A Kinetic Framework for Fluids with Partial Ordering

Umberto Zerbinati*

Mathematical Institute – University of Oxford

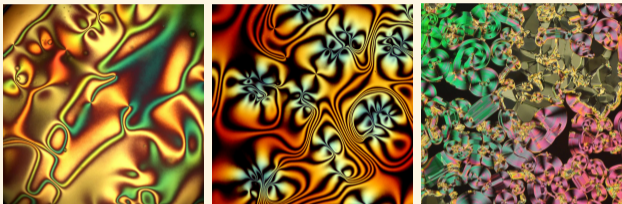Modelling of Materials, 23rd October 2024

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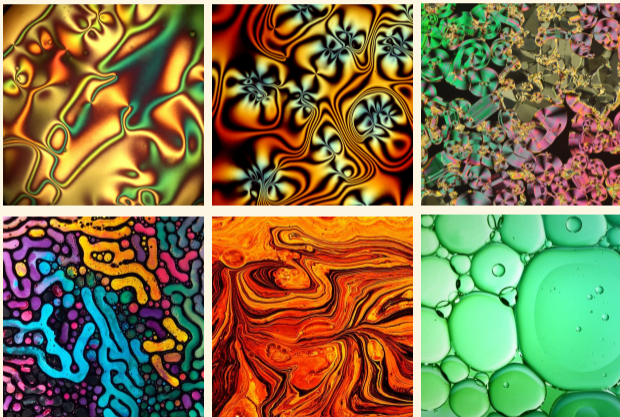
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Partially ordered fluids are ubiquitous in nature and have a wide range of applications.

▸ **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 seeks to describe the evolution of the fluid using a statistical description and knowledge of the microscopic interactions.

Oxford
Mathematics

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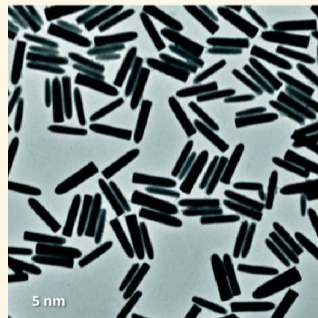Kinetic Theory of Ordered Fluids

Prague, 23rd Oct. '24

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- Typically, this is done by considering only binary interactions between fluid constituents. This is a good approximation for dilute systems.

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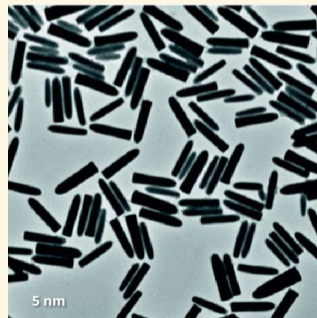*J. Am. Chem. Soc.* 2011 133 (8), 2346-2349 (A. Kuijk, A. van Blaaderen, A. Imhof).


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A KINETIC THEORY APPROACH

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- In certain cases, the partial ordering of the fluid is a consequence of the dilute nature of the system.

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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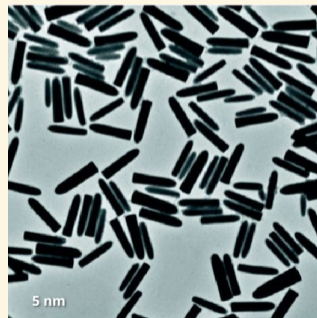
ORDER PARAMETER MANIFOLD

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 $\forall \underline{\underline{Q}} \in$ 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
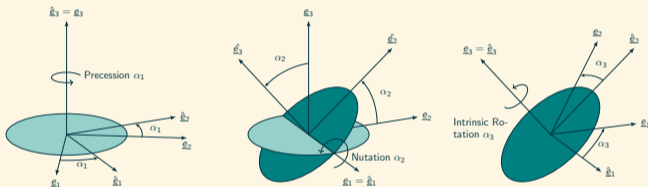
📑 *Variational Theories for Liquid Crystals*, (E. Virga), *The Physics of Liquid Crystals*, (P.G. de Gennes, J. Prost).

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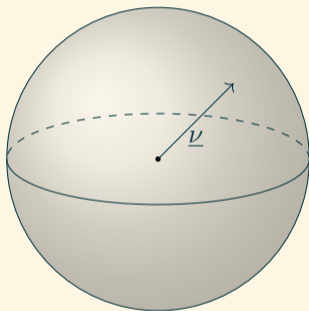
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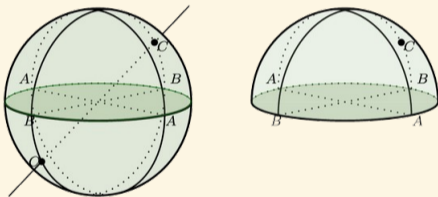
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▸ For head-tail symmetric calamitic molecules, we can use $\mathbb{RP}^2$.

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 $\underline{v}_i$, the order parameter ν_i and its total time derivative $\underline{\dot{\nu}}_i$.

