UNIVERSITY OF OXFORD
Mathematical Institute

A Kinetic Framework for Fluids with Partial Ordering

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**Mathematical Institute – University of Oxford*

Modelling of Materials, 23rd October 2024

Oxford Mathematics

ORDERED FLUIDS

Partially ordered fluids are ubiquitous in nature and have a wide range of applications.

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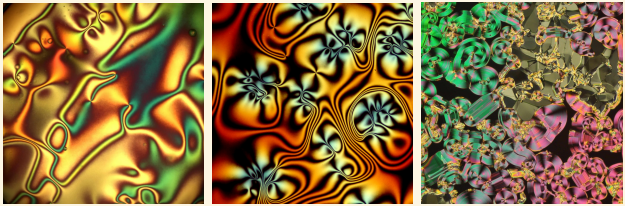

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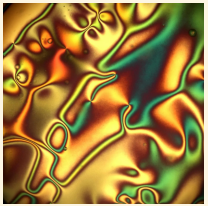
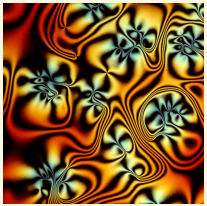
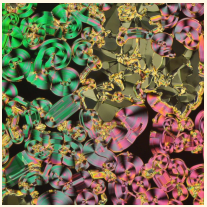


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- **Ferrofluids**, i.e. a colloidal suspension made of nanoscale ferromagnetic or ferrimagnetic particles.

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- **Liquid crystals**, here depicted in nematic and smectic phases.
- **Ferrofluids**, i.e. a colloidal suspension made of nanoscale ferromagnetic or ferrimagnetic particles.
- **Gas saturated magma melts** and other fluids with non-diffusive bubbles.

A KINETIC THEORY APPROACH

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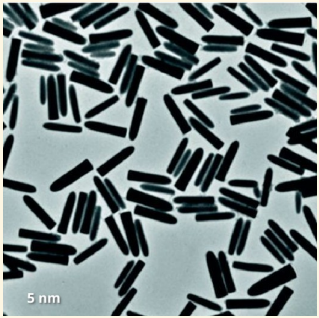

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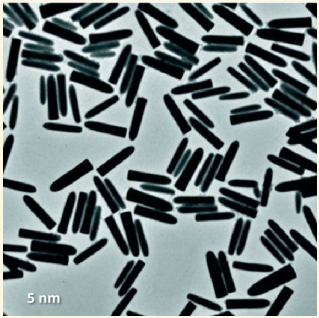

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Onsager's Approach To Liquid Crystals

Onsager first explained the emergence of nematic ordering in liquid crystals by a truncation of the Mayer cluster expansion, valid for dilute systems.

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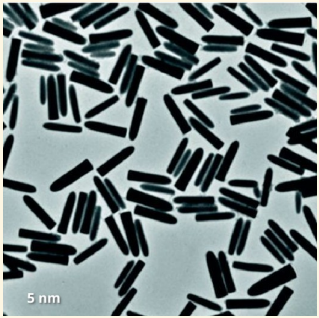

ORDER PARAMETER MANIFOLD

1

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Order Parameter Manifold

We say that the tuple $(\mathcal{M}, \mathcal{A})$ is an order parameter manifold if $\mathcal{M}$ is a smooth manifold with a fixed parametrization, and $\mathcal{A}$ is a Lie group action of SO(3) on $\mathcal{M}$, i.e. the map $\mathcal{A}$ is smooth enough to be differentiable.

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Furthermore, we say that a field $\nu : \mathbb{E}^3 \to \mathcal{M}$ is an order parameter field if $\forall \underline{c} \in \mathbb{R}^3$ and $\forall \underline{\underline{Q}} \in \mathrm{SO}(3)$ we have

$$\nu(\underline{\underline{Q}}\mathbf{x} + \underline{c}) = \mathcal{A}(\underline{\underline{Q}}, \nu(\mathbf{x})), \quad \forall \mathbf{x} \in \mathbb{E}^3.$$

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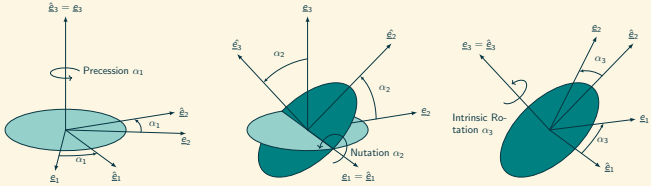
- We need to understand the action of rotations on the manifold $\mathcal{M}$.

