangle\!\rangle, \qquad \boldsymbol{\omega}_0 := \langle\!\langle \boldsymbol{\omega} \rangle\!\rangle.$$

The Hydrodynamic Equations – Curtiss Balance Laws

Testing (1) against the first two **collision invariants** and integrating, Curtiss obtained the following **balance laws**:

$$\partial_t \rho + \nabla_{\boldsymbol{r}} \cdot (\rho \boldsymbol{v}_0) = 0,$$

$$\rho\Big[\partial_t \boldsymbol{v}_0 + (\nabla_{\boldsymbol{r}} \boldsymbol{v}_0)\boldsymbol{v}_0\Big] + \nabla_{\boldsymbol{r}} \cdot (\rho \mathbb{P}) = 0,$$

where ρ is the **density** defined as $\rho(\boldsymbol{r}) = mn(\boldsymbol{r})$ and $\mathbb{P}$ is the **pressure tensor** defined as $\mathbb{P} := \langle\!\langle \boldsymbol{V} \otimes \boldsymbol{V} \rangle\!\rangle$, with V being the **peculiar velocity** $\boldsymbol{V} := \boldsymbol{v} - \boldsymbol{v}_0$.

The hydrodynamic equations – surprise balance laws

For the third collision invariant we took a different route than Curtiss, which led to the following balance law

$$\rho\Big[\partial_t \boldsymbol{\eta} + (\nabla_{\boldsymbol{r}} \boldsymbol{\eta})\boldsymbol{v}_0\Big] + \nabla_{\boldsymbol{r}} \cdot (\rho \mathbb{N}) = \boldsymbol{\xi},$$

where $\boldsymbol{\eta}$ is the **macroscopic intrinsic angular momentum** defined as $\boldsymbol{\eta}(\boldsymbol{r}) := \langle\!\langle \mathbb{I} \cdot \omega \rangle\!\rangle$ and $\mathbb{N}$ is the **couple tensor** defined as $\mathbb{N} := \langle\!\langle \boldsymbol{V} \otimes (\mathbb{I}\boldsymbol{\omega}) \rangle\!\rangle$. Here ξ_l is defined in tensor notation as $\langle\!\langle mn(\varepsilon_{lki} v_i v_k)\boldsymbol{e}_l \rangle\!\rangle$ and we proved that $\boldsymbol{\xi}$ vanishes.

Maxwell–Boltzmann distribution

Curtiss gives an expression for the Maxwell–Boltzmann distribution, i.e. the distribution $f^{(0)}$ such that $C[f^{(0)}, f^{(0)}]$ vanishes:

$$f^{(0)}(\boldsymbol{v},\boldsymbol{\omega}) = \frac{n\sin(\alpha_2)Q}{\int Q\sin(\alpha_2)d\boldsymbol{\alpha}}\frac{m^{\frac{3}{2}}}{(2\pi\langle\!\langle\theta\rangle\!\rangle)^3}(\Gamma)^{\frac{1}{2}}\exp\left[-m\frac{|\boldsymbol{V}|}{2\langle\!\langle\theta\rangle\!\rangle}-\frac{\boldsymbol{\Omega}\cdot\mathbb{I}\cdot\boldsymbol{\Omega}}{2\langle\!\langle\theta\rangle\!\rangle}\right],$$

where the **peculiar angular velocity** defined as $\boldsymbol{\Omega} := \boldsymbol{\omega} - \boldsymbol{\omega}_0$, $\Gamma = \prod_{i=1}^{3}\Gamma_i$, Γ_i are the moments of inertia of the spherocylinder we are considering and $Q := \exp\left[\frac{\boldsymbol{\omega}_0\cdot\mathbb{I}\cdot\boldsymbol{\omega}_0}{2\theta}\right]$.

Maxwell–Boltzmann distribution

Curtiss gives an expression for the Maxwell–Boltzmann distribution, i.e. the distribution $f^{(0)}$ such that $C[f^{(0)}, f^{(0)}]$ vanishes:

$$f^{(0)}(\boldsymbol{v}, \boldsymbol{\omega}) = \frac{n \sin(\alpha_2) Q}{\int Q \sin(\alpha_2) d\boldsymbol{\alpha}} \frac{m^{\frac{3}{2}}}{(2\pi \langle\!\langle \theta \rangle\!\rangle)^3} (\Gamma)^{\frac{1}{2}} \exp\left[-m \frac{|\boldsymbol{V}|}{2\langle\!\langle \theta \rangle\!\rangle} - \frac{\boldsymbol{\Omega} \cdot \mathbb{I} \cdot \boldsymbol{\Omega}}{2\langle\!\langle \theta \rangle\!\rangle}\right],$$

where the **peculiar angular velocity** defined as $\boldsymbol{\Omega} := \boldsymbol{\omega} - \boldsymbol{\omega}_0$, $\Gamma = \prod_{i=1}^{3} \Gamma_i$, Γ_i are the moments of inertia of the spherocylinder we are considering and $Q := \exp\left[\frac{\boldsymbol{\omega}_0 \cdot \mathbb{I} \cdot \boldsymbol{\omega}_0}{2\theta}\right]$.

