

# A Nematic Theory For a Nonspherical Rarefied Gas



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Università di Catania*

Numerical Analysis Group Internal Seminar, 2nd May 2023, Oxford



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# A Kinetic Theory For Nematic Liquid Crystals



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# A Kinetic Theory For Nematic Liquid Crystals And Simulations

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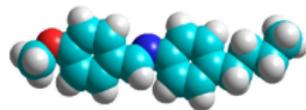


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# The molecules

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

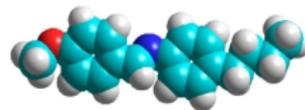


5CB

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



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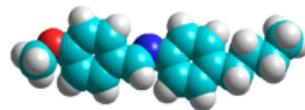


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- ▶ Molecules are **achiral**, i.e. they can be superimposed with their mirror images.



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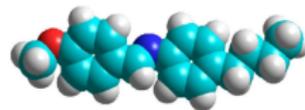


5CB

# 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**.



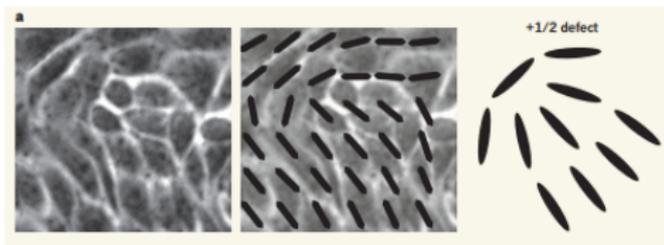
MBBA



5CB

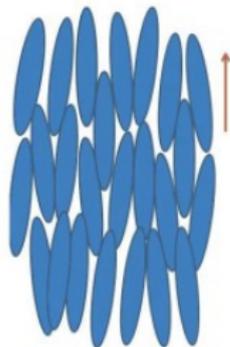
# The applications

Nematic molecules seem to be ubiquitous in our life they can be found at the heart of modern liquid crystal displays while at the same time being the structure of our epithelium.



# The nematic ordering

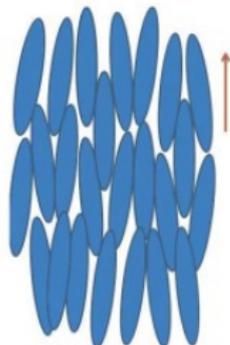
Onsager first related the ability of certain colloidal particles to have a partial ordering before they freeze (hence retaining the ability to flow) to the particle geometry. The greater the elongation of the molecule, the more likely the colloidal will form a nematic ordering.



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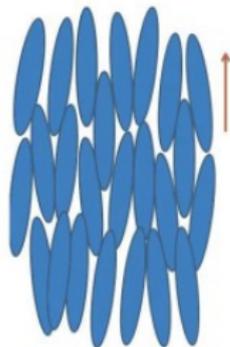
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- ▶ There is an **enthalpic drive**, i.e. the van der Waals forces favor alignment.
- ▶ There is an **entropic drive**, i.e. aligned elongated molecules are more loosely packed, i.e. we have fewer constraints on the velocity and position.



- ▶ The anisotropic behavior of ordered fluids is described by **Frank's constants**. Measuring Frank's constants is an expensive and time-consuming process. We want to derive the value of **Frank's constants** from a kinetic point of view.

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- ▶ Develop a **compressible** and **thermally coupled** model for the flow of fluids with a **nematic order**.

# Kinetic Theory

# Kinetic Theory of Spherical Molecules

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- ▶ **Statistical** description of a thermodynamic system composed of **spherical** particles.



Ludwig Eduard Boltzmann,  
1844–1906

# Kinetic Theory of Spherical Molecules

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- ▶ Reduce particles interactions to only **binary collisions**.



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# Kinetic Theory of Spherical Molecules

- ▶ **Statistical** description of a thermodynamic system composed of **spherical** particles.
- ▶ Reduce particles interactions to only **binary collisions**.
- ▶ **Stosszahlansatz**, i.e. is the assumption that the velocities of colliding particles are **uncorrelated** and independent of position.



Ludwig Eduard Boltzmann,  
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# Kinetic Theory of Non-Spherical Molecules

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Charles Francis Curtiss,  
1921–2007

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# Kinetic Theory of Non-Spherical Molecules

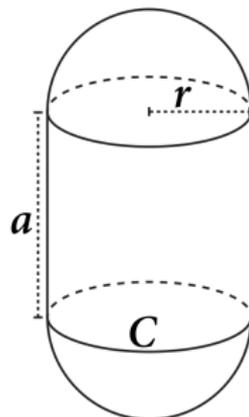
- ▶ In 1956 derived the first kinetic theory for **non-spherical** molecules.
- ▶ In 1963 together with J.S. Dahler, used the **BBGKY** formalism to derive a kinetic theory for **non-spherical** molecules.
- ▶ Fostered a kinetic theory “school” who was very active in development of a theory for **hard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



Charles Francis Curtiss,  
1921–2007

# Curtiss collision operator

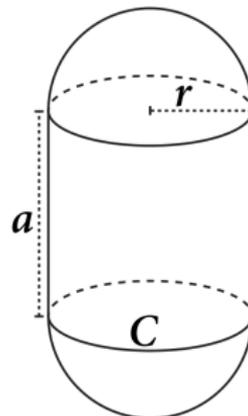
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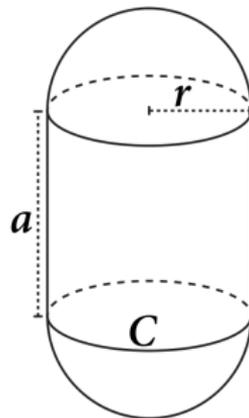
- ▶ He considered a larger configuration space made by **position**, **velocity**, the **Euler angles** for describing the orientation of each molecule, and the **angular velocity** with respect to a fixed coordinate system.