AN EXAMPLE: NEMATIC LIQUID CRYSTALS



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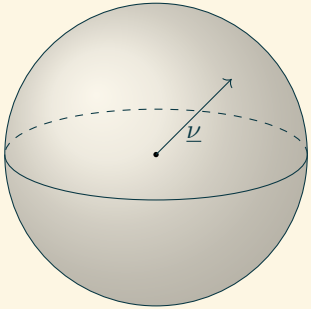

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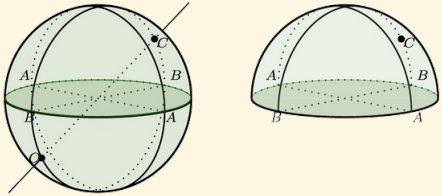

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- We can also represent the state of a calamitic molecule using a director field $\underline{\nu} \in \mathbb{S}^2$.
- For head-tail symmetric calamitic molecules, we can use $\mathbb{RP}^2$.

EMBEDDING RESULTS

Emedding theorems

- Any compact orientable 2-manifold can be embedded in $\mathbb{R}^3$.

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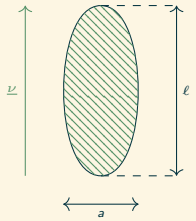
THE MICROSCOPIC WORLD

2

LAGRANGIAN MECHANICS OF THE CONSTITUENTS

We will here assume that the fluid is composed of a set of constituents, each of which is described by a position $\mathbf{x}_i$, a velocity $\underline{\nu}_i$, the order parameter ν_i and its total time derivative $\dot{\underline{\nu}}_i$.



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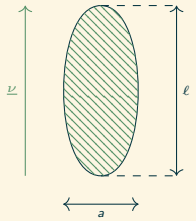
$$\mathcal{L}_i := \frac{1}{2} m_1 (\dot{\underline{x}}_i \cdot \dot{\underline{x}}_i + \frac{1}{2} \dot{\underline{\nu}}_i \cdot \underline{\underline{\Omega}}_i(\nu_i) \dot{\underline{\nu}}_i.$$



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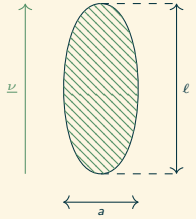
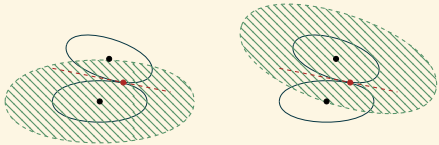


We assume the interaction between the constituents is given by a potential $\mathcal{W}(|\mathbf{x}_i - \mathbf{x}_j|, \nu_i, \nu_j)$, i.e.

$$\mathcal{L}_{i,j} = \mathcal{L}_i(\mathbf{x}_i, \Xi_i) + \mathcal{L}_j(\mathbf{x}_j, \Xi_j) + \mathcal{W}(|\mathbf{x}_i - \mathbf{x}_j|, \nu_i, \nu_j),$$

where $\Xi_i := (\underline{v}_i, \nu_i, \dot{\underline{\nu}}_i)$.



NOETHER'S THEOREM: SYMMETRIES AND CONSERVATION LAWS

Noether's theorem

If a Lagrangian $\mathcal{L}$ is invariant under a group action with infinitesimal generators G then

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{q}_{1,2}} \cdot G\right) = 0, \qquad q_{1,2} = (\mathbf{x}_1, \mathbf{x}_2, \nu_1, \nu_2)\,.$$

In other words for any physical symmetry of the system, there is a conserved quantity.

Analytical Mechanics: An Introduction, (A. Fasano, S. Marmi).

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- The Lagrangian $\mathcal{L}$ is invariant under translations, i.e. the linear momentum is conserved.
- The Lagrangian $\mathcal{L}$ is independent of time and the kinetic energy is a homogeneous quadratic form of the conjugate moments, i.e. the energy is conserved.