Notice in particular that we assumed ω_0 is the kinetic temperature of the system measured in energy units.

Novel Momentum Closure

Momentum closure around the equilibrium

Now we can use the Maxwell–Boltzmann distribution to compute an approximation of the **pressure tensor** near the equilibrium, i.e.

$$\mathbb{P}^{(0)} = \frac{\Gamma}{3m}\langle\langle\theta\rangle\rangle \boldsymbol{Id}.$$

$$\left[\partial_t \boldsymbol{v}_0 + (\nabla_{\boldsymbol{r}} \boldsymbol{v}_0)\boldsymbol{v}_0\right] = -\frac{1}{\rho}\nabla p,$$

Momentum closure around the equilibrium

Now we can use the Maxwell–Boltzmann distribution to compute an approximation of the **pressure tensor** near the equilibrium, i.e.

$$\mathbb{P}^{(0)} = \frac{\Gamma}{3m}\langle\langle\theta\rangle\rangle \boldsymbol{Id}.$$

$$\left[\partial_t \boldsymbol{v}_0 + (\nabla_{\boldsymbol{r}} \boldsymbol{v}_0)\boldsymbol{v}_0\right] = -\frac{1}{\rho}\nabla p,$$

Isotropicity

Unfortunately the same procedure results in a **vanishing** $\mathbb{N}^{(0)}$.

Noether's Theorem and Momentum Coupling

Let us consider the equation for the angular momentum, and observe that under the assumption $\mathbb{N}^{(0)} = 0$ it reads

$$\dot{\boldsymbol{\eta}} = \boldsymbol{\xi} = 0.$$

In particular, this is a consequence of Noether's theorem since when $\mathbb{N}^{(0)} = 0$ we have a **rotationally invariant** Lagrangian.

Noether's Theorem and Momentum Coupling

Let us consider the equation for the angular momentum, and observe that under the assumption $\mathbb{N}^{(0)} = 0$ it reads

$$\dot{\boldsymbol{\eta}} = \boldsymbol{\xi} = 0.$$

In particular, this is a consequence of Noether's theorem since when $\mathbb{N}^{(0)} = 0$ we have a **rotationally invariant** Lagrangian.

Isotropicity

Near the thermal equilibrium is the fluid isotropic? No!

The nematic ordering and the inertia tensor

We know that for a **slender body** the inertia tensor can be decomposed as,

$$\mathbb{I} = \lambda_1 (I - \boldsymbol{\nu} \otimes \boldsymbol{\nu}) + \mathcal{O}(\varepsilon)$$

where $\varepsilon = (\frac{r}{a})^2$. Furthermore, the macroscopic kinetic energy can be computed as

$$m\frac{1}{2}|\boldsymbol{v}_0|^2 + \frac{1}{2}\boldsymbol{\omega}_0 \cdot \mathbb{I}\boldsymbol{\omega}_0 = \frac{1}{2}m|\boldsymbol{v}_0|^2 + \frac{\lambda_1}{2}|\dot{\boldsymbol{\nu}}|^2 + \mathcal{O}(\varepsilon),$$

as $\varepsilon \to 0$ we retrieve the same energy that is the starting point for **Ericksen theory of anisotropic fluids**.

Balance laws for kinetic temperature

We need another way to formulate the **constitutive relation** for the **couple tensor**. We begin by observing that from $\psi^{(4)}$ we get the following balance law:

$$\dot{\psi}_0+\nabla_{\boldsymbol{r}}\boldsymbol{v}_0:(\rho\mathbb{P})+\nabla_{\boldsymbol{r}}\boldsymbol{\omega}_0:(\rho\mathbb{N})-\nabla\cdot\left[\mathbb{P}^T\boldsymbol{v}_0+\mathbb{N}^T\boldsymbol{\omega}_0\right]+\nabla_{\boldsymbol{r}}\cdot Q=0$$

where $\psi_0=\langle\langle\theta\rangle\rangle$, $Q=\frac{1}{2}\langle\langle\boldsymbol{V}(m|\boldsymbol{V}|^2+\boldsymbol{\Omega}\cdot\mathbb{I}\boldsymbol{\Omega})\rangle\rangle$, and

$$\theta=\frac{m}{2}\boldsymbol{V}\cdot\boldsymbol{V}+\frac{1}{2}\boldsymbol{\Omega}\cdot\mathbb{I}\cdot\boldsymbol{\Omega}.$$