## 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,

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

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

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$$C[f, f] = - \iiint\!\!\!\int (f'_1 f' - f_1 f)(\mathbf{k} \cdot \mathbf{g}) S(\mathbf{k}) d\mathbf{k} d\mathbf{v}_1 d\alpha_1 d\varsigma_1$$

with  $S(\mathbf{k})d\mathbf{k}$  being the surface element of the excluded volume and  $\mathbf{g} = \mathbf{v} - \mathbf{v}_1$ . 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.

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

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<sup>1</sup>The inertia tensor for the spherocylinder we are considering.

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- ▶  $\psi^{(4)} = \frac{1}{2}m\mathbf{v} \cdot \mathbf{v} + \frac{1}{2}\boldsymbol{\omega} \cdot \mathbb{I} \cdot \boldsymbol{\omega}$ , the **kinetic energy of the system**.

---

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## The hydrodynamic equations – notation

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

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

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

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

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

$$\mathbf{v}_0 := \langle\langle \mathbf{v} \rangle\rangle, \quad \boldsymbol{\omega}_0 := \langle\langle \boldsymbol{\omega} \rangle\rangle.$$

# The Hydrodynamic Equations – Curtiss Balance Laws

Testing  $C[f, f]$  against the first two **collision invariants** and integrating, Curtiss obtained the following **balance laws**:

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

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

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

# 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

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

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

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

where the **peculiar angular velocity** defined as  $\boldsymbol{\Omega} := \boldsymbol{\omega} - \boldsymbol{\omega}_0$ ,  $\Gamma = \prod_{i=1}^3 \Gamma_i$ ,  $\Gamma_i$  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  $\boldsymbol{\omega}_0$  and the **peculiar kinetic energy**  $\theta = \frac{m}{2} \mathbf{V} \cdot \mathbf{V} + \frac{1}{2} \boldsymbol{\Omega} \cdot \mathbb{I} \cdot \boldsymbol{\Omega}$  are fixed.

# Anisotropic Behavior

## Momentum closure around the equilibrium

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

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

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

### Isotropy

**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

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

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

## Isotropy

Near the thermal equilibrium is the fluid isotropic? **No!**

## The nematic ordering and the inertia tensor

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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

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

as  $\varepsilon \rightarrow 0$  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:

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

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

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

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

## The Oseen-Frank stored energy

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

Making use of the fact that  $\dot{\nu} = \omega_0 \times \nu = (\nabla \nu) \nu_0$  we can rewrite part of the stored energy as

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

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

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

## Nematic law of angular momentum

### Anisotropy

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

### Static equation

The equation corresponding to the balance law of angular momentum in the static case becomes,

$$\nabla \cdot (p \nabla \boldsymbol{\nu}) + (\nabla \boldsymbol{\nu}^T \nabla p) + |\nabla \boldsymbol{\nu}|^2 \boldsymbol{\nu} = 0.$$

- ▶ Using a Noll–Coleman argument for the closure of the momentum hierarchy allows us to capture the anisotropy of acoustic waves in rarefied liquid crystals.

**Thank you for your attention!**

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- ▶ We hope to use similar techniques to the one presented today to compute all Frank constants from  $\mathbb{I}$ .

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- ▶ Using a Noll–Coleman argument for the closure of the momentum hierarchy allows us to capture the anisotropy of acoustic waves in rarefied liquid crystals.
- ▶ We hope to use similar techniques to the one presented today to compute all Frank constants from  $\mathbb{I}$ .
- ▶ We hope to adopt finite-element discretisation together with multi-scale methods to simulate the integro-differential equation arising from our model.

**Thank you for your attention!**

## Noll–Coleman procedure

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

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

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

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

## Noll–Coleman procedure

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

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

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

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

# The system of PDE

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

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

$$\nabla_{\mathbf{r}} \cdot \left( p_K \frac{\lambda_1}{2} \nabla_{\mathbf{r}} \boldsymbol{\nu} \right) = \lambda \boldsymbol{\nu},$$

$$\rho \left[ \partial_t \psi_0 + \nabla_{\mathbf{r}} \psi_0 \cdot \mathbf{v}_0 \right] + \left( p_K I + p_K \frac{\lambda_1}{2} \nabla_{\mathbf{r}} \boldsymbol{\nu}^T \nabla_{\mathbf{r}} \boldsymbol{\nu} \right) : \nabla_{\mathbf{r}} \mathbf{v}_0 = 0.$$