NOETHER'S THEOREM: SYMMETRIES AND CONSERVATION LAWS

Infinitesimal Generator of $\mathcal{A}$

For fixed $\nu \in \mathcal{M}$, the orbit map

$$\mathcal{A}_\nu : \mathrm{SO}(3) \to \mathrm{SO}(3)\nu, \quad \underline{\underline{Q}} \mapsto \mathcal{A}(\underline{\underline{Q}}, \nu),$$

is differentiable at the identity.

We will denote by $A_\nu : \mathrm{SO}(3) \to T_\nu\mathcal{M}$ the differential of $\mathcal{A}_\nu$ at the identity.
Composing the canonical isomorphism $\mathbb{R}^3 \to SO(3)$ with the differential of the orbit map we obtain a map $A_\nu : \mathbb{R}^3 \to T_\nu\mathcal{M}$.

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Assuming that the Lagrangian $\mathcal{L}$ is frame-indifferent, i.e. invariant under the action of SO(3), we have:

$$G = (\underline{r} \times \mathbf{x}, \underline{r} \times \underline{x}, A_\nu \mathbf{r}, A_\nu \underline{r}),$$

where $\underline{r}$ is the rotation axis. Thus, the angular momentum is conserved.

BBGKY HIERARCHY

3

HAMILTONIAN MECHANICS OF THE CONSTITUENTS

We introduce the Hamiltonian formalism associated to the Lagrangian $\mathcal{L}$ introduced in the previous section. As usual, we introduce the conjugate momenta to the generalised coordinates, i.e.

$$\underline{p_i} \coloneqq \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{x}}_i} = m\dot{\mathbf{x}}_i, \qquad \underline{\varsigma_i} \coloneqq \frac{\partial \mathcal{L}}{\partial \underline{\dot{\nu}_i}} = \underline{\underline{\Omega}}(\nu)\,\underline{\dot{\nu}_i}.$$

We then introduce the Hamiltonian $\mathcal{H}$ of the full system of N constituents, only interacting in pairs, as

$$\mathcal{H} \coloneqq \sum_{i=1}^{N} \frac{1}{2m}\underline{p_i}\cdot\underline{p_i} + \frac{1}{2}\underline{\varsigma_i}\cdot\underline{\underline{\Omega}}(\nu)^{-1}\,\underline{\varsigma_i} + \sum_{1\le i<j\le N} \mathcal{W}(|\mathbf{x}_i-\mathbf{x}_j|,\nu_i,\nu_j).$$

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The Legendre transform of the Lagrangian $\mathcal{L}$ is always well-defined, assuming $\underline{\underline{\Omega}}(\nu)$ is symmetric and positive definite for all $\nu \in \mathcal{M}$.

STATISTICAL MECHANICS APPROACH

We will also denote $\Gamma_i := (\mathbf{x}_i, \underline{p}_i, \nu_i, \underline{\varsigma}_i)$ the phase space point of the i-th constituent, and introduce

$$\pi\left(\{\Gamma_i\}_{i=1}^N\right) := \sum_{i=1}^N \delta\left(\Gamma_i - \Gamma_i^*(t)\right)$$

the **Klimontovich distribution function**, where $\Gamma_i^*(t)$ is the configuration of the i-th constituent at time t.

We will denote π_s the marginals of the Klimontovich distribution function, with respect to $\Gamma^{(s)} = (\Gamma_{s+1}, \dots, \Gamma_N)$, i.e.

$$\pi_s\left(\{\Gamma_i\}_{i=1}^s\right) := \int \pi\left(\{\Gamma_i\}_{i=1}^N\right) d\Gamma^{(s)}.$$

The distribution function π_s is called the **s-particle distribution function**, and represents the probability of finding s particles in the phase space point $\Gamma_1, \dots, \Gamma_s$.

BOGOLIUBOV–BORN–GREEN–KIRKWOOD–YVON HIERARCHY

An Introduction to the Theory of the Boltzmann Equation, (S. Harris),
Statistical Physics of Particles, (M. Kardar),
Statistical Mechanics, 2nd Edition (K. Huang).