Balance laws for kinetic temperature

We need another way to formulate the **constitutive relation** for the **couple tensor**. We begin by observing that from $\psi^{(4)}$ we get the following balance law:

$$\dot{\psi}_0+\nabla_{\boldsymbol{r}}\boldsymbol{v}_0:(\rho\mathbb{P})+\nabla_{\boldsymbol{r}}\boldsymbol{\omega}_0:(\rho\mathbb{N})-\nabla\cdot\left[\mathbb{P}^T\boldsymbol{v}_0+\mathbb{N}^T\boldsymbol{\omega}_0\right]+\nabla_{\boldsymbol{r}}\cdot Q=0$$

where $\psi_0=\langle\langle\theta\rangle\rangle$, $Q=\frac{1}{2}\langle\langle\boldsymbol{V}(m|\boldsymbol{V}|^2+\boldsymbol{\Omega}\cdot\mathbb{I}\boldsymbol{\Omega})\rangle\rangle$, and

$$\theta=\frac{m}{2}\boldsymbol{V}\cdot\boldsymbol{V}+\frac{1}{2}\boldsymbol{\Omega}\cdot\mathbb{I}\cdot\boldsymbol{\Omega}.$$

This is a **kinetic derivation** of **Leslie's rate of work hypothesis**.

The Oseen-Frank stored energy

"Whenever possible, substitute constructions out of known entities for inferences to unknown entities." – B. Russell

Making use of the fact that $\dot{\boldsymbol{\nu}} = \boldsymbol{\omega} \times \boldsymbol{\nu} = \partial_t \boldsymbol{\nu} (\nabla \boldsymbol{\nu}) \boldsymbol{\nu}$ we can rewrite part of the stored energy as

$$\psi_{OF}(\boldsymbol{\nu}, \nabla \boldsymbol{\nu}) = \frac{1}{2} \boldsymbol{\Omega} \cdot \mathbb{I} \boldsymbol{\Omega} = \frac{\lambda_{\mathbf{1}}}{2} tr \left[\nabla \boldsymbol{\nu}^T \mathbb{P}^{(0)} \nabla \boldsymbol{\nu} \right].$$

The Oseen-Frank stored energy

“Whenever possible, substitute constructions out of known entities for inferences to unknown entities.” – B. Russell

Making use of the fact that $\dot{\boldsymbol{\nu}} = \boldsymbol{\omega} \times \boldsymbol{\nu} = \partial_t \boldsymbol{\nu} (\nabla \boldsymbol{\nu}) \boldsymbol{\nu}$ we can rewrite part of the stored energy as

$$\psi_{OF}(\boldsymbol{\nu}, \nabla \boldsymbol{\nu}) = \frac{1}{2} \boldsymbol{\Omega} \cdot \mathbb{I} \boldsymbol{\Omega} = \frac{\boldsymbol{\lambda_1}}{2} tr\left[\nabla \boldsymbol{\nu}^T \mathbb{P}^{(0)} \nabla \boldsymbol{\nu} \right].$$

Using $\mathbb{P}^{(0)}$ we get a **stored energy functional** very similar to the **Oseen-Frank** energy

$$\psi_{OF} = p \frac{\boldsymbol{\lambda_1}}{2} tr\left[\nabla \boldsymbol{\nu}^T \nabla \boldsymbol{\nu} \right].$$

Noll–Coleman procedure

Since we are happy with our **pressure tensor**, we make the following **ansatz**

$$\psi = \psi(\nu, \nabla\nu)$$

where ν is the **nematic director**. Expanding the total derivative and using the Ericksen identity we get the following expression in tensor notation

$$\dot{\psi} = \varepsilon_{iqp}\Big[(\nu_q \frac{\partial\psi}{\partial(\nu_p)} + \partial_k(\nu_q)\frac{\partial\psi}{\partial(\partial_k\nu_p)})\omega_i^0 + \nu_q \frac{\partial\psi}{\partial(\partial_k\nu_p)}\partial_k\omega_i^0\Big] \\ - \frac{\partial\psi}{\partial(\partial_k\nu_p)}\partial_q(\nu_p)\partial(v_q^0)$$

