

LIQUID CRYSTAL THEORIES

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PLAN OF THE PRESENTATION

Liquid crystal dynamics: several models, two important ones

Affine Euler-Poincaré reduction

Geometry of non-viscous Ericksen-Leslie nematodynamics

Nonviscous Eringen micropolar model

Eringen implies Ericksen-Leslie

In the variational formulation, the terms modeling dissipation have been eliminated. Reason: want to understand the geometric nature of these equations. The dissipative terms are added later. Think: Euler versus Navier-Stokes.

HARVARD MODEL

- Forster D., Lubensky T., Martin P., Swift J., Pershan P., Hydrodynamics of liquid crystals, *Phys. Rev. Lett.* **26** (1971) 1016–1019.
- Landau L., Pitaevskii L., Lifshitz E., Kosevich A., *Theory of Elasticity*, 3rd edition; *Theoretical Physics*, Vol. 7, 1986 (Ch.VI, §41).

$$\partial_t \rho + \operatorname{div}(\rho u) = 0,$$

$$\partial_t(\rho u) + \operatorname{Div}(\rho u \otimes u) + \nabla p = \operatorname{Div}(\sigma^R) + \operatorname{Div}(\sigma^D),$$

$$\frac{D}{Dt} d_i = \Omega_{ki} d_k + \lambda(\delta_{il} - d_i d_l) d_k A_{kl} + \frac{h_i}{\beta},$$

$$p = p(\rho), \quad \frac{D}{Dt} := \frac{\partial}{\partial t} + u \cdot \nabla, \quad \lambda, \beta \text{ constants}$$

$$(\rho, u, d) \Big|_{t=0} = (\rho_0, u_0, d_0), \quad \|d_0\| = 1, \quad \text{initial conditions}$$

Equations in $\mathbb{R} \times \mathbb{R}^3$: conservation of mass, linear momentum, and constraint $\|d\| = 1$ (third equation). Describes the flow of a compressible isentropic material. All written in standard Euclidean coordinates.

ρ density, p pressure, $u = (u_1, u_2, u_3)^T$ spatial velocity, $d = (d_1, d_2, d_3)^T$ orientational order parameter representing the macroscopic average of the molecular directors,

$$\operatorname{div}(a) := \sum_{i=1}^3 \frac{\partial a_i}{\partial x_i} \quad \text{divergence of vector field } a = (a_1, a_2, a_3)^T$$

$$\operatorname{Div}(\tau)_i := \sum_{j=1}^3 \frac{\partial \tau_{ij}}{\partial x_j} \quad \text{divergence of a 2-tensor } \tau = (\tau_{ij})$$

$$A := \frac{1}{2}(\nabla u + (\nabla u)^T), \quad \text{symmetric part of strain rate}$$

$$\Omega := \frac{1}{2}(\nabla u - (\nabla u)^T), \quad \text{skew-symmetric part of strain rate = vorticity}$$

$$W(\rho, d) := \frac{1}{2}K_1 \underbrace{(\operatorname{div} d)^2}_{\text{splay}} + \frac{1}{2}K_2 \underbrace{\|d \times \operatorname{curl} d\|^2}_{\text{bend}} + \frac{1}{2}K_3 \underbrace{(d \cdot \operatorname{curl} d)^2}_{\text{twist}}$$

Oseen-Zöcher-Frank free energy, $K_i \geq 0$ depend on ρ but not on x

$$h := H - (d \cdot H)d, \quad \text{molecular field, } H_i := \partial_k \pi_{ki} - \frac{\partial W}{\partial d_i}, \quad \pi_{ki} := \frac{\partial W}{\partial (\partial_k d_i)}$$

The reactive (non-dissipative) symmetrized part of the stress tensor

$$\sigma_{ik}^R := -\frac{1}{2}(d_i h_k + d_k h_i) - \frac{1}{2}(\pi_{kl} \partial_i d_l + \pi_{il} \partial_k d_l) - \frac{1}{2} \partial_l [(\pi_{ik} - \pi_{ki}) d_l - \pi_{kl} d_i - \pi_{il} d_k],$$

The dissipative part of the stress tensor

$$\sigma_{ij}^D := \mu_1 A_{ij} + \mu_2 (A_{ik} d_k d_j + A_{jk} d_i d_k) + \mu_3 \delta_{ij} A_{kk} + \mu_4 d_i d_j d_k d_l A_{kl} + \mu_5 [\delta_{ij} d_k d_l A_{kl} + d_i d_j A_{kk}].$$

μ_1, \dots, μ_5 constants depending on the material.

If $W \equiv 0$, then 1+2+4+5 is compressible Navier Stokes in \mathbb{R}^3 .

- Many papers by F.-H. Lin and his group in the incompressible case about a simplified version (replaces $\|d\| = 1$ by penalty term $\frac{1}{\epsilon^2} (\|d\|^2 - 1)^2$ added to W and neglects some terms). Results in 2D.
- Global existence of weak solutions with large initial data in 3D still open. No results on the classical solvability for the main initial and initial-boundary problems for the full system.

If $\|d_0\| = 1$, then $\|d\| = 1$ for $t > 0$ as long as the solution to the system remains smooth.

$$m(t) := \int_{\mathbb{R}^3} \rho \, dx, \quad \text{total mass}$$

$$P(t) := \int_{\mathbb{R}^3} \rho u \, dx, \quad \text{linear momentum}$$

$$E(t) := \frac{1}{2} \int_{\mathbb{R}^3} \rho \|u\|^2 \, dx + \int_{\mathbb{R}^3} \Psi(\rho) \, dx + \int_{\mathbb{R}^3} W(\rho, d) \, dx$$

$$= \underbrace{E_k(t)}_{\text{kinetic}} + \underbrace{E_i(t)}_{\text{internal}} + \underbrace{E_d(t)}_{\text{deformation}} \geq 0, \quad \text{total energy}$$

$$\Psi(\rho) := \int_0^\rho \frac{p'(\xi)}{\xi} \, d\xi \geq 0, \quad |Du|^2 := \sum_{i,j=1}^3 \left(\frac{\partial u_i}{\partial x_j} \right)^2$$

$$\frac{d}{dt} E(t) = - \int_{\mathbb{R}^3} \left(\sigma_{ik}^D A_{ik} + \frac{\|h\|^2}{\beta} \right) \, dx \leq -\theta \int_{\mathbb{R}^3} |Du|^2 \, dx,$$

$$\text{if } \beta > 0, \quad \mu_1 > 0, \quad \mu_1 + \mu_3 \geq 0, \quad \mu_4 \geq 0, \quad \theta := \frac{\mu_1}{2} - 2|\mu_2| - 4|\mu_5| > 0.$$

DEFINITION: Solution (ρ, u, d) to the Cauchy problem is in the class \mathfrak{K} if the solution is classical, $\rho \geq 0$, $u \in H^1(\mathbb{R}^3)$, the mass $m(t)$, linear momentum $P(t)$, and total energy are finite for all $t \geq 0$, for which the solution exists, and, in addition, the mass and linear momentum are conserved, i.e., $m(t) = m = \text{const}$, $P(t) = P = \text{const}$.

Thus, if the solution belongs to the class \mathfrak{K} , then

$$\rho \in L^1(\mathbb{R}^3), \Psi(\rho) \in L^1(\mathbb{R}^3), \sqrt{\rho}u \in L^2(\mathbb{R}^3), W \in L^1(\mathbb{R}^3),$$

ASSUMPTION: $\exists \gamma > 1$, $A > 0$ constants such that $\Psi(\rho) \geq A\rho^\gamma$.

Then with $\gamma \geq \frac{6}{5}$, $\|P\| \neq 0$, there exists $C > 0$ constant, such that for the solutions from the class \mathfrak{K} the following inequality holds:

$$\int_{\mathbb{R}^3} |Du|^2 dx \geq C E_i(t)^{-\frac{1}{3(\gamma-1)}}.$$

THEOREM (Ratiu-Rozanova): Suppose $\beta > 0$, $\mu_1 > 0$, $\mu_1 + \mu_3 \geq 0$, $\mu_4 \geq 0$, $\Psi(\rho) \geq A\rho^\gamma$, $A > 0$, $\gamma \geq \frac{6}{5}$. Then there is no global in time solution to the Cauchy problem in the class \mathfrak{K} .

The assumption $\Psi(\rho) \geq A\rho^\gamma$ with $\gamma \geq 6/5$ is physically realistic.

The other inequalities hold for the constants at temperature 55° which is well within the range of the liquid crystal phase according to experimental data. If one looks at these experimental papers and our inequalities the conclusion is that loss of smoothness is related to high temperature.

PROBLEM WITH THE HARVARD MODEL: There is no known geometric interpretation! The model deliberately confuses the fact that one is in \mathbb{R}^3 and that $\dim \text{SO}(3) = 3$.

The next models are much more natural: they are heavily geometric and can be easily generalized to any dimensions.

LIQUID CRYSTAL DYNAMICS

Director theory due to Oseen, Frank, Zöcher, Ericksen and Leslie

Micropolar, **microstretch**, and **microporphic theories**, due to Eringen, which take into account the microinertia of the particles and which is applicable, for example, to *liquid crystal polymers*

Ordered micropolar approach, due to Lhuillier and Rey, which combines the director theory with the micropolar models.

We discuss only nematic liquid crystals (no chirality $\mathbf{n} \cdot \text{curl } \mathbf{n}$). We set all dissipation equal to zero; want to understand the conservative case first.

$\mathcal{D} \subset \mathbb{R}^3$ bounded domain with smooth boundary. All boundary conditions are ignored: in all integration by parts the boundary terms vanish. We fix a volume form μ on \mathcal{D} .