Let f_s denote the normalised π_s. We obtain the following expression for the BBGKY hierarchy,

$$\frac{\partial f_s}{\partial t} + \{\pi_s, \mathcal{H}_s\} = \int \sum_{i=1}^{s} \frac{\partial f_{s+1}}{\partial \underline{p}_i} \cdot \frac{\partial \mathcal{W}(|\mathbf{x}_i - \mathbf{x}_{s+1}|, \nu_i, \nu_{s+1})}{\partial \mathbf{x}_i} \, d\Gamma_{s+1}$$
$$+ \int \sum_{i=1}^{s} \frac{\partial f_{s+1}}{\partial \underline{\varsigma}_i} \cdot \frac{\partial \mathcal{W}(|\mathbf{x}_i - \mathbf{x}_{s+1}|, \nu_i, \nu_{s+1})}{\partial \nu_i} \, d\Gamma_{s+1},$$

where $\mathcal{H}_s = \left(\sum_{i=1}^{s} \frac{|\underline{p}_i|^2}{2m} + \frac{1}{2}\underline{\varsigma}_i \cdot \underline{\underline{\Omega}}(\nu)^{-1} \underline{\varsigma}_i \right) + \sum_{1 \le i < j \le s} \mathcal{W}(|\mathbf{x}_i - \mathbf{x}_j|, \nu_i, \nu_j)$.

BOGOLIUBOV–BORN–GREEN–KIRKWOOD–YVON HIERARCHY

The first two terms of the BBGKY hierarchy, under the assumption that there are no three-body interactions, amount to

$$\frac{\partial f_1}{\partial t} + \frac{\underline{p}_1}{m} \cdot \frac{\partial f_1}{\partial \mathbf{x}_1} + \underline{\underline{\Omega}}(\nu_1)^{-1}\underline{\varsigma}_1 \frac{\partial f_1}{\partial \nu_1} =$$
$$+ \int \frac{\partial \mathcal{W}(|\mathbf{x}_1 - \mathbf{x}_2|, \nu_1, \nu_2)}{\partial \mathbf{x}_1} \left(\frac{\partial f_2}{\partial \underline{p}_1} - \frac{\partial f_2}{\partial \underline{p}_2} \right)$$
$$+ \int \frac{\partial \mathcal{W}(|\mathbf{x}_1 - \mathbf{x}_2|, \nu_1, \nu_2)}{\partial \nu_1} \left(\frac{\partial f_2}{\partial \underline{\varsigma}_1} - \frac{\partial f_2}{\partial \underline{\varsigma}_2} \right)$$

$$\frac{\partial f_2}{\partial t} + \frac{\underline{p}_1}{m} \cdot \frac{\partial f_2}{\partial \mathbf{x}_1} + \underline{\underline{\Omega}}(\nu_1)^{-1}\underline{\varsigma}_1 \cdot \frac{\partial f_2}{\partial \nu_1}$$
$$+ \frac{\underline{p}_2}{m} \cdot \frac{\partial f_2}{\partial \mathbf{x}_2} + \underline{\underline{\Omega}}(\nu_2)^{-1}\underline{\varsigma}_2 \cdot \frac{\partial f_2}{\partial \nu_2}$$
$$- \frac{\partial \mathcal{W}(|\mathbf{x}_1 - \mathbf{x}_2|, \nu_1, \nu_2)}{\partial \mathbf{x}_1} \left(\frac{\partial f_2}{\partial \underline{p}_1} - \frac{\partial f_2}{\partial \underline{p}_2} \right)$$
$$- \frac{\partial \mathcal{W}(|\mathbf{x}_1 - \mathbf{x}_2|, \nu_1, \nu_2)}{\partial \nu_1} \frac{\partial f_2}{\partial \underline{\varsigma}_1} = 0$$

BOGOLIUBOV–BORN–GREEN–KIRKWOOD–YVON HIERARCHY

To highlight the same timescale separation in the second term of the hierarchy we introduce fast and slow varying coordinates, i.e.

$$\mathbf{x} = \mathbf{x}_2 - \mathbf{x}_1, \qquad \mathbf{X} = \frac{1}{2}\left(\mathbf{x}_2 + \mathbf{x}_1\right).$$

We then boxed the terms that are quickly varying in the second equation of the BBGKY hierarchy, i.e.