Noll–Coleman procedure

Substituting this expression in the Theorem of power expanded and considering thermodynamic processes for which the exact divergences disappear, we get:

$$\begin{aligned}\left[\mathbb{P}_{ij} + \frac{\partial \psi}{\partial(\partial_j \nu_p)}\partial_i(\nu_p)\right]\partial_j(\nu_i) + \left[N_{ij} - \varepsilon_{iqp}\nu_q \frac{\partial \psi}{\partial(\partial_j \nu_p)}\right]\partial_j(\omega_i^0) \\ \left[P_{pq} - \frac{\partial \psi}{\partial(\partial_p \nu_k)\partial_q(\nu_k)}\right]\varepsilon_{iqp}\omega_i^0 \geq 0.\end{aligned}$$

Since the above expression must hold for all thermodynamic processes for which the exact divergences disappear, we get the following **constitutive relations**:

$$\mathbb{P} = \nabla \boldsymbol{\nu}^T \frac{\partial \psi}{\partial(\nabla \boldsymbol{\nu})} + \mathbb{P}^{(0)}, \qquad N_{ij} = \varepsilon_{iqp}\nu_q \frac{\partial \psi}{\partial(\partial_j \nu_p)} = \boldsymbol{\nu} \times \frac{\partial \psi}{\partial(\nabla \boldsymbol{\nu})}.$$

Compressible Leslie–Ericksen equations

This leads to the following set of equations, which can be seen as a generalisation of the Leslie–Ericksen that take into account the compressibility of the fluid:

Compressible Leslie–Ericksen equations

This leads to the following set of equations, which can be seen as a generalisation of the Leslie–Ericksen that take into account the compressibility of the fluid:

$$\partial_t \rho + \nabla_{\boldsymbol{r}} \cdot (\rho \boldsymbol{v}_0) = 0,$$

Compressible Leslie–Ericksen equations

This leads to the following set of equations, which can be seen as a generalisation of the Leslie–Ericksen that take into account the compressibility of the fluid:

$$\partial_t \rho + \nabla_{\boldsymbol{r}} \cdot (\rho \boldsymbol{v}_0) = 0,$$

$$\rho\Big[\partial_t \boldsymbol{v}_0 + (\nabla_{\boldsymbol{r}} \boldsymbol{v}_0)\boldsymbol{v}_0\Big] + \nabla_{\boldsymbol{r}} \cdot \Big(p_K I + p_K \frac{\lambda_1}{2} \nabla_{\boldsymbol{r}} \boldsymbol{\nu}^T \nabla_{\boldsymbol{r}} \boldsymbol{\nu}\Big) = 0,$$

Compressible Leslie–Ericksen equations

This leads to the following set of equations, which can be seen as a generalisation of the Leslie–Ericksen that take into account the compressibility of the fluid:

$$\partial_t \rho + \nabla_{\boldsymbol{r}} \cdot (\rho \boldsymbol{v}_0) = 0,$$

$$\rho\Big[\partial_t \boldsymbol{v}_0 + (\nabla_{\boldsymbol{r}} \boldsymbol{v}_0)\boldsymbol{v}_0\Big] + \nabla_{\boldsymbol{r}} \cdot \Big(p_K I + p_K \frac{\lambda_1}{2} \nabla_{\boldsymbol{r}} \boldsymbol{\nu}^T \nabla_{\boldsymbol{r}} \boldsymbol{\nu}\Big) = 0,$$

$$\rho\Big[\partial_t \boldsymbol{\nu} + (\nabla_{\boldsymbol{r}} \boldsymbol{\nu})\boldsymbol{v}_0\Big] + \nabla_{\boldsymbol{r}} \cdot \Big(p_K \frac{\lambda_1}{2} \nabla_{\boldsymbol{r}} \boldsymbol{\nu}\Big) = \tau \boldsymbol{\nu},$$