ERICKSEN-LESLIE DIRECTOR THEORY

For nematic and cholesteric liquid crystals

Key assumption: only the direction and not the sense of the molecules matter. The preferred orientation of the molecules around a point is described by a unit vector $\mathbf{n} : \mathcal{D} \rightarrow S^2$, called the *director*, and \mathbf{n} and $-\mathbf{n}$ are assumed to be equivalent.

Ericksen-Leslie equations (*Ericksen [1966], Leslie [1968]*) in a domain \mathcal{D} , constraint $\|\mathbf{n}\| = 1$, are:

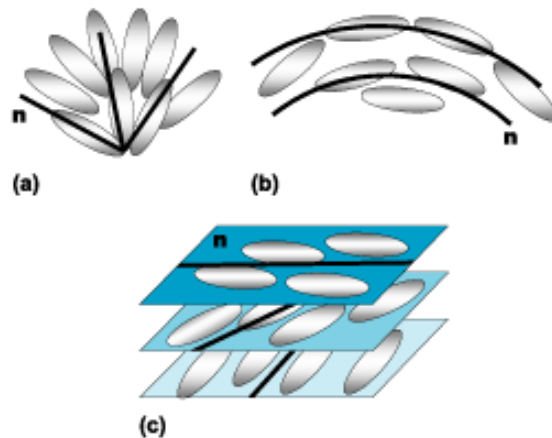
$$\left\{ \begin{array}{l} \rho \left(\frac{\partial}{\partial t} \mathbf{u} + \nabla_{\mathbf{u}} \mathbf{u} \right) = \text{grad} \frac{\partial F}{\partial \rho^{-1}} - \partial_j \left(\rho \frac{\partial F}{\partial \mathbf{n}_{,j}} \cdot \nabla \mathbf{n} \right), \\ \rho J \frac{D^2}{Dt^2} \mathbf{n} - 2q\mathbf{n} + \mathbf{h} = 0, \quad \mathbf{h} = \rho \frac{\partial F}{\partial \mathbf{n}} - \partial_i \left(\rho \frac{\partial F}{\partial \mathbf{n}_{,i}} \right) \\ \frac{\partial}{\partial t} \rho + \text{div}(\rho \mathbf{u}) = 0, \quad \frac{D}{Dt} := \frac{\partial}{\partial t} + \nabla_{\mathbf{u}} = \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \end{array} \right.$$

\mathbf{u} *Eulerian velocity*, ρ *mass density*, $\mathbf{n} : \mathcal{D} \rightarrow \mathbb{R}^3$ *director* (\mathbf{n} equivalent to $-\mathbf{n}$), J *microinertia constant*, and $F(\mathbf{n}, \mathbf{n}_{,i})$ is the *free energy*:

A standard choice for F is the *Oseen-Zöcher-Frank free energy*:

$$\rho F(\rho^{-1}, \mathbf{n}, \nabla \mathbf{n}) = \frac{1}{2} K_1 \underbrace{(\operatorname{div} \mathbf{n})^2}_{\text{splay}} + \frac{1}{2} K_2 \underbrace{(\mathbf{n} \cdot \operatorname{curl} \mathbf{n})^2}_{\text{twist}} + \frac{1}{2} K_3 \underbrace{\|\mathbf{n} \times \operatorname{curl} \mathbf{n}\|^2}_{\text{bend}},$$

associated to the basic type of director distortions nematics:



(a) splay, (b) bend, (c) twist

WHAT IS THE VARIATIONAL/HAMILTONIAN STRUCTURE OF THESE EQUATIONS?

ERINGEN MICROPOLAR THEORY

First key assumption: Replace point particles by *small deformable bodies*: **microfluids**. Examples: *liquid crystals, blood, polymer melts, bubbly fluids, suspensions with deformable particles, biological fluids*. Eringen [1978], [1979], [1981],...

A material particle P in a microfluid is characterized by its position X and by a vector Ξ attached to P that denotes the orientation and intrinsic deformation of P . Both X and Ξ have their own motions: $X \mapsto x = \eta(X, t)$ and $\Xi \mapsto \xi = \chi(X, \Xi, t)$ called, respectively, the *macromotion* and *micromotion*.

Second key assumption: Material bodies are very small, so a linear approximation in Ξ is permissible for the micromotion:

$$\xi = \chi(X, t)\Xi,$$

where $\chi(X, t) \in \text{GL}(3)^+ := \{A \in \text{GL}(3) \mid \det(A) > 0\}$.

The classical Eringen theory considers only three possible groups in the description of the micromotion of the particles:

$$GL(3)^+(\textit{micromorphic}) \supset K(3)(\textit{microstretch}) \supset SO(3)(\textit{micropolar}),$$

$$K(3) = \left\{ A \in GL(3)^+ \mid \text{there exists } \lambda \in \mathbb{R} \text{ such that } AA^T = \lambda I_3 \right\}$$

is a closed subgroup of $GL(3)^+$; associated to rotations and stretch.

The general theory admits other groups describing the micromotion.

We will study only micropolar fluids, i.e., the **order parameter group** is

$$\mathcal{O} := SO(3)$$

.

Eringen's equations for non-dissipative micropolar liquid crystals:

$$\left\{ \begin{array}{l} \rho \frac{D}{Dt} \mathbf{u}_l = \partial_l \frac{\partial \Psi}{\partial \rho^{-1}} - \partial_k \left(\rho \frac{\partial \Psi}{\partial \gamma_k^a} \gamma_l^a \right), \quad \rho \sigma_l = \partial_k \left(\rho \frac{\partial \Psi}{\partial \gamma_k^l} \right) - \varepsilon_{lmn} \rho \frac{\partial \Psi}{\partial \gamma_m^a} \gamma_n^a, \\ \frac{D}{Dt} \rho + \rho \operatorname{div} \mathbf{u} = 0, \quad \frac{D}{Dt} j_{kl} + (\varepsilon_{kpr} j_{lp} + \varepsilon_{lpr} j_{kp}) \nu_r = 0, \\ \frac{D}{Dt} \gamma_l^a = \partial_l \nu_a + \nu_{ab} \gamma_l^b - \gamma_r^a \partial_l u_r, \quad \frac{D}{Dt} := \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \quad \text{mat. deriv.} \end{array} \right.$$

sum on repeated indices, $\mathbf{u} \in \mathfrak{X}(\mathcal{D})$ Eulerian velocity, $\rho \in \mathcal{F}(\mathcal{D})$ mass density, $\boldsymbol{\nu} \in \mathcal{F}(\mathcal{D}, \mathbb{R}^3)$ microrotation rate, where we use the standard isomorphism between $\mathfrak{so}(3)$ and \mathbb{R}^3 , $j_{kl} \in \mathcal{F}(\mathcal{D}, \operatorname{Sym}(3))$ microinertia tensor (symmetric), σ_k spin inertia is defined by

$$\sigma_k := j_{kl} \frac{D}{Dt} \nu_l + \varepsilon_{klm} j_{mn} \nu_l \nu_n = \frac{D}{Dt} (j_{kl} \nu_l),$$

$\gamma = (\gamma_i^{ab}) \in \Omega^1(\mathcal{D}, \mathfrak{so}(3))$ wryness tensor, related to (η, χ) by

$$\gamma = -\eta_*(\nabla \chi) \chi^{-1} =: \hat{\gamma} = (\widehat{\gamma}_i^a),$$

and $\Psi = \Psi(\rho^{-1}, j, \gamma) : \mathbb{R} \times \operatorname{Sym}(3) \times \mathfrak{gl}(3) \rightarrow \mathbb{R}$ is the free energy.

VARIATIONAL/HAMILTONIAN STRUCTURE?

Result: Well posedness of the full EL system with viscosity

RELATION BETWEEN ERICKSEN-LESLIE AND ERINGEN?

Eringen's claim: Eringen theory recovers Ericksen-Leslie theory in the rod-like assumption $j = J(\mathbf{I} - \mathbf{n} \otimes \mathbf{n})$ with the choice $\gamma = \nabla \mathbf{n} \times \mathbf{n}$.

Once we have the Euler-Poincaré formulation, it will be clear that $\gamma = \nabla \mathbf{n} \times \mathbf{n}$ **cannot** be considered as a definition!

Eringen's claim has been controversial due to mistakes; fights over the past 25 years. Since then, this remains an open problem.

We solve this problem using techniques of geometric mechanics:

- (1) find under what assumptions, Eringen reduces to Ericksen-Leslie
- (2) find correct relation between γ and \mathbf{n} with these assumptions

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AFFINE EULER-POINCARÉ REDUCTION

Right G -representation on V , $(v, g) \in V \times G \mapsto vg \in V$, induces:

- right G -representation on V^* : $(a, g) \in V^* \times G \mapsto ag \in V^*$
- right \mathfrak{g} -representation on V : $(v, \xi) \in V \times \mathfrak{g} \mapsto v\xi \in V$
- right \mathfrak{g} -representation on V^* : $(a, \xi) \in V^* \times \mathfrak{g} \mapsto a\xi \in V^*$

Duality pairings: $\langle \cdot, \cdot \rangle_{\mathfrak{g}} : \mathfrak{g}^* \times \mathfrak{g} \rightarrow \mathbb{R}$ and $\langle \cdot, \cdot \rangle_V : V^* \times V \rightarrow \mathbb{R}$

Affine right representation: $\theta_g(a) = ag + c(g)$, where $c \in \mathcal{F}(G, V^*)$ is a right group one-cocycle, i.e., $c(fg) = c(f)g + c(g)$, $\forall f, g \in G$. This implies that $c(e) = 0$ and $c(g^{-1}) = -c(g)g^{-1}$. Note that

$$\left. \frac{d}{dt} \right|_{t=0} \theta_{\exp(t\xi)}(a) = a\xi + dc(\xi), \quad \xi \in \mathfrak{g}, \quad a \in V^*,$$

where $dc : \mathfrak{g} \rightarrow V^*$ is defined by $dc(\xi) := T_e c(\xi)$. Useful to introduce:

- $\mathbf{dc}^T : V \rightarrow \mathfrak{g}^*$ by $\langle \mathbf{dc}^T(v), \xi \rangle_{\mathfrak{g}} := \langle \mathbf{dc}(\xi), v \rangle_V$, for $\xi \in \mathfrak{g}$, $v \in V$
- $\diamond : V \times V^* \rightarrow \mathfrak{g}^*$ by $\langle v \diamond a, \xi \rangle_{\mathfrak{g}} := -\langle a\xi, v \rangle_V$ for $\xi \in \mathfrak{g}$, $v \in V$, $a \in V^*$
- then: $\langle a\xi + \mathbf{dc}(\xi), v \rangle_V = \langle \mathbf{dc}^T(v) - v \diamond a, \xi \rangle_{\mathfrak{g}}$

- the semidirect product $S = G \ltimes V$ with group multiplication

$$(g_1, v_1)(g_2, v_2) := (g_1g_2, v_2 + v_1g_2), \quad g_i \in G, \quad v_i \in V$$

- its Lie algebra $\mathfrak{s} = \mathfrak{g} \ltimes V$ with bracket

$$\mathbf{ad}_{(\xi_1, v_1)}(\xi_2, v_2) := [(\xi_1, v_1), (\xi_2, v_2)] = ([\xi_1, \xi_2], v_1\xi_2 - v_2\xi_1)$$

- then for $(\xi, v) \in \mathfrak{s}$ and $(\mu, a) \in \mathfrak{s}^* = \mathfrak{g}^* \times V^*$ we have

$$\mathbf{ad}_{(\xi, v)}^*(\mu, a) = (\mathbf{ad}_{\xi}^* \mu + v \diamond a, a\xi)$$

In a physical problem (like liquid crystals) we are given:

- $L : TG \times V^* \rightarrow \mathbb{R}$ right G -invariant under the action
 $(v_h, a) \in T_h G \times V^* \xrightarrow{g} (v_h g, \theta_g(a)) = (v_h g, a g + c(g)) \in T_{hg} G \times V^*$.

- So, if $a_0 \in V^*$, define $L_{a_0} : TG \rightarrow \mathbb{R}$ by $L_{a_0}(v_g) := L(v_g, a_0)$. Then L_{a_0} is right invariant under the lift to TG of right translation of $G_{a_0}^c$ on G , where $G_{a_0}^c$ is the θ -isotropy group of a_0 .

- Right G -invariance of L permits us to define $l : \mathfrak{g} \times V^* \rightarrow \mathbb{R}$ by

$$l(v_g g^{-1}, \theta_{g^{-1}}(a_0)) = L(v_g, a_0).$$

- Curve $g(t) \in G$, let $\xi(t) := \dot{g}(t)g(t)^{-1} \in \mathfrak{g}$, $a(t) = \theta_{g(t)^{-1}}(a_0) \in V^*$
 Then $a(t)$ as the unique solution of the following affine differential equation with time dependent coefficients

$$\dot{a}(t) = -a(t)\xi(t) - \mathbf{d}c(\xi(t)),$$

with initial condition $a(0) = a_0 \in V^*$.

The following are equivalent:

(i) With a_0 held fixed, Hamilton's variational principle

$$\delta \int_{t_1}^{t_2} L_{a_0}(g(t), \dot{g}(t)) dt = 0,$$

holds, for variations $\delta g(t)$ of $g(t)$ vanishing at the endpoints.

(ii) $g(t)$ satisfies the Euler-Lagrange equations for L_{a_0} on G .

(iii) The constrained variational principle

$$\delta \int_{t_1}^{t_2} l(\xi(t), a(t)) dt = 0,$$

holds on $\mathfrak{g} \times V^*$, upon using variations of the form

$$\delta \xi = \frac{\partial \eta}{\partial t} - [\xi, \eta], \quad \delta a = -a\eta - \mathbf{d}c(\eta),$$

where $\eta(t) \in \mathfrak{g}$ vanishes at the endpoints.

(iv) The affine Euler-Poincaré equations hold on $\mathfrak{g} \times V^*$:

$$\frac{\partial}{\partial t} \frac{\delta l}{\delta \xi} = -\text{ad}_\xi^* \frac{\delta l}{\delta \xi} + \frac{\delta l}{\delta a} \diamond a - \mathbf{d}c^\top \left(\frac{\delta l}{\delta a} \right).$$

Lagrangian Approach to Continuum Theories of Perfect Complex Fluids

To apply the previous theorem to complex fluids one makes two key observations:

1. Complex fluids have internal degrees of freedom encoded by the order parameter Lie group \mathcal{O}

2. New kind of advection equation:
$$\frac{D}{Dt}\gamma_l^a = \partial_l \nu_a + \nu_{ab}\gamma_l^b - \gamma_r^a \partial_l u_r$$

Geometrically, this means:

1. Enlarge the “particle relabeling group” $\text{Diff}(\mathcal{D})$ to the semidirect product $G = \text{Diff}(\mathcal{D}) \ltimes \mathcal{F}(\mathcal{D}, \mathcal{O})$, $\mathcal{F}(\mathcal{D}, \mathcal{O}) := \{\chi : \mathcal{D} \rightarrow \mathcal{O} \text{ smooth}\}$

2. The usual advection equations (for the mass density, the entropy, the magnetic field, etc) need to be augmented by a new advected quantity on which the group G acts by an *affine representation*.

Algebraic structure of the symmetry group of complex fluids:

$\text{Diff}(\mathcal{D})$ acts on $\mathcal{F}(\mathcal{D}, \mathfrak{o})$ via the *right* action

$$(\eta, \chi) \in \text{Diff}(\mathcal{D}) \times \mathcal{F}(\mathcal{D}, \mathfrak{o}) \mapsto \chi \circ \eta \in \mathcal{F}(\mathcal{D}, \mathfrak{o}).$$

Therefore, the group multiplication is given by

$$(\eta, \chi)(\varphi, \psi) = (\eta \circ \varphi, (\chi \circ \varphi)\psi).$$

Fix a volume form μ on \mathcal{D} , so identify densities with functions, one-form densities with one-forms, etc.

The **Lie algebra** \mathfrak{g} of the semidirect product group is

$$\mathfrak{g} = \mathfrak{X}(\mathcal{D}) \ltimes \mathcal{F}(\mathcal{D}, \mathfrak{o}) \ni (\mathbf{u}, \nu),$$

and the Lie bracket is computed to be

$$\text{ad}_{(\mathbf{u}, \nu)}(\mathbf{v}, \zeta) = (\text{ad}_{\mathbf{u}} \mathbf{v}, \text{ad}_{\nu} \zeta + \mathbf{d}\nu \cdot \mathbf{v} - \mathbf{d}\zeta \cdot \mathbf{u}),$$

where $\text{ad}_{\mathbf{u}} \mathbf{v} = -[\mathbf{u}, \mathbf{v}]$, $\text{ad}_{\nu} \zeta \in \mathcal{F}(\mathcal{D}, \mathfrak{o})$ is given by $\text{ad}_{\nu} \zeta(x) := \text{ad}_{\nu(x)} \zeta(x)$, and $\mathbf{d}\nu \cdot \mathbf{v} \in \mathcal{F}(\mathcal{D}, \mathfrak{o})$ is given by $\mathbf{d}\nu \cdot \mathbf{v}(x) := \mathbf{d}\nu(x)(\mathbf{v}(x))$.

The **dual Lie algebra** is identified with

$$\mathfrak{g}^* = \Omega^1(\mathcal{D}) \otimes \mathcal{F}(\mathcal{D}, \mathfrak{o}^*) \ni (\mathbf{m}, \kappa),$$

through the pairing

$$\langle (\mathbf{m}, \kappa), (\mathbf{u}, \nu) \rangle = \int_{\mathcal{D}} (\mathbf{m} \cdot \mathbf{u} + \kappa \cdot \nu) \mu.$$

The dual map to $\text{ad}_{(\mathbf{u}, \nu)}$ is

$$\text{ad}_{(\mathbf{u}, \nu)}^*(\mathbf{m}, \kappa) = \left(\mathcal{L}_{\mathbf{u}}\mathbf{m} + (\text{div } \mathbf{u})\mathbf{m} + \kappa \cdot \mathbf{d}\nu, \text{ad}_{\nu}^* \kappa + \text{div}(\mathbf{u}\kappa) \right).$$

Explanation of the symbols:

- $\kappa \cdot \mathbf{d}\nu \in \Omega^1(\mathcal{D})$ denotes the one-form defined by

$$(\kappa \cdot \mathbf{d}\nu)(v_x) := \kappa(x)(\mathbf{d}\nu(v_x))$$

- $\text{ad}_{\nu}^* \kappa \in \mathcal{F}(\mathcal{D}, \mathfrak{o}^*)$ denotes the \mathfrak{o}^* -valued mapping defined by

$$(\text{ad}_{\nu}^* \kappa)(x) := \text{ad}_{\nu(x)}^*(\kappa(x)).$$

- $\mathbf{u}\kappa$ is the 1-contravariant tensor field with values in \mathfrak{o}^* defined by

$$(\mathbf{u}\kappa)(\alpha_x) := \alpha_x(\mathbf{u}(x))\kappa(x) \in \mathfrak{o}^*.$$

So $\mathbf{u}\kappa$ is a generalization of the notion of a vector field. $\mathfrak{X}(\mathcal{D}, \mathfrak{o}^*)$ denotes the space of all \mathfrak{o}^* -valued 1-contravariant tensor fields.