$$\frac{\partial f_2}{\partial t} + \frac{1}{2}\frac{\underline{p}_2 + \underline{p}_1}{m} \cdot \frac{\partial f_2}{\partial \underline{X}} + \underline{\underline{\Omega}}(\nu_1)^{-1}\underline{\varsigma}_1 \cdot \frac{\partial f_2}{\partial \nu_1} + \underline{\underline{\Omega}}(\nu_2)^{-1}\underline{\varsigma}_2 \cdot \frac{\partial f_2}{\partial \nu_2} + \boxed{\frac{\underline{p}_2 - \underline{p}_1}{m} \cdot \frac{\partial f_2}{\partial \mathbf{x}}}$$
$$- \boxed{\frac{\partial \mathcal{W}(|\mathbf{x}_1 - \mathbf{x}_2|, \nu_1, \nu_2)}{\partial \mathbf{x}_1} \cdot \left(\frac{\partial f_2}{\partial \underline{p}_1} - \frac{\partial f_2}{\partial \underline{p}_2}\right)} - \frac{\partial \mathcal{W}(|\mathbf{x}_1 - \mathbf{x}_2|, \nu_1, \nu_2)}{\partial \nu_1} \cdot \frac{\partial f_2}{\partial \underline{\varsigma}_1} = 0$$

EMBEDDED BOGOLIUBOV–BORN–GREEN–KIRKWOOD–YVON HIERARCHY

Using the embedding results previously discussed, we can use the fast and slow varying coordinates also for the order parameters, i.e.

$$\underline{n} = \underline{\nu}_2 - \underline{\nu}_1, \qquad \underline{N} = \frac{1}{2}\left(\underline{\nu}_2 + \underline{\nu}_1\right).$$

We then introduce $\underline{A} = \frac{1}{2}\left(\underline{\underline{\Omega}}_2(\underline{\nu}a_1)^{-1}\underline{\varsigma}_1 + \underline{\underline{\Omega}}_2(\underline{\nu}_2)^{-1}\underline{\varsigma}_2\right)$, $\underline{B} = \left(\underline{\underline{\Omega}}_2(\underline{\nu}_2)^{-1}\underline{\varsigma}_2 - \Omega_1(\underline{\nu}_1)^{-1}\underline{\varsigma}_1\right)$, i.e.

$$\frac{\partial f_2}{\partial t} + \frac{1}{2}\frac{\underline{p}_2+\underline{p}_1}{m}\cdot\frac{\partial f_2}{\partial \underline{X}} + \underline{A}\cdot\frac{\partial f_2}{\partial \underline{N}} + \boxed{\underline{B}\cdot\frac{\partial f_2}{\partial n}} + \boxed{\frac{\underline{p}_2-\underline{p}_1}{m}\cdot\frac{\partial f_2}{\partial \mathbf{x}}}$$
$$- \boxed{\frac{\partial \mathcal{W}(|\mathbf{x}_1-\mathbf{x}_2|,\nu_1,\nu_2)}{\partial \mathbf{x}_1}\cdot\left(\frac{\partial f_2}{\partial \underline{p}_1} - \frac{\partial f_2}{\partial \underline{p}_2}\right)} - \boxed{\frac{\partial \mathcal{W}(|\mathbf{x}_1-\mathbf{x}_2|,\nu_1,\nu_2)}{\partial \nu_1}\cdot\left(\frac{\partial f_2}{\partial \underline{\varsigma}_1} - \frac{\partial f_2}{\partial \underline{\varsigma}_2}\right)} = 0.$$

BOLTZMANN–CURTISS EQUATION

4

J. Chem. Phys. 1956, 24, 225–241 (C. F. Curtiss),
J. Chem. Phys. 1963, 38, 2352–2363 (C. F. Curtiss, J. S. Dahler).

We can obtain from the embedded BBGKY hierarchy the following **Boltzmann** type equation,

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

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

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

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

COLLISION INVARIANTS

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

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

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- $\psi^{(3)} = \mathbb{I} \cdot \omega + \mathbf{x} \times m\underline{v}$, the **angular momentum**;
- $\psi^{(4)} = \frac{1}{2} m\underline{v} \cdot \underline{v} + \frac{1}{2}\underline{\omega} \cdot \mathbb{I} \cdot \underline{\omega}$, the **kinetic energy of the system**.