Compressible Leslie–Ericksen equations

This leads to the following set of equations, which can be seen as a generalisation of the Leslie–Ericksen that take into account the compressibility of the fluid:

$$
\begin{aligned}
&\partial_t \rho + \nabla_{\boldsymbol{r}} \cdot (\rho \boldsymbol{v}_0) = 0,\\
&\rho\Big[\partial_t \boldsymbol{v}_0 + (\nabla_{\boldsymbol{r}} \boldsymbol{v}_0)\boldsymbol{v}_0\Big] + \nabla_{\boldsymbol{r}} \cdot \Big(p_K I + p_K \frac{\lambda_1}{2} \nabla_{\boldsymbol{r}} \boldsymbol{\nu}^T \nabla_{\boldsymbol{r}} \boldsymbol{\nu}\Big) = 0,\\
&\rho\Big[\partial_t \boldsymbol{\nu} + (\nabla_{\boldsymbol{r}} \boldsymbol{\nu})\boldsymbol{v}_0\Big] + \nabla_{\boldsymbol{r}} \cdot \Big(p_K \frac{\lambda_1}{2} \nabla_{\boldsymbol{r}} \boldsymbol{\nu}\Big) = \tau \boldsymbol{\nu},\\
&\rho\Big[\partial_t \psi_0 + \nabla_{\boldsymbol{r}} \psi_0 \cdot \boldsymbol{v}_0\Big] + \Big(p_K I + p_K \frac{\lambda_1}{2} \nabla_{\boldsymbol{r}} \boldsymbol{\nu}^T \nabla_{\boldsymbol{r}} \boldsymbol{\nu}\Big) : \nabla_{\boldsymbol{r}} \boldsymbol{v}_0 = 0.
\end{aligned}
$$

Static problem

Compressible Oseen–Frank energy

We will now consider the equation for the **director** $\boldsymbol{\nu}$ in the static regime, i.e. $\dot{\boldsymbol{\nu}} = 0$, i.e.

$$\nabla_{\boldsymbol{r}} \cdot \left(p_K \frac{\lambda_1}{2} \nabla_{\boldsymbol{r}} \boldsymbol{\nu} \right) = \tau \boldsymbol{\nu}.$$

Compressible Oseen–Frank energy

We will now consider the equation for the **director** $\boldsymbol{\nu}$ in the static regime, i.e. $\dot{\boldsymbol{\nu}} = 0$, i.e.

$$\nabla_{\boldsymbol{r}} \cdot \left(p_K \frac{\lambda_1}{2} \nabla_{\boldsymbol{r}} \boldsymbol{\nu} \right) = \tau \boldsymbol{\nu}.$$

In particular, this equation can be seen as Euler–Lagrange of for the minimisation of the **compressible Oseen–Frank energy**, i.e.

$$\boldsymbol{\nu} = \underset{\boldsymbol{\eta} \in V(\mathcal{S}, \mathbb{S}^2)}{argmin} \; I[\nabla_{\boldsymbol{r}} \boldsymbol{\eta}] = \frac{1}{2} \int_{\mathcal{S}} \Phi(\nabla \boldsymbol{\eta}) \, d\boldsymbol{r} = \frac{1}{2} \int_{\mathcal{S}} \lambda_1 p |\nabla_{\boldsymbol{r}} \boldsymbol{\eta}|^2 \, d\boldsymbol{r}.$$

Euler–Lagrange equations

We know that because $\boldsymbol{\nu}$ is a minimizer the first variation of the energy must vanish, i.e.

$$\frac{d}{d\varepsilon}\, I[\nabla \boldsymbol{\nu}_\varepsilon] = \frac{d}{d\varepsilon}\,\frac{1}{2}\int_{\mathcal{S}} \lambda_1 p |\nabla_{\boldsymbol{r}} \boldsymbol{\nu}_\varepsilon|^2 \, d\boldsymbol{r} = \int_{\mathcal{S}} \lambda_1 p \, \nabla_{\boldsymbol{r}} \boldsymbol{\nu}_\varepsilon \cdot \nabla_{\boldsymbol{r}} \left(\frac{d}{d\varepsilon}\, \boldsymbol{\nu}_\varepsilon \right) \, d\boldsymbol{r}.$$

Euler–Lagrange equations

We know that because $\boldsymbol{\nu}$ is a minimizer the first variation of the energy must vanish, i.e.

$$\frac{d}{d\varepsilon} I[\nabla \boldsymbol{\nu}_\varepsilon] = \frac{d}{d\varepsilon} \frac{1}{2} \int_{\mathcal{S}} \lambda_1 p |\nabla_{\boldsymbol{r}} \boldsymbol{\nu}_\varepsilon|^2 \, d\boldsymbol{r} = \int_{\mathcal{S}} \lambda_1 p \, \nabla_{\boldsymbol{r}} \boldsymbol{\nu}_\varepsilon \cdot \nabla_{\boldsymbol{r}} \left(\frac{d}{d\varepsilon} \boldsymbol{\nu}_\varepsilon \right) \, d\boldsymbol{r}.$$