- $\text{div}(\mathbf{u})$ denotes the divergence of the vector field \mathbf{u} with respect to the fixed volume form μ . Recall that it is defined by the condition

$$(\text{div } \mathbf{u})\mu = \mathcal{L}_{\mathbf{u}}\mu.$$

This operator can be naturally extended to the space $\mathfrak{X}(\mathcal{D}, \mathfrak{o}^*)$ as follows. For $w \in \mathfrak{X}(\mathcal{D}, \mathfrak{o}^*)$ we write $w = w_a \varepsilon^a$ where (ε^a) is a basis of \mathfrak{o}^* and $w_a \in \mathfrak{X}(\mathcal{D})$. We define $\text{div} : \mathfrak{X}(\mathcal{D}, \mathfrak{o}^*) \rightarrow \mathcal{F}(\mathcal{D}, \mathfrak{o}^*)$ by

$$\text{div } w := (\text{div } w_a) \varepsilon^a.$$

Note that if $w = \mathbf{u}\kappa$ we have

$$\text{div}(\mathbf{u}\kappa) = \mathbf{d}\kappa \cdot \mathbf{u} + (\text{div } \mathbf{u})\kappa.$$

Split the space of advected quantities in two: usual ones and new ones that involve affine actions and cocycles.

GEOMETRY OF THE ERICKSEN-LESLIE EQUATIONS

- **Symmetry group:** $G = \text{Diff}(\mathcal{D}) \otimes \mathcal{F}(\mathcal{D}, SO(3)) \ni (\eta, \chi)$, macromotion and micromotion.

- **Advected variables:** $V^* = \mathcal{F}(\mathcal{D}) \times \mathcal{F}(\mathcal{D}, \mathbb{R}^3) \ni (\rho, \mathbf{n})$, mass density and director field.

- **Representation of G on V^* :**

$$(\rho, \mathbf{n}) \mapsto \left(J(\eta)(\rho \circ \eta), \chi^{-1}(\mathbf{n} \circ \eta) \right).$$

- **Associated infinitesimal actions and diamond operations:**

$\mathbf{n}\mathbf{u} = \nabla \mathbf{n} \cdot \mathbf{u}$, $\mathbf{n}\boldsymbol{\nu} = \mathbf{n} \times \boldsymbol{\nu}$, $\mathbf{m} \diamond_1 \mathbf{n} = -\nabla \mathbf{n}^T \cdot \mathbf{m}$ and $\mathbf{m} \diamond_2 \mathbf{n} = \mathbf{n} \times \mathbf{m}$,
where $\boldsymbol{\nu}, \mathbf{m}, \mathbf{n} \in \mathcal{F}(\mathcal{D}, \mathbb{R}^3)$.

- No cocycle.

- EP equations for $(\text{Diff}(\mathcal{D}) \otimes \mathcal{F}(\mathcal{D}, \text{SO}(3))) \otimes (\mathcal{F}(\mathcal{D}) \times \mathcal{F}(\mathcal{D}, \mathbb{R}^3))$:

$$\begin{cases} \frac{\partial}{\partial t} \frac{\delta \ell}{\delta \mathbf{u}} = -\mathcal{L}_{\mathbf{u}} \frac{\delta \ell}{\delta \mathbf{u}} - \text{div} \mathbf{u} \frac{\delta \ell}{\delta \mathbf{u}} - \frac{\delta \ell}{\delta \boldsymbol{\nu}} \cdot \mathbf{d}\boldsymbol{\nu} + \rho \mathbf{d} \frac{\delta \ell}{\delta \rho} - \left(\nabla \mathbf{n}^\top \cdot \frac{\delta \ell}{\delta \mathbf{n}} \right)^\flat, \\ \frac{\partial}{\partial t} \frac{\delta \ell}{\delta \boldsymbol{\nu}} = \boldsymbol{\nu} \times \frac{\delta \ell}{\delta \boldsymbol{\nu}} - \text{div} \left(\frac{\delta \ell}{\delta \boldsymbol{\nu}} \mathbf{u} \right) + \mathbf{n} \times \frac{\delta \ell}{\delta \mathbf{n}}, \end{cases}$$

- The advection equations are:

$$\begin{cases} \frac{\partial}{\partial t} \rho + \text{div}(\rho \mathbf{u}) = 0, \\ \frac{\partial}{\partial t} \mathbf{n} + \nabla \mathbf{n} \cdot \mathbf{u} + \mathbf{n} \times \boldsymbol{\nu} = 0. \end{cases}$$

- Reduced Lagrangian for nematic and cholesteric liquid crystals:

$$\ell(\mathbf{u}, \boldsymbol{\nu}, \rho, \mathbf{n}) := \frac{1}{2} \int_{\mathcal{D}} \rho \|\mathbf{u}\|^2 \mu + \frac{1}{2} \int_{\mathcal{D}} \rho J \|\boldsymbol{\nu}\|^2 \mu - \int_{\mathcal{D}} \rho F(\rho^{-1}, \mathbf{n}, \nabla \mathbf{n}) \mu.$$

- EP equations for this ℓ : yield

$$(motion) \quad \begin{cases} \rho \left(\frac{\partial}{\partial t} \mathbf{u} + \nabla_{\mathbf{u}} \mathbf{u} \right) = \text{grad} \frac{\partial F}{\partial \rho^{-1}} - \partial_i \left(\rho \frac{\partial F}{\partial \mathbf{n}_{,i}} \cdot \nabla \mathbf{n} \right), \\ \rho J \frac{D}{Dt} \boldsymbol{\nu} = \mathbf{h} \times \mathbf{n}, \end{cases}$$

$$(advection) \quad \begin{cases} \frac{\partial}{\partial t} \rho + \text{div}(\rho \mathbf{u}) = 0, \\ \frac{D}{Dt} \mathbf{n} = \boldsymbol{\nu} \times \mathbf{n}, \end{cases}$$

- Recovering the Ericksen-Leslie equations:

Observation: if $\boldsymbol{\nu}$ and \mathbf{n} are solutions of the EP equations then:

(i) $\|\mathbf{n}_0\| = 1$ implies $\|\mathbf{n}\| = 1$ for all time.

(ii) $\frac{D}{Dt}(\mathbf{n} \cdot \boldsymbol{\nu}) = 0$. Therefore, $\mathbf{n}_0 \cdot \boldsymbol{\nu}_0 = 0$ implies $\mathbf{n} \cdot \boldsymbol{\nu} = 0$ for all time.

(iii) Suppose that $\mathbf{n}_0 \cdot \boldsymbol{\nu}_0 = 0$ and $\|\mathbf{n}_0\| = 1$. Then

$$\frac{D}{Dt}\mathbf{n} = \boldsymbol{\nu} \times \mathbf{n} \quad \text{becomes} \quad \boldsymbol{\nu} = \mathbf{n} \times \frac{D}{Dt}\mathbf{n}$$

and

$$\rho J \frac{D}{Dt}\boldsymbol{\nu} = \mathbf{h} \times \mathbf{n} \quad \text{becomes} \quad \rho J \frac{D^2}{Dt^2}\mathbf{n} - 2q\mathbf{n} + \mathbf{h} = 0.$$

Therefore:

If $(\mathbf{u}, \boldsymbol{\nu}, \rho, \mathbf{n})$ is a solution of the Euler-Poincaré equations with initial conditions \mathbf{n}_0 and $\boldsymbol{\nu}_0$ satisfying $\|\mathbf{n}_0\| = 1$ and $\mathbf{n}_0 \cdot \boldsymbol{\nu}_0 = 0$, then $(\mathbf{u}, \rho, \mathbf{n})$ is a solution of the Ericksen-Leslie equations.

Conversely:

if $(\mathbf{u}, \rho, \mathbf{n})$ is a solution of the Ericksen-Leslie equations, define

$$\boldsymbol{\nu} := \mathbf{n} \times \frac{D}{Dt}\mathbf{n} \in \mathcal{F}(\mathcal{D}, \mathbb{R}^3).$$

Then, $(\mathbf{u}, \boldsymbol{\nu}, \rho, \mathbf{n})$ is a solution of the Euler-Poincaré equations.

Use these equations plus add dissipation, get well posedness.

WELL POSEDNESS OF INCOMPRESSIBLE MODEL

Viscous Ericksen-Leslie nematodynamics of liquid crystals:

$$\begin{cases} \frac{D\mathbf{u}}{Dt} - \mu\Delta\mathbf{u} = -\nabla p - \frac{\partial}{\partial x_j} \left(\frac{\partial F}{\partial \mathbf{n}_{x_j}} \cdot \nabla \mathbf{n} \right) + \mathbf{F} + f, & \operatorname{div} \mathbf{u} = 0, \\ \frac{D^2\mathbf{n}}{Dt^2} - 2q\mathbf{n} + \mathbf{h} = g + \mathbf{G}, & \|\mathbf{n}\| = 1, \end{cases}$$

$\mu > 0$ viscosity coefficient, $J > 0$ moment of inertia constant, $\mathbf{F}(x, t)$, $\mathbf{G}(x, t)$ given external forces, f , g dissipative part of the stress tensor and dissipative part of intrinsic body force, respectively (they depend on \mathbf{u} , \mathbf{n} and their derivatives), we are interested in the non-dissipative case so we assume $f = g = 0$,

$$F(\mathbf{n}, \nabla \mathbf{n}) := \frac{1}{2} \left(K_1 (\operatorname{div} \mathbf{n})^2 + K_2 (\mathbf{n} \cdot \operatorname{curl} \mathbf{n})^2 + K_3 \|\mathbf{n} \times \operatorname{curl} \mathbf{n}\|^2 \right)$$

is the *Oseen-Zöcher-Frank free energy*, molecular field is

$$\mathbf{h} := \frac{\partial F}{\partial \mathbf{n}} - \frac{\partial}{\partial x_j} \left(\frac{\partial F}{\partial \mathbf{n}_{x_j}} \right)$$

and the pressure p and the Lagrange multiplier q are determined, respectively, by the conditions $\operatorname{div} \mathbf{u} = 0$ and $\|\mathbf{n}\| = 1$.