THE HYDRODYNAMIC EQUATIONS – NOTATION

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

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

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

$$\langle\!\langle \cdot \rangle\!\rangle(\mathbf{x}) \coloneqq \frac{1}{n(\mathbf{x})} \iiint \cdot \, f(\mathbf{x}, \underline{v}, \underline{\alpha}, \underline{\varsigma}) d\underline{v} d\underline{\alpha} d\underline{\varsigma}.$$

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

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

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

THE HYDRODYNAMIC EQUATIONS – CURTISS BALANCE LAWS

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

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

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

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

THE HYDRODYNAMIC EQUATIONS – SURPRISE BALANCE LAWS

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

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

where $\underline{\eta}$ is the **macroscopic intrinsic angular momentum** defined as $\underline{\eta}(\mathbf{x}) := \langle\langle \mathbb{I} \cdot \omega \rangle\rangle$ and $\mathbb{N}$ is the **couple tensor** defined as $\mathbb{N} := \langle\langle \underline{V} \otimes (\mathbb{I}\underline{\omega}) \rangle\rangle$. Here ξ_I is defined in tensor notation as $\langle\langle mn(\varepsilon_{Iki} v_i v_k)\underline{e}_I \rangle\rangle$ and we proved that $\underline{\xi}$ vanishes.

MAXWELL–BOLTZMANN DISTRIBUTION

J. Chem. Phys. 1956, 24, 225–241 (C. F. Curtiss),
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Curtiss gives an expression for the Maxwell–Boltzmann distribution, i.e. the distribution $f^{(0)}$ such that $C[f^{(0)}, f^{(0)}]$ vanishes:

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

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

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Notice in particular that we assumed $\underline{\omega}_0$ is the kinetic temperature of the system measured in energy units.

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.

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

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

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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

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

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

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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,

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

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

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

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

Multiscale Model. Simul. 2024, accepted (P. E. Farrell, G. Russo, U. Z.),

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:

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

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

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

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

THE OSEEN-FRANK STORED ENERGY

Multiscale Model. Simul. 2024, accepted (P. E. Farrell, G. Russo, U. Z.),

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

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

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

$$\psi_{OF} = p \frac{\lambda_1}{2} tr \Big[\nabla \underline{\nu}^T \nabla \underline{\nu} \Big].$$

NOLL–COLEMAN PROCEDURE

Multiscale Model. Simul. 2024, accepted (P. E. Farrell, G. Russo, U. Z.),

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

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

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

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

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

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

COMPRESSIBLE LESLIE–ERICKSEN EQUATIONS

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This leads to the following set of equations, which can be seen as an inviscid compressible generalisation of the Leslie–Ericksen equations:

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

A VLASOV–TYPE EQUATION

5

VLASOV–TYPE EQUATION

From the separation of timescales in the BBGKY hierarchy we obtain the following identity,

$$\frac{\underline{p}_2 - \underline{p}_1}{m} \cdot \frac{\partial f_2}{\partial \mathbf{x}} = \frac{\partial \mathcal{W}}{\partial \mathbf{x}_1}\left(|\mathbf{x}_1 - \mathbf{x}_2|, \nu_1, \nu_2\right) \cdot \left(\frac{\partial f_2}{\partial \underline{p}_1} - \frac{\partial f_2}{\partial \underline{p}_2}\right).$$

Substituting this identity in the second equation of the BBGKY hierarchy we obtain the following equation,

$$\frac{\partial f_1}{\partial t} + \frac{\underline{p}_1}{m} \cdot \frac{\partial f_1}{\partial \mathbf{x}_1} + \underline{\underline{\Omega}}(\nu_1)^{-1}\underline{\varsigma}_1 \cdot \frac{\partial f_1}{\partial \nu_1} = \int \frac{\underline{p}_2 - \underline{p}_1}{m} \cdot \frac{\partial f_2}{\partial \mathbf{x}}\, d\Gamma_2 + \int \frac{\partial \mathcal{W}(|\mathbf{x}_1 - \mathbf{x}_2|, \nu_1, \nu_2)}{\partial \nu_1} \cdot \frac{\partial f_2}{\partial \underline{\varsigma}_1}\, d\Gamma_2.$$

WEAK-ORDER INTERACTIONS

We might be tempted to assume interactions are **weak**,

$$f_2(\Gamma_1, \Gamma_2, t) = f_1(\Gamma_1, t) f_1(\Gamma_2, t).$$

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Weak-order Interactions

We will say that a kinetic equation is governed by **weak-order interactions** if the derivative of the two-particle distribution function factorises as,

$$\partial_{\nu_i} f_2(\Gamma_1, \Gamma_2, t) = f_1(\Gamma_i, t) \partial_{\nu_i} f_1(\Gamma_j, t),$$
$$\partial_{\varsigma_i} f_2(\Gamma_1, \Gamma_2, t) = f_1(\Gamma_j, t) \partial_{\varsigma_i} f_1(\Gamma_i, t),$$

for $i \neq j$ and $i, j = 1, 2$.

