NonEquilibrium Thermodynamics of Flowing Systems: 3

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Schedule:

1. 4/13/07, 9:30 am Introduction. One mode viscoelasticity.
2. 4/13/07, 10:15 am