Assume $K_1 > 0$, $K_2 = K_3 > 0$; includes the important case of the one constant approximation. Define linear differential operator \mathcal{L}

$$\mathcal{L}\mathbf{v} := (K_2 - K_1)\nabla(\operatorname{div} \mathbf{v}) - K_2\Delta\mathbf{v}.$$

Define

$$\boldsymbol{\nu} := \mathbf{n} \times \frac{D}{Dt}\mathbf{n} \in \mathcal{F}(\mathcal{D}, \mathbb{R}^3).$$

With these hypotheses and notations, the EL system becomes the first order system

$$\frac{D\mathbf{u}}{Dt} - \mu\Delta\mathbf{u} = -\nabla p + (\mathcal{L}\mathbf{n} \cdot \nabla\mathbf{n}) + \mathbf{F}, \quad \operatorname{div} \mathbf{u} = 0,$$

$$J\frac{D\boldsymbol{\nu}}{Dt} = \mathcal{L}\mathbf{n} \times \mathbf{n} + \mathbf{G}, \quad \frac{D\mathbf{n}}{Dt} = \boldsymbol{\nu} \times \mathbf{n},$$

unknowns \mathbf{u} , $\boldsymbol{\nu}$, \mathbf{n} ; initial conditions satisfy $\|\mathbf{n}_0\| \equiv 1$, $\boldsymbol{\nu}_0 \cdot \mathbf{n}_0 = 0$.

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Conversely, if the initial conditions of the system above satisfy

$$\|\mathbf{n}(x, 0)\| = 1, \quad \mathbf{n}(x, 0) \perp \boldsymbol{\nu}(x, 0),$$

at time $t = 0$, then for any $t > 0$ we have

$$\|\mathbf{n}\| \equiv 1, \quad \boldsymbol{\nu} = \mathbf{n} \times \frac{D\mathbf{n}}{Dt}, \quad 2q = \mathbf{n} \cdot \mathbf{h} - J\|\boldsymbol{\nu}\|^2,$$

and this system turns into the EL system with unknowns \mathbf{u} , \mathbf{n} .

Thus, under these hypotheses on the initial conditions, the first order system above is equivalent to the original Ericksen-Leslie system. From now on we shall study this system instead of the original EL system.

Periodic case. $Q_T := (0, T) \times \mathbb{T}$, $\mathbb{T} = \mathbb{R}^3/\mathbb{Z}^3$ the 3-dimensional flat torus. Initial conditions

$$\mathbf{u}(0, x) = \mathbf{u}_0, \quad \boldsymbol{\nu}(0, x) = \boldsymbol{\nu}_0, \quad \mathbf{n}(0, x) = \mathbf{n}_0.$$

Here \mathbf{u} , $\boldsymbol{\nu}$, \mathbf{n} are unknown vector fields, p is an unknown scalar function, and $J > 0$, $K_1 > 0$, $K_2 = K_3 > 0$, $\mu > 0$ are given constants.

Notations:

- $L_2(\mathbb{T}) := \{ \mathbf{v} : \mathbb{T} \rightarrow \mathbb{R}^3 \mid \|\mathbf{v}\|_2^2 := \int_{\mathbb{T}} \|\mathbf{v}\|^2 dx < \infty \}$;
- $(\mathbf{u}, \mathbf{v}) := \int_{\mathbb{T}} \mathbf{u} \cdot \mathbf{v} dx$ is the inner product in $L_2(\mathbb{T})$;
- $W_2^m(\mathbb{T})$ is the Sobolev space of functions on \mathbb{T} having m distributional derivatives in $L_2(\mathbb{T})$;
- $Sol(\mathbb{T}) := \{ \mathbf{v} : \mathbb{T} \rightarrow \mathbb{R}^3 \mid \mathbf{v} \in C^\infty(\mathbb{T}), \operatorname{div} \mathbf{v} = 0 \}$;
- $Sol(Q_T) := \{ \mathbf{v} \in C^\infty(Q_T) \mid \mathbf{v}(t, \cdot) \in Sol(\mathbb{T}), \forall t \in (0, T) \}$;
- $Sol_2(\mathbb{T})$ is the closure of $Sol(\mathbb{T})$ in the norm $L_2(\mathbb{T})$;
- $Sol_2^m(\mathbb{T})$ is the closure of $Sol(\mathbb{T})$ in the norm $W_2^m(\mathbb{T})$.

- A quadruple $(\mathbf{u}, \boldsymbol{\nu}, \mathbf{n}, \nabla p)$ is a *strong solution* in the domain Q_T if
- (i) \mathbf{u} is a time-dependent vector field in $L_2((0, T); Sol_2^2(\mathbb{T}))$, $\mathbf{u}_t \in L_2(Q_T)$;
 - (ii) $\boldsymbol{\nu}$ is a vector field in $L_\infty((0, T); W_2^1(\mathbb{T}))$, $\boldsymbol{\nu}_t \in L_\infty((0, T); L_2(\mathbb{T}))$;
 - (iii) \mathbf{n} is a vector field in $L_\infty((0, T); W_2^3(\mathbb{T}))$, $\mathbf{n}_t \in L_\infty((0, T); W_2^2(\mathbb{T}))$;
 - (iv) $\nabla p \in L_2(Q_T)$;
 - (v) $(\mathbf{u}, \mathbf{n}, \boldsymbol{\nu}) \rightharpoonup (\mathbf{u}_0, \mathbf{n}_0, \boldsymbol{\nu}_0)$ weakly in $L_2(\mathbb{T})$ as $t \rightarrow 0$;
 - (vi) the equations hold almost everywhere.

(Chechkin, Ratiu, Romanov, Samokhin) Suppose

$$\mathbf{u}_0 \in Sol_2^2(\mathbb{T}),$$

$$\boldsymbol{\nu}_0 \in W_2^2(\mathbb{T}),$$

$$\mathbf{n}_0 \in W_2^3(\mathbb{T}),$$

$$\mathbf{F} \in L_2((0, T); W_2^1(\mathbb{T})),$$

$$\mathbf{G} \in L_1((0, T); W_2^2(\mathbb{T})).$$

Then there exists some $0 < T_0 < T$ such that the solution exists and is unique in Q_{T_0} .

Similar result in bounded domains with boundary conditions

$$\mathbf{u}|_{\partial\Omega} = 0, \mathbf{n} - \mathbf{n}_1|_{\partial\Omega} = 0, \boldsymbol{\nu}|_{\partial\Omega} = 0 \text{ for all } t > 0,$$

where \mathbf{n}_1 is a given constant vector field on Ω .

GEOMETRY OF THE ERINGEN EQUATIONS

- **Symmetry group**: same group as before $G = \text{Diff}(\mathcal{D}) \otimes \mathcal{F}(\mathcal{D}, \mathcal{O})$.
- **Advection variables**: $V^* = \mathcal{F}(\mathcal{D}) \times \mathcal{F}(\mathcal{D}, \text{Sym}(3)) \times \Omega^1(\mathcal{D}, \mathfrak{so}(3)) \ni (\rho, j, \gamma)$, mass density, microinertia tensor, strain.
- **Representation**: $(\eta, \chi) \in \text{Diff}(\mathcal{D}) \otimes \mathcal{F}(\mathcal{D}, \text{SO}(3))$ acts *linearly* on the advected quantities $(\rho, j) \in \mathcal{F}(\mathcal{D}) \times \mathcal{F}(\mathcal{D}, \text{Sym}(3))$, by

$$(\rho, j) \mapsto (J(\eta)(\rho \circ \eta), \chi^T(j \circ \eta)\chi), \quad \chi^T = \chi^{-1}.$$
- **Affine representation**: $(\eta, \chi) \in \text{Diff}(\mathcal{D}) \otimes \mathcal{F}(\mathcal{D}, \text{SO}(3))$ acts on $\gamma \in \Omega^1(\mathcal{D}, \mathfrak{so}(3))$ by an *affine* representation

$$\gamma \mapsto \chi^{-1}(\eta^*\gamma)\chi + \chi^{-1}\nabla\chi.$$

Note that γ transforms as a connection.

So, Eringen's wryness tensor is a connection one-form.

- The **reduced Lagrangian** of Eringen's theory:

$$\ell : [\mathfrak{X}(\mathcal{D}) \otimes \mathcal{F}(\mathcal{D}, \mathbb{R}^3)] \otimes [\mathcal{F}(\mathcal{D}) \oplus \mathcal{F}(\mathcal{D}, \text{Sym}(3)) \oplus \Omega^1(\mathcal{D}, \mathfrak{so}(3))] \rightarrow \mathbb{R}$$

$$\ell(\mathbf{u}, \boldsymbol{\nu}, \rho, j, \gamma) = \frac{1}{2} \int_{\mathcal{D}} \rho \|\mathbf{u}\|^2 \mu + \frac{1}{2} \int_{\mathcal{D}} \rho (j \boldsymbol{\nu} \cdot \boldsymbol{\nu}) \mu - \int_{\mathcal{D}} \rho \Psi(\rho^{-1}, j, \gamma) \mu.$$

- The **affine Euler-Poincaré equations** for ℓ are:

$$\left\{ \begin{array}{l} \rho \left(\frac{\partial}{\partial t} \mathbf{u} + \nabla_{\mathbf{u}} \mathbf{u} \right) = \text{grad} \frac{\partial \Psi}{\partial \rho^{-1}} - \partial_k \left(\rho \frac{\partial \Psi}{\partial \gamma_k^a} \gamma^a \right), \\ j \frac{D}{Dt} \boldsymbol{\nu} - (j \boldsymbol{\nu}) \times \boldsymbol{\nu} = -\frac{1}{\rho} \text{div} \left(\rho \frac{\partial \Psi}{\partial \gamma} \right) + \gamma^a \times \frac{\partial \Psi}{\partial \gamma^a}, \\ \frac{\partial}{\partial t} \rho + \text{div}(\rho \mathbf{u}) = 0, \quad \frac{D}{Dt} j + [j, \boldsymbol{\nu}] = 0, \\ \frac{\partial}{\partial t} \gamma + \mathcal{L}_{\mathbf{u}} \gamma + \mathbf{d}^{\gamma} \boldsymbol{\nu} = 0, \quad \hat{\boldsymbol{\nu}} = \boldsymbol{\nu} \in \mathcal{F}(\mathcal{D}, \mathfrak{so}(3)), \end{array} \right.$$

where \mathbf{d}^{γ} is the covariant γ -derivative defined by

$$\mathbf{d}^{\gamma} \boldsymbol{\nu}(\mathbf{v}) := \mathbf{d}\boldsymbol{\nu}(\mathbf{v}) + [\gamma(\mathbf{v}), \boldsymbol{\nu}].$$

This system is identical Eringen's equations.