VLASOV–TYPE EQUATION

Under the assumption of weak-order interactions we can rewrite the first equation of the BBGKY hierarchy as,

$$\frac{\partial f}{\partial t} + \dot{\underline{x}} \cdot \nabla_{\mathbf{x}} f + \dot{\underline{\nu}} \cdot \nabla_{\nu} f + \mathcal{V} \cdot \nabla_{\varsigma} f = C[f, f],$$

where the collision operator $C[f, f]$ can be written using the transition "probability" W as,

$$C[f_1, f_1] = \int d\Xi_1' \, d\Xi_2' d\Xi_2 \int_0^{\frac{\pi}{2}} \int_0^{2\pi} W\left(\Xi_1', \Xi_2' \mapsto \Xi_1, \Xi_2\right) f_1(\Gamma_1', t) f_1(\Gamma_2', t) - W\left(\Xi_1, \Xi_2 \mapsto \Xi_1', \Xi_2'\right) f_1(\Gamma_1, t) f_1(\Gamma_2, t) \, d\theta_2 \, d\varphi_2.$$

BOLTZMANN INEQUALITY AND THERMALISATION

J. Stat. Phys. Volume 26, 795–801 (C. Cercignani, M. Lampis).

As we said before the collision operator $C[f, f]$ considered here guarantees that the system thermalises to a Maxwellian distribution. In particular, we can prove

$$\int d\Xi \, \log(f(\Gamma, t)) C[f, f] \leq 0,$$

which is a generalisation of the **Boltzmann inequality** for Boltzmann's equation with internal degrees of freedom. Following the classical calculus of variation approach we can prove that the unique Maxwellian with prescribed collision invariants is

$$\bar{f}(\Gamma, t) = \exp\left(a + \underline{b} \cdot \underline{p} + c(\underline{p} \times \mathbf{x} + \underline{w}_\nu \times \underline{\varsigma}) + d(m^{-1}\underline{p} \cdot \underline{p} + \varsigma \cdot \underline{\underline{\Omega}}(\nu)^{-1}\varsigma)\right).$$

THE HYDRODYNAMIC EQUATIONS

Testing the Vlasov–type equation against the first three collision invariants we obtain the following balance laws,

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

$$\rho \Big[\partial_t \underline{v}_0 + (\nabla_{\mathbf{x}} \underline{v}_0) \underline{v}_0 \Big] + \nabla_{\mathbf{x}} \cdot (\rho \mathbb{P}) = 0, \quad \mathbb{P} = \langle\langle \underline{V} \otimes \underline{V} \rangle\rangle.$$

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Angular Momentum

The action of infinitesimal generators A_ν can be identified via the canonical isomorphism between $\mathbb{R}^3$ and $T_\nu \mathcal{M}$ as the cross-product between a vector $\underline{w}_\nu$ and the rotation vector $\underline{r}$. For this reason, the angular momentum is defined as

$$\underline{\eta} = \langle\!\langle \underline{w}_\nu \times \underline{\underline{\Omega}}(\nu) \dot{\underline{\nu}} \rangle\!\rangle$$

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$$\rho \Big[\partial_t \underline{\eta} + (\nabla_{\mathbf{x}} \underline{\eta}) \underline{v}_0 \Big] + \nabla_{\mathbf{x}} \cdot (\rho \mathbb{N}) = \underline{\xi}, \quad \mathbb{N} = \langle\!\langle \underline{V} \otimes \underline{\eta} \rangle\!\rangle.$$