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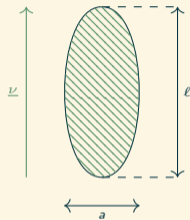
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$$\mathcal{L}_i := \frac{1}{2} m_1 (\underline{\dot{x}}_i \cdot \underline{\dot{x}}_i) + \frac{1}{2} \underline{\dot{\nu}}_i \cdot \underline{\underline{\Omega}}_i(\nu_i) \underline{\dot{\nu}}_i.$$
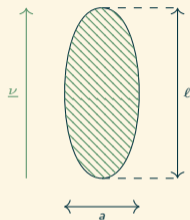
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We assume the interaction between the constituents is given by a potential $\mathcal{W}(|\mathbf{x}_i - \mathbf{x}_j|, \nu_i, \nu_j)$, i.e.

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

where $\Xi_i := (\underline{v}_i, \nu_i, \underline{\dot{\nu}}_i)$.
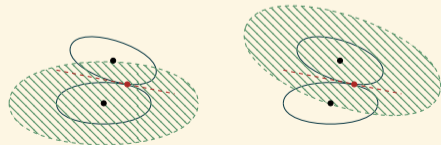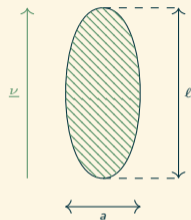
NOETHER'S THEOREM: SYMMETRIES AND CONSERVATION LAWS

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

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

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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   R.J. Knops).

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.

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

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

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

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The Legendre transform of the Lagrangian $\mathcal{L}$ is always well-defined, assuming $\underline{\Omega}(\nu)$ 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 $\Gamma^{(s)} = (\Gamma_{s+1}, \ldots, \Gamma_N)$, 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 $\Gamma_1, \ldots, \Gamma_s$.

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

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

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

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

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 $\underline{A} = \frac{1}{2}\left(\underline{\Omega}_2(\underline{\nu}a_1)^{-1}\underline{\varsigma}_1 + \underline{\Omega}_2(\underline{\nu}_2)^{-1}\underline{\varsigma}_2\right)$, $\underline{B} = \left(\underline{\Omega}_2(\underline{\nu}_2)^{-1}\underline{\varsigma}_2 - \Omega_1(\underline{\nu}_1)^{-1}\underline{\varsigma}_1\right)$, 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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▶ $\psi^{(4)} = \frac{1}{2} m\underline{v} \cdot \underline{v} + \frac{1}{2}\underline{\omega} \cdot \mathbb{I} \cdot \underline{\omega}$, the **kinetic energy of the system**.

THE HYDRODYNAMIC EQUATIONS – NOTATION

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

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

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

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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

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

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

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

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_l is defined in tensor notation as $\langle\!\langle mn(\varepsilon_{lki}v_iv_k)\underline{e}_l \rangle\!\rangle$ and we proved that $\underline{\xi}$ vanishes.

MAXWELL–BOLTZMANN DISTRIBUTION

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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** $\mathbb{N}^{(0)}$.

Oxford
Mathematics

U. Zerbinati

Kinetic Theory of Ordered Fluids

Prague, 23rd Oct. '24

21 / 37

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

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

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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

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Making use of the fact that $\dot{\underline{\nu}} = \underline{\omega} \times \underline{\nu} = \partial_t \underline{\nu} (\nabla \underline{\nu}) \underline{v}$ 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

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

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

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

NOLL–COLEMAN PROCEDURE

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

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**,

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

This leads to equations of a **reversible nature**, compatible with **Loschmidt's paradox**.

Thus, we have no guarantee that the system described thermalises to a Maxwellian distribution.

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Thus, we have no guarantee that the system described thermalises to a Maxwellian distribution.

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,

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

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

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

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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

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

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,

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

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

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

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

THE ISSUE WITH NOLL–COLEMAN CLOSURE

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

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

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

$$\dot\psi_0+\mathbb{P}:\nabla_{\mathbf{x}}\underline{v}+\mathbb{M}:\nabla_{\mathbf{x}}\underline{\eta}+\langle\!\langle\mathcal{V}\cdot\underline{\underline{\Lambda}}\,\underline{\dot\nu}\rangle\!\rangle=-\nabla_{\mathbf{x}}\cdot\mathfrak{Q}.$$

with the internal energy ψ_0 being defined as,

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

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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On any sphere like manifold, i.e.text

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We can use the following identity to prove that the

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

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

CONCLUSION

▶ We derived a general kinetic framework to study the dynamics of a system with partial ordering.

Oxford
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- Using this framework, via the use of a larger embedding space, we used this framework to study calamitic fluids.
  - Using a Noll–Coleman argument for the closure of the momentum hierarchy allows us to retrieve the **Ericksen stress tensor**.
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THANK YOU!

A Kinetic Framework for Fluids with Partial Ordering

Umberto Zerbinati*