The general affine Euler-Poincaré theory applied to many other complex fluids: spin chain, Yang-Mills MHD (classical and superfluid), Hall MHD, multivelocitv superfluids (classical and superfluid), HBVK dynamics for superfluid ^4He , Volovik-Dotsenko spin glasses, microfluids, Lhuillier-Rey equations (see Gay-Balmaz & Ratiu [2009]).

Kelvin-Noether circulation theorem for micropolar liquid crystals

$$\frac{d}{dt} \oint_{C_t} \mathbf{u}^b = \oint_{C_t} \frac{\partial \Psi}{\partial j} dj + \frac{\partial \Psi}{\partial \gamma} \mathbf{i}_- d\gamma - \frac{1}{\rho} \operatorname{div} \left(\rho \frac{\partial \Psi}{\partial \gamma} \right) \gamma.$$

The γ -circulation formulated in \mathbb{R}^3

$$\frac{d}{dt} \oint_{C_t} \gamma = \oint_{C_t} \nu \times \gamma$$

ERINGEN IMPLIES ERICKSEN-LESLIE

Physically, the Eringen equations should imply the Ericksen-Leslie equations. *Eringen [1993]* proposes

$$j := J(I_3 - \mathbf{n} \otimes \mathbf{n}), \quad \gamma := \nabla \mathbf{n} \times \mathbf{n}$$

to pass from his equations to the Ericksen-Leslie equations. This is FALSE! Two arguments: brute force computation and symmetry considerations. So, one needs to do something else.

However, not all is wrong:

1. it is true that there is $\Psi(j, \gamma)$ such that

$$\Psi (J(I_3 - \mathbf{n} \otimes \mathbf{n}), \nabla \mathbf{n} \times \mathbf{n}) = F(\mathbf{n}, \nabla \mathbf{n}).$$

2. the definition $j := J(I_3 - \mathbf{n} \otimes \mathbf{n})$ is geometrically consistent.

WE SHALL USE THE TOOLS OF GEOMETRIC MECHANICS
TO GIVE A DEFINITIVE ANSWER.

Note: For simplicity, we consider motionless nematics. The present approach easily generalizes to the flowing case.

STEP I: γ -formulation of Ericksen-Leslie

The material Lagrangian for nematic motionless liquid crystals $\mathcal{L} : T\mathcal{F}(\mathcal{D}, \text{SO}(3)) \rightarrow \mathbb{R}$, $\mathcal{D} \subset \mathbb{R}^3$, is thus given by

$$\mathcal{L}(\chi, \dot{\chi}) = \frac{1}{2}J \int_{\mathcal{D}} \|\dot{\chi}\mathbf{n}_0\|^2 \mu - \int_{\mathcal{D}} F(\chi\mathbf{n}_0, \nabla(\chi\mathbf{n}_0)) \mu,$$

where, usually $\mathbf{n}_0 = \hat{\mathbf{z}}$, J is the microinertia constant, and F is the Oseen-Frank free energy:

$$F(\mathbf{n}, \nabla\mathbf{n}) = K_2 \underbrace{(\mathbf{n} \cdot \text{curl } \mathbf{n})}_{\text{chirality}} + \frac{1}{2}K_{11} \underbrace{(\text{div } \mathbf{n})^2}_{\text{splay}} + \frac{1}{2}K_{22} \underbrace{(\mathbf{n} \cdot \text{curl } \mathbf{n})^2}_{\text{twist}} + \frac{1}{2}K_{33} \underbrace{\|\mathbf{n} \times \text{curl } \mathbf{n}\|^2}_{\text{bend}}.$$

IDEA: Apply two different EP reductions to this Lagrangian.

FIRST EULER-POINCARÉ REDUCTION FOR NEMATICS

Write $\mathcal{L}(\chi, \dot{\chi}) = L_{\mathbf{n}_0}(\chi, \dot{\chi})$, where the Lagrangian

$$L_{\mathbf{n}_0} : T\mathcal{F}(\mathcal{D}, SO(3)) \rightarrow \mathbb{R}$$

is invariant under the right action

$$(\chi, \mathbf{n}_0) \mapsto (\chi\psi, \psi^{-1}\mathbf{n}_0)$$

of $\psi \in \mathcal{F}(\mathcal{D}, SO(3))_{\mathbf{n}_0}$ (the G_{a_0} of the general theory). So get the reduced Euler-Poincaré Lagrangian

$$\ell_1(\boldsymbol{\nu}, \mathbf{n}) = \frac{1}{2}J \int_{\mathcal{D}} \|\boldsymbol{\nu} \times \mathbf{n}\|^2 \mu - \int_{\mathcal{D}} F(\mathbf{n}, \nabla \mathbf{n}) \mu,$$

$\hat{\boldsymbol{\nu}} = \dot{\chi}\chi^{-1}$, $\mathbf{n} = \chi\mathbf{n}_0$. The Euler-Poincaré equations are

$$\begin{cases} \frac{d}{dt} \frac{\delta \ell_1}{\delta \boldsymbol{\nu}} = \boldsymbol{\nu} \times \frac{\delta \ell_1}{\delta \boldsymbol{\nu}} + \mathbf{n} \times \frac{\delta \ell_1}{\delta \mathbf{n}} \\ \partial_t \mathbf{n} + \mathbf{n} \times \boldsymbol{\nu} = 0 \end{cases}$$

More explicitly, upon denoting $\mathbf{h} = -\delta\ell_1/\delta\mathbf{n}$, one has

$$\begin{cases} J\partial_t\boldsymbol{\nu} = \mathbf{h} \times \mathbf{n} \\ \partial_t\mathbf{n} + \mathbf{n} \times \boldsymbol{\nu} = 0, \end{cases}$$

which are the Ericksen-Leslie equations of nematodynamics if $\|\mathbf{n}_0\| = 1$ and $\boldsymbol{\nu}_0 \cdot \mathbf{n}_0 = 0$:

$$J\frac{d^2\mathbf{n}}{dt^2} - 2 \underbrace{\left(\mathbf{n} \cdot \mathbf{h} + J \mathbf{n} \cdot \frac{d^2\mathbf{n}}{dt^2} \right)}_{=q} \mathbf{n} + \mathbf{h} = 0.$$

Since there is no macromotion, $\frac{d}{dt} = \frac{D}{Dt}$.

SECOND EULER-POINCARÉ REDUCTION FOR NEMATICS

Start with the **same** Lagrangian. If \mathbf{n}_0 is constant, we can write

$$\begin{aligned}\mathcal{L}(\chi, \dot{\chi}) &= \frac{1}{2}J \int_{\mathcal{D}} \|\dot{\chi}\mathbf{n}_0\|^2 \mu - \int_{\mathcal{D}} F(\chi\mathbf{n}_0, \nabla(\chi\mathbf{n}_0)) \mu \\ &= \frac{1}{2}J \int_{\mathcal{D}} \|\dot{\chi}\mathbf{n}_0\|^2 \mu - \int_{\mathcal{D}} F(\chi\mathbf{n}_0, (\nabla\chi) \chi^{-1} \cdot \chi\mathbf{n}_0) \mu,\end{aligned}$$

and we view \mathcal{L} as

$$\mathcal{L}(\chi, \dot{\chi}) = L_{(\mathbf{n}_0, \gamma_0=0)}(\chi, \dot{\chi}).$$

This Lagrangian is invariant under the right action

$$(\chi, \mathbf{n}_0, \gamma_0) \mapsto (\chi\psi, \psi^{-1}\mathbf{n}_0, \psi^{-1}\gamma_0\psi + \psi^{-1}\nabla\psi)$$

of the isotropy subgroup $\mathcal{F}(\mathcal{D}, SO(3))_{(\mathbf{n}_0, 0)} = \mathcal{F}(\mathcal{D}, S^1) \cap SO(3) = S^1$
(the $G_{a_0}^c$ of the general theory).

So we get the reduced affine Euler-Poincaré Lagrangian

$$\ell_2(\boldsymbol{\nu}, \mathbf{n}, \boldsymbol{\gamma}) = \frac{1}{2} J \int_{\mathcal{D}} \|\boldsymbol{\nu} \times \mathbf{n}\|^2 \mu - \int_{\mathcal{D}} F(\mathbf{n}, -\boldsymbol{\gamma} \times \mathbf{n}) \mu.$$

$$\hat{\boldsymbol{\nu}} = \dot{\chi} \chi^{-1}, \quad \mathbf{n} = \chi \mathbf{n}_0, \quad \boldsymbol{\gamma} = -(\nabla \chi) \chi^{-1} \in \Omega^1(\mathcal{D}, \mathfrak{so}(3)).$$

\leadsto **The correct relation between $\boldsymbol{\gamma}$ and \mathbf{n} is $\nabla \mathbf{n} = \mathbf{n} \times \boldsymbol{\gamma}$ and not $\boldsymbol{\gamma} := \nabla \mathbf{n} \times \mathbf{n}$.** Note: $\boldsymbol{\gamma}$ is NOT determined by \mathbf{n} ! It does not matter.