We compute , $\frac{d}{d\varepsilon} \boldsymbol{\nu}_\varepsilon$, i.e. $\displaystyle \frac{d}{d\varepsilon} \boldsymbol{\nu}_\varepsilon \Big|_{\varepsilon=0} = (I - \boldsymbol{\nu} \otimes \boldsymbol{\nu}) \widetilde{\boldsymbol{\nu}}$,

Euler–Lagrange equations

We know that because $\boldsymbol{\nu}$ is a minimizer the first variation of the energy must vanish, i.e.

$$\frac{d}{d\varepsilon} I[\nabla \boldsymbol{\nu}_\varepsilon] = \frac{d}{d\varepsilon}\frac{1}{2}\int_{\mathcal{S}} \lambda_1 p |\nabla_{\boldsymbol{r}} \boldsymbol{\nu}_\varepsilon|^2 \, d\boldsymbol{r} = \int_{\mathcal{S}} \lambda_1 p \, \nabla_{\boldsymbol{r}} \boldsymbol{\nu}_\varepsilon \cdot \nabla_{\boldsymbol{r}} \left(\frac{d}{d\varepsilon} \boldsymbol{\nu}_\varepsilon \right) \, d\boldsymbol{r}.$$

We compute , $\frac{d}{d\varepsilon}\boldsymbol{\nu}_\varepsilon$, i.e. $\displaystyle \frac{d}{d\varepsilon}\boldsymbol{\nu}_\varepsilon \bigg|_{\varepsilon=0} = (I - \boldsymbol{\nu} \otimes \boldsymbol{\nu})\, \widetilde{\boldsymbol{\nu}},$ yielding the following **Euler–Lagrange** equations in weak form

$$\int_{\mathcal{S}} \lambda_1 \nabla_{\boldsymbol{r}} \cdot (p \nabla_{\boldsymbol{r}} \boldsymbol{\nu}) \, (I - \boldsymbol{\nu} \otimes \boldsymbol{\nu}) \, \widetilde{\boldsymbol{\nu}} \, d\boldsymbol{r} = 0.$$

Euler–Lagrange equations

We know that because $\boldsymbol{\nu}$ is a minimizer the first variation of the energy must vanish, i.e.

$$\frac{d}{d\varepsilon}\, I[\nabla\boldsymbol{\nu}_\varepsilon] = \frac{d}{d\varepsilon}\,\frac{1}{2}\int_{\mathcal{S}} \lambda_1 p|\nabla_{\boldsymbol{r}}\boldsymbol{\nu}_\varepsilon|^2\, d\boldsymbol{r} = \int_{\mathcal{S}} \lambda_1 p\, \nabla_{\boldsymbol{r}}\boldsymbol{\nu}_\varepsilon \cdot \nabla_{\boldsymbol{r}}\left(\frac{d}{d\varepsilon}\,\boldsymbol{\nu}_\varepsilon\right)\, d\boldsymbol{r}.$$

We compute , $\frac{d}{d\varepsilon}\boldsymbol{\nu}_\varepsilon$, i.e. $\displaystyle \frac{d}{d\varepsilon}\,\boldsymbol{\nu}_\varepsilon\bigg|_{\varepsilon=0} = (I - \boldsymbol{\nu}\otimes\boldsymbol{\nu})\,\widetilde{\boldsymbol{\nu}}$, yielding the following **Euler–Lagrange** equations in weak form

$$\int_{\mathcal{S}} \lambda_1 \nabla_{\boldsymbol{r}} \cdot (p\nabla_{\boldsymbol{r}}\boldsymbol{\nu})\,(I - \boldsymbol{\nu}\otimes\boldsymbol{\nu})\,\widetilde{\boldsymbol{\nu}}\, d\boldsymbol{r} = 0.$$

$$\boxed{\lambda_1 \nabla_{\boldsymbol{r}} \cdot (p\nabla_{\boldsymbol{r}}\boldsymbol{\nu}) = \tau\boldsymbol{\nu} \text{ in } \mathcal{S}.}$$

The $\mathbb{S}^2$ constraint and the harmonic maps

We can think of $\tau : \mathcal{S} \to \mathbb{R}$ as a **Lagrange multiplier** that enforces the constraint $\boldsymbol{\nu} \in \mathbb{S}^2$.