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BOLTZMANN H-THEOREM

H-Theorem

Boltzmann inequality is the standard tool used to prove the **H-Theorem** for the Boltzmann equation. Testing the Vlasov–type equation with $\psi = \log(f)$ we obtain the following inequality,

$$\rho\dot{\mathcal{H}} + \nabla_{\mathbf{x}} \cdot (\rho \underline{J}) + \mathcal{N} + \mathcal{F} \leq 0,$$

$$\mathcal{H} = \int d\Xi \, \log(f(\Gamma, t)) f(\Gamma, t).$$

$$\mathcal{J} = \int d\Xi \, v \log(f(\Gamma, t)) f(\Gamma, t).$$

$$\mathcal{N} = \int d\Xi \, \underline{\dot{\nu}} \cdot \nabla_{\nu} \log(f(\Gamma, t)) f(\Gamma, t).$$

$$\mathcal{F} = \int d\Xi \, \mathcal{V} \cdot \nabla_{\underline{\nu}} \log(f(\Gamma, t)) f(\Gamma, t).$$

THE ISSUE WITH NOLL–COLEMAN CLOSURE

If we test with the forth collision invariant the Vlasov type equation, we obtain

$$\partial_t\Big(\rho\langle\!\langle \frac{1}{2}(\underline{\nu}\cdot\underline{\nu}) + \frac{1}{2}\dot{\underline{\nu}}\cdot\underline{\underline{\Lambda}}\,\dot{\underline{\nu}}\rangle\!\rangle\Big) + \nabla_{\mathbf{x}}\cdot\Big[\rho\langle\!\langle \underline{\nu}\frac{1}{2}(\underline{\nu}\cdot\underline{\nu}) + \underline{\nu}\frac{1}{2}\dot{\underline{\nu}}\cdot\underline{\underline{\Lambda}}\,\dot{\underline{\nu}}\rangle\!\rangle\Big] + \rho\langle\!\langle \mathcal{V}\cdot\underline{\underline{\Lambda}}\,\dot{\underline{\nu}}\rangle\!\rangle = 0.$$

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Playing the same game we did for the Curtiss-Boltzmann equation, we obtain

$$\dot{\psi}_0+\mathbb{P}:\nabla_{\mathbf{x}}\underline{\mathbf{v}}+\mathbb{M}:\nabla_{\mathbf{x}}\underline{\eta}+\langle\!\langle\mathcal{V}\cdot\underline{\underline{\Lambda}}\,\dot{\underline{\nu}}\rangle\!\rangle=-\nabla_{\mathbf{x}}\cdot\mathfrak{Q}.$$

with the internal energy ρ_0 being defined as,

$$\psi_0=\frac{1}{2}\langle\!\langle v\cdot v\rangle\!\rangle+\frac{1}{2}\lambda(\dot{\underline{\nu}}\cdot\dot{\underline{\nu}})-\frac{1}{2}|\underline{\mathbf{v}}|^2-\frac{1}{2}\underline{\eta}\cdot\underline{\underline{\Lambda}}^{-1}\,\underline{\eta},$$

THE $\mathbb{S}^{m-1}$ TYPE MANIFOLD

We can express the total time derivative of

$$\underline{\dot{\nu}} = \underline{\underline{\Lambda}}^{-1}\underline{\eta} \times \underline{w}_\nu - \underline{w}_\nu(\underline{w}_\nu \cdot \underline{\dot{\nu}}).$$

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We can use the following identity to prove that the

$$\begin{aligned}\dot{\underline{\nu}} \cdot (\underline{\eta} \times \underline{w}_\nu) &= (\dot{\underline{\nu}} \cdot \Lambda\dot{\underline{\nu}}) - \dot{\underline{\nu}} \cdot \underline{w}_\nu(\underline{w}_\nu \cdot \Lambda\dot{\underline{\nu}}) \\ &= \underline{\eta} \cdot \underline{\underline{\Lambda}}^{-1}\underline{\eta}.\end{aligned}$$

This implies the internal energy has no dependence on the internal degrees of freedom.

CONCLUSION

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  - From the kinetic theory of spherocylindrical molecules, we derived a **compressible** and thermally coupled model for the flow of fluids with a nematic order.

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- We have dervied a Vlasov–type equation for the dynamics of a system with partial ordering, that doesn't require the use of large embedding space.

THANK YOU!

A Kinetic Framework for Fluids with Partial Ordering

Umberto Zerbinati*