Notations:

$\boldsymbol{\gamma} = \hat{\boldsymbol{\gamma}}$. For $\boldsymbol{\gamma} = \gamma_i dx^i \in \Omega^1(\mathcal{D}; \mathbb{R}^3)$, define $\boldsymbol{\gamma} \times \mathbf{n} \in \Omega^1(\mathcal{D}, \mathbb{R}^3)$ by $\boldsymbol{\gamma} \times \mathbf{n} = (\gamma_i \times \mathbf{n}) dx^i$, or

$$(\boldsymbol{\gamma} \times \mathbf{n})(v_x) = \boldsymbol{\gamma}(v_x) \times \mathbf{n}, \quad v_x \in T_x \mathcal{D}.$$

Important: $L(\chi, \dot{\chi}, \mathbf{n}_0, \boldsymbol{\gamma}_0)$ may not be defined when $\boldsymbol{\gamma}_0 \neq 0$. ℓ_2 is only defined on the orbit of $\boldsymbol{\gamma}_0 = 0$, i.e., if $\boldsymbol{\gamma} = -(\nabla \chi) \chi^{-1}$. However, this does not affect reduction, as long as the expression $L(\chi, \dot{\chi}, \mathbf{n}_0, 0)$ is invariant under the isotropy group of $\boldsymbol{\gamma}_0 = 0$. This occurs in the reduction for molecular strand dynamics with nonlocal interactions (*Ellis, Gay-Balmaz, Holm, Putkaradze, Ratiu [2010]*).

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The affine Euler-Poincaré equations are

$$\begin{cases} \frac{d}{dt} \frac{\delta \ell_2}{\delta \boldsymbol{\nu}} = \boldsymbol{\nu} \times \frac{\delta \ell_2}{\delta \boldsymbol{\nu}} + \operatorname{div} \frac{\delta \ell_2}{\delta \boldsymbol{\gamma}} + \operatorname{Tr} \left(\boldsymbol{\gamma} \times \frac{\delta \ell_2}{\delta \boldsymbol{\gamma}} \right) + \mathbf{n} \times \frac{\delta \ell_2}{\delta \mathbf{n}} \\ \partial_t \mathbf{n} + \mathbf{n} \times \boldsymbol{\nu} = 0 \\ \partial_t \boldsymbol{\gamma} + \boldsymbol{\gamma} \times \boldsymbol{\nu} + \nabla \boldsymbol{\nu} = 0, \quad \gamma_0 = 0. \end{cases}$$

If $\gamma_0 \neq 0$, these reduced equations still make sense, and they are an extension of EL dynamics to account for disclination dynamics. Note that these equations consistently preserve the relation $\nabla \mathbf{n} = \mathbf{n} \times \boldsymbol{\gamma}$, since

$$\left(\frac{\partial}{\partial t} - \boldsymbol{\nu} \times \right) (\nabla \mathbf{n} - \mathbf{n} \times \boldsymbol{\gamma}) = 0.$$

EP equations for ℓ_1 and AEP equations ℓ_2 are equivalent since they are induced by the SAME Euler-Lagrange equations for $\mathcal{L}(\boldsymbol{\chi}, \dot{\boldsymbol{\chi}})$ on $T\mathcal{F}(\mathcal{D}, \operatorname{SO}(3))$.

Moreover, the AEP equations allow for a generalization of Ericksen-Leslie to the case with disclinations.

STEP II: Eringen micropolar theory contains Ericksen-Leslie director theory as a particular case

Recall:

1. Eringen's Lagrangian (motionless case = no macro motion)

$$\mathcal{L}(\chi, \dot{\chi}) = \frac{1}{2} \int_{\mathcal{D}} \text{Tr} \left((i_0 \chi^{-1} \dot{\chi})^T \chi^{-1} \dot{\chi} \right) \mu - \int_{\mathcal{D}} \Psi(\chi j_0 \chi^{-1}, \chi \nabla \chi^{-1} + \chi \gamma_0 \chi^{-1}) \mu,$$

was interpreted as $\mathcal{L} = L_{(j_0, \gamma_0)}$, where $i_0 := \frac{1}{2} \text{Tr}(j_0) I_3 - j_0$. This Lagrangian is invariant under the right affine action

$$(\chi, j_0, \gamma_0) \mapsto (\chi \psi, \psi^{-1} j_0 \psi, \psi^{-1} \gamma_0 \psi + \psi^{-1} \nabla \psi)$$

of the isotropy subgroup $\mathcal{F}(\mathcal{D}, SO(3))_{(j_0, \gamma_0)}$.

2. Reduced Lagrangian

$$\ell_2(\nu, j, \gamma) = \frac{1}{2} \int_{\mathcal{D}} (j \nu) \cdot \nu \mu - \int_{\mathcal{D}} \Psi(j, \gamma) \mu.$$

3. Eringen's equation are the affine Euler-Poincaré equations for:

$$G = \mathcal{F}(\mathcal{D}, SO(3))$$

$$V^* = \mathcal{F}(\mathcal{D}, \text{Sym}(3)) \times \Omega^1(\mathcal{D}, \mathfrak{so}(3)).$$

II.1 Rod-like assumption

Take as initial condition $j_0 = J(\mathbf{I} - \mathbf{n}_0 \otimes \mathbf{n}_0)$.

This definition is $\mathcal{F}(\mathcal{D}, SO(3))$ -equivariant, so that $j = J(\mathbf{I} - \mathbf{n} \otimes \mathbf{n})$ for all time.

Consider $\mathcal{L}(\chi, \dot{\chi}) = L_{(\mathbf{n}_0, \gamma_0)}(\chi, \dot{\chi}) := L_{(j_0 = J(\mathbf{I} - \mathbf{n}_0 \otimes \mathbf{n}_0), \gamma_0)}(\chi, \dot{\chi})$. This Lagrangian is invariant under the right action

$$(\chi, \mathbf{n}_0, \gamma_0) \mapsto (\chi\psi, \psi^{-1}\mathbf{n}_0, \psi^{-1}\gamma_0\psi + \psi^{-1}\nabla\psi)$$

of the isotropy subgroup $\mathcal{F}(\mathcal{D}, SO(3))_{(\mathbf{n}_0, \gamma_0)}$.

Reduced Lagrangian

$$\begin{aligned} \ell'_2(\boldsymbol{\nu}, \mathbf{n}, \gamma) &:= \ell_2(\boldsymbol{\nu}, J(\mathbf{I} - \mathbf{n} \otimes \mathbf{n}), \gamma) \\ &= \frac{J}{2} \int_{\mathcal{D}} \|\boldsymbol{\nu} \times \mathbf{n}\|^2 \mu - \int_{\mathcal{D}} \Psi(J(\mathbf{I} - \mathbf{n} \otimes \mathbf{n}), \gamma) \mu, \end{aligned}$$

Affine Euler-Poincaré equations for ℓ'_2 are equivalent to Eringen's equations in which the rod-like assumption has been assumed.

It remains to show that these equations contain as particular case, the Ericksen-Leslie equations.

II.2 No disclination assumption $\gamma_0 = 0$

Same step as earlier: suppose that \mathbf{n}_0 is constant and take $\gamma_0 = 0$. So the evolution of γ is given by

$$\gamma = \theta_{\chi^{-1}}(0) = -(\nabla\chi)\chi^{-1}.$$

Since $\mathbf{n} = \chi\mathbf{n}_0$, we get $\nabla\mathbf{n} = \mathbf{n} \times \gamma$.

II.3 Recovering the Oseen-Frank free energy

Recall that $\Psi = \Psi(j, \gamma)$, rod-like assumption $j = J(\mathbf{I} - \mathbf{n} \otimes \mathbf{n})$, and

$$\begin{aligned} F(\mathbf{n}, \nabla\mathbf{n}) = & K_2 \underbrace{(\mathbf{n} \cdot \text{curl } \mathbf{n})}_{\text{chirality}} + \frac{1}{2}K_{11} \underbrace{(\text{div } \mathbf{n})^2}_{\text{splay}} + \frac{1}{2}K_{22} \underbrace{(\mathbf{n} \cdot \text{curl } \mathbf{n})^2}_{\text{twist}} \\ & + \frac{1}{2}K_{33} \underbrace{\|\mathbf{n} \times \text{curl } \mathbf{n}\|^2}_{\text{bend}}; \end{aligned}$$

$K_2 \neq 0$ for cholesterics, $K_2 = 0$ for nematics.

So we need to show that there exists $\Psi = \Psi(j, \gamma)$ such that

$$\Psi(j, \gamma) = \Psi(J(\mathbf{I} - \mathbf{n} \otimes \mathbf{n}), \gamma) = F(\mathbf{n}, \mathbf{n} \times \gamma) = F(\mathbf{n}, \nabla\mathbf{n}).$$

Lemma The Oseen-Frank free energy can be expressed in terms of $\Psi = \Psi(j, \gamma)$ as

$$\begin{aligned} \Psi(j, \gamma) = & \frac{K_2}{J} \text{Tr}(j\gamma) + \frac{K_{11}}{J} \left(\text{Tr}((\gamma^A)^2) (\text{Tr}(j) - J) - 2 \text{Tr}(j(\gamma^A)^2) \right) \\ & + \frac{1}{2} \frac{K_{22}}{J^2} \text{Tr}^2(j\gamma) - \frac{K_{33}}{J} \text{Tr} \left(((\gamma j)^A - J\gamma^A)^2 \right). \end{aligned}$$

So we can rewrite the reduced Eringen Lagrangian in the rod-like assumption

$$\begin{aligned} \ell'_2(\boldsymbol{\nu}, \mathbf{n}, \gamma) &= \ell_2(\boldsymbol{\nu}, J(\mathbf{I} - \mathbf{n} \otimes \mathbf{n}), \gamma) \\ &= \frac{J}{2} \int_{\mathcal{D}} \|\boldsymbol{\nu} \times \mathbf{n}\|^2 \mu - \int_{\mathcal{D}} \Psi(J(\mathbf{I} - \mathbf{n} \otimes \mathbf{n}), \gamma) \mu \end{aligned}$$

as

$$\ell'_2(\boldsymbol{\nu}, \mathbf{n}, \gamma) = \frac{J}{2} \int_{\mathcal{D}} \|\boldsymbol{\nu} \times \mathbf{n}\|^2 \mu - \int_{\mathcal{D}} F(\mathbf{n}, \mathbf{n} \times \gamma) \mu,$$

Same substitution in the unreduced Eringen Lagrangian in the rod-like assumption yields $\mathcal{L}(\chi, \dot{\chi}) = L_{(\mathbf{n}_0, \gamma_0=0)}(\chi, \dot{\chi})$.