The $\mathbb{S}^2$ constraint and the harmonic maps

We can think of $\tau : \mathcal{S} \to \mathbb{R}$ as a **Lagrange multiplier** that enforces the constraint $\boldsymbol{\nu} \in \mathbb{S}^2$.

$$\begin{aligned}\tau &= \boldsymbol{\nu} \cdot \nabla_{\boldsymbol{r}} \cdot (p \nabla_{\boldsymbol{r}} \boldsymbol{\nu}) \\ &= \boldsymbol{\nu} \cdot \left[\nabla_{\boldsymbol{r}} \boldsymbol{\nu}^T \nabla_{\boldsymbol{r}} p + p \Delta_{\boldsymbol{r}} \boldsymbol{\nu} \right] = \boldsymbol{\nu} \cdot \left[\nabla_{\boldsymbol{r}} \boldsymbol{\nu}^T \nabla_{\boldsymbol{r}} p - p |\nabla_{\boldsymbol{r}} \boldsymbol{\nu}|^2 \right],\end{aligned}$$

The $\mathbb{S}^2$ constraint and the harmonic maps

We can think of $\tau : \mathcal{S} \to \mathbb{R}$ as a **Lagrange multiplier** that enforces the constraint $\boldsymbol{\nu} \in \mathbb{S}^2$.

$$\begin{aligned}\tau &= \boldsymbol{\nu} \cdot \nabla_{\boldsymbol{r}} \cdot (p \nabla_{\boldsymbol{r}} \boldsymbol{\nu}) \\ &= \boldsymbol{\nu} \cdot \left[\nabla_{\boldsymbol{r}} \boldsymbol{\nu}^T \nabla_{\boldsymbol{r}} p + p \Delta_{\boldsymbol{r}} \boldsymbol{\nu} \right] = \boldsymbol{\nu} \cdot \left[\nabla_{\boldsymbol{r}} \boldsymbol{\nu}^T \nabla_{\boldsymbol{r}} p - p |\nabla_{\boldsymbol{r}} \boldsymbol{\nu}|^2 \right],\end{aligned}$$

Harmonic maps

Substituting this expression in (1) we get that $\boldsymbol{\nu}$ mush be an **harmonic map** from $\mathcal{S}$ to $\mathbb{S}^2$, i.e.

$$\lambda_1 p \left(\Delta_{\boldsymbol{r}} \boldsymbol{\nu} + |\nabla_{\boldsymbol{r}} \boldsymbol{\nu}|^2 \boldsymbol{\nu} \right) = 0,$$

since the pressure p is positive.

Liquid crystal defects: the hedgehog

An intersting example of a universal solution is the **hedgehog** solution, i.e.

$$\hat{\boldsymbol{\nu}} : \mathcal{S} \to \mathbb{S}^2 \qquad \boldsymbol{r} \mapsto \frac{\boldsymbol{r}}{|\boldsymbol{r}|}.$$

Liquid crystal defects: the hedgehog

An intersting example of a universal solution is the **hedgehog** solution, i.e.

$$\hat{\boldsymbol{\nu}} : \mathcal{S} \to \mathbb{S}^2 \qquad \boldsymbol{r} \mapsto \frac{\boldsymbol{r}}{|\boldsymbol{r}|}.$$

The hedgehog map is the only admissible class of solution to the weak formulation of the harmonic map equation in $W^{1,2}(\mathcal{S})$.

$$I[\nabla_{\boldsymbol{r}}\hat{\boldsymbol{\nu}}] = \frac{1}{2}\int_{B_R(\mathbf{0})} \lambda_1 p |\nabla_{\boldsymbol{r}}\hat{\boldsymbol{\nu}}|^2 \, d\boldsymbol{r} = \frac{\lambda_1}{2}\pi \|p\|_{L^\infty(\mathcal{S})}$$

$$= \lambda_1 \|p\|_{L^\infty(\mathcal{S})} \int_0^R s^2 \frac{2}{s^2} \, ds = 2\pi\lambda_1 \|p\|_{L^\infty(\mathcal{S})} R.$$

Liquid crystal defects: the two-dimensional hedgehog

Another extremely interesting universal solution to the harmonic map equation is the **two-dimensional hedgehog**, i.e.

$$\overline{\boldsymbol{\nu}} : \mathcal{S} \to \mathbb{S}^2 \qquad \boldsymbol{r} \mapsto \begin{pmatrix} R^{-1}\boldsymbol{r}_1 & R^{-1}\boldsymbol{r}_2 & 0 \end{pmatrix}, \qquad R := \sqrt{\boldsymbol{r}_1^2 + \boldsymbol{r}_2^2}.$$

Liquid crystal defects: the two-dimensional hedgehog

Another extremely interesting universal solution to the harmonic map equation is the **two-dimensional hedgehog**, i.e.

$$\overline{\boldsymbol{\nu}} : \mathcal{S} \to \mathbb{S}^2 \qquad \boldsymbol{r} \mapsto \begin{pmatrix} R^{-1}\boldsymbol{r}_1 & R^{-1}\boldsymbol{r}_2 & 0 \end{pmatrix}, \qquad R := \sqrt{\boldsymbol{r}_1^2 + \boldsymbol{r}_2^2}.$$

Line defects

Notice that the two-dimensional hedgehog is a vector field orthogonal to a family of cylinders, and it presents a **line singularity** passing through the origin. Line singularities are not admissible in $\mathcal{W}^{1,2}(\mathcal{S}, \mathbb{S}^2)$.

Liquid crystal defects: the two–dimensional hedgehog

The two–dimensional hedgehog is a universal solution and if we compute the energy of the two-dimensional hedgehog on a cylinder $\mathcal{S}$ of radius R and height L we obtain

$$I[\nabla_{\boldsymbol{r}}\overline{\boldsymbol{\nu}}] = \frac{\lambda_1}{2}\int_{\mathcal{S}} p|\nabla_{\boldsymbol{r}}\overline{\boldsymbol{\nu}}|^2 \, d\boldsymbol{r} = \lambda_1 \pi L \int_0^R p\, s \cdot \frac{2}{s^2}\, ds,$$

hence choosing the pressure field p as $p(\boldsymbol{r}) = \sqrt{\boldsymbol{r}_1^2 + \boldsymbol{r}_2^2}$ we obtain $I[\nabla_{\boldsymbol{r}}\overline{\boldsymbol{\nu}}] = 2\pi\lambda_1 L < \infty$.

Conclusions

- Using a Noll–Coleman argument for the closure of the momentum hierarchy allows us to retrieve the **Ericksen stress tensor**.

Conclusions

- Using a Noll–Coleman argument for the closure of the momentum hierarchy allows us to retrieve the **Ericksen stress tensor**.
- From the kinetic theory of spherocylindrical molecules, we derived a **compressible** and thermally coupled model for the flow of fluids with a nematic order.

Conclusions

- Using a Noll–Coleman argument for the closure of the momentum hierarchy allows us to retrieve the **Ericksen stress tensor**.
- From the kinetic theory of spherocylindrical molecules, we derived a **compressible** and thermally coupled model for the flow of fluids with a nematic order.
- From the kinetic theory of spherocylindrical molecules, we can only derive the **poor–man** Oseen–Frank energy.

Conclusions

- Using a Noll–Coleman argument for the closure of the momentum hierarchy allows us to retrieve the **Ericksen stress tensor**.
- From the kinetic theory of spherocylindrical molecules, we derived a **compressible** and thermally coupled model for the flow of fluids with a nematic order.
- From the kinetic theory of spherocylindrical molecules, we can only derive the **poor–man** Oseen–Frank energy.
- We have given a new physical meaning to J. L. Ericksen's **variable degree of orientation**;

Dreaming of the future

- Use L. Ambrosio works on the regularity of the minimisers of the Ericksen's energy with variable degree of orientation to prove the existence of minimisers for the compressible Oseen–Frank energy even when the pressure field is not fixed;

Dreaming of the future

- Use L. Ambrosio works on the regularity of the minimisers of the Ericksen's energy with variable degree of orientation to prove the existence of minimisers for the compressible Oseen–Frank energy even when the pressure field is not fixed;
- Derive from a kinetic theory of spherocylindrical molecules, Virga's energy functional for nematic Korteweg fluids;

Dreaming of the future

- Use L. Ambrosio works on the regularity of the minimisers of the Ericksen's energy with variable degree of orientation to prove the existence of minimisers for the compressible Oseen–Frank energy even when the pressure field is not fixed;
- Derive from a kinetic theory of spherocylindrical molecules, Virga's energy functional for nematic Korteweg fluids;
- Interpret the **smectic energy functional** within the framework here proposed;

Dreaming of the future

- Use L. Ambrosio works on the regularity of the minimisers of the Ericksen's energy with variable degree of orientation to prove the existence of minimisers for the compressible Oseen–Frank energy even when the pressure field is not fixed;
- Derive from a kinetic theory of spherocylindrical molecules, Virga's energy functional for nematic Korteweg fluids;
- Interpret the **smectic energy functional** within the framework here proposed;
- Study numerically the equations derived in this work, focusing on C^1 conforming FEM, VEM and **lightning-VEM**.