II.4 Recovering Ericksen-Leslie theory

1. Interpret now this $\mathcal{L}(\chi, \dot{\chi})$ as $L_{\mathbf{n}_0}(\chi, \dot{\chi})$ instead of $L_{(\mathbf{n}_0, \gamma=0)}(\chi, \dot{\chi})$.
2. Check that this Lagrangian is $\mathcal{F}(\mathcal{D}, SO(3))_{\mathbf{n}_0}$ -invariant under the action $(\chi, \mathbf{n}_0) \mapsto (\chi\psi, \psi^{-1}\mathbf{n}_0)$.
3. Implement Euler-Poincaré reduction associated to the action $(\chi, \mathbf{n}_0) \mapsto (\chi\psi, \psi^{-1}\mathbf{n}_0)$ and obtain the reduced Lagrangian

$$\ell'_1(\boldsymbol{\nu}, \mathbf{n}) = \frac{J}{2} \int_{\mathcal{D}} \|\boldsymbol{\nu} \times \mathbf{n}\|^2 \mu - \int_{\mathcal{D}} F(\mathbf{n}, \nabla \mathbf{n}) \mu$$

(Previously we considered affine Euler-Poincaré reduction associated to the action $(\chi, \mathbf{n}_0, \gamma_0) \mapsto (\chi\psi, \psi^{-1}\mathbf{n}_0, \psi^{-1}\gamma_0\psi + \psi^{-1}\nabla\psi)$, with reduced Lagrangian ℓ'_2).

By general reduction theory: EP equations for ℓ'_1 and AEP equations ℓ'_2 are equivalent since they are induced by the SAME Euler-Lagrange equations for $\mathcal{L}(\chi, \dot{\chi})$ on $T\mathcal{F}(\mathcal{D}, SO(3))$.

It remains to show that the EP equations for ℓ'_1 are the Ericksen-Leslie equations. True, by direct verification.

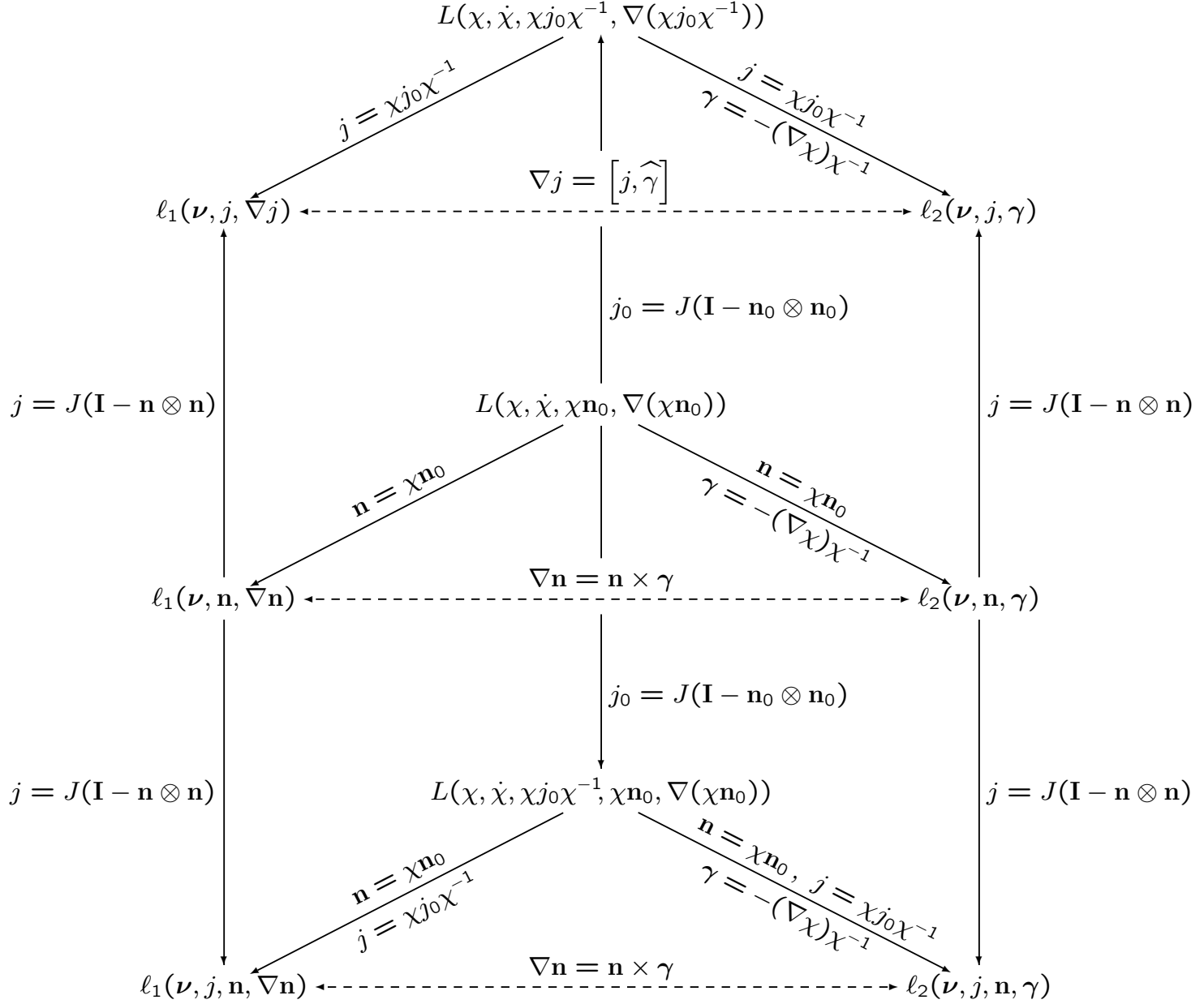
We have thus proved:

THEOREM: The Eringen micropolar theory of liquid crystals contains as a particular case the Ericksen-Leslie director theory. More precisely, the Ericksen-Leslie theory is recovered by assuming rod-like molecules: $j = J(\mathbf{I} - \mathbf{n} \otimes \mathbf{n})$ and absence of disclinations $\gamma_0 = 0$.

Summary of method:

- This is shown by considering two distinct Euler-Poincaré reductions associated with distinct advected quantities.
- This allows us to replace the non-consistent definition $\gamma := \nabla \mathbf{n} \times \mathbf{n}$ by the relation $\nabla \mathbf{n} = \mathbf{n} \times \gamma$ and to solve the inconsistencies in Eringen's approach.

$$\widehat{\nu} := \dot{\chi}\chi^{-1}$$



Final remarks: 1.) All the discussion here can be easily extended to moving liquid crystals. One applies EP, respectively affine EP, theory, as discussed earlier. Then the same considerations as above show that Eringen micropolar theory contains Ericksen-Leslie nematicodynamics.

2.) Other inconsistencies in the micropolar description: Eringen defines a **smectic liquid crystal** by $\text{Tr}(\gamma) = \gamma_1^1 + \gamma_2^2 + \gamma_3^3 = 0$. *This is not preserved by the evolution $\gamma = \eta_* \left(\chi \gamma_0 \chi^{-1} + \chi \nabla \chi^{-1} \right)$.* Consistent with the statement: the equation

$$\frac{\partial \gamma}{\partial t} + \mathcal{L}_u \gamma + d\nu + \gamma \times \nu = 0$$

does not imply that if $\text{Tr}(\gamma_0) = 0$ then $\text{Tr}(\gamma) = 0$ for all time.

Is Eringen's definition of smectic incorrect? Instead of the trace need an $\mathcal{F}(\mathcal{D}, \text{SO}(3))$ -invariant function (of γ) under the action

$$\mathbf{v} \mapsto \chi^{-1} \mathbf{v} + \chi^{-1} \nabla \chi, \quad \mathbf{v} \in \mathcal{F}(\mathcal{D}, \mathbb{R}^3), \quad \chi \in \mathcal{F}(\mathcal{D}, \text{SO}(3)).$$

We do not know how to choose a physically reasonable function of this type.

3.) Other difficulties in liquid crystals dynamics may be solved by using the tools of geometric mechanics (disclinations, defects,...)

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References

Gay-Balmaz, F. and Ratiu T.S. [2009] The geometric structure of complex fluids, *Advances in Applied Math.*, **42**, 176–275.

Gay-Balmaz, F., Ratiu, T.S., and Tronci, C. [2013] Equivalent theories of liquid crystal dynamics, *Arch. Rational Mechanics Analysis*, **210**, 773–811, doi: 10.1007/s00205-013-0673-1.

Chechkin, G.A., Ratiu, T.S., Romanov, M.S., and Samokhin, V.N. [2014] Existence and uniqueness theorems for the two-dimensional Ericksen-Leslie system, preprint.

Chechkin, G.A., Ratiu, T.S., Romanov, M.S., and Samokhin, V.N. [2014] Existence and uniqueness theorems for the full three-dimensional Ericksen-Leslie system, preprint.

Ratiu, T.S. and Rozanova, O. [2014] Nonexistence of smooth solutions for the general compressible Ericksen-Leslie equations in three dimensions, *Physica D*, **276**(1), 7–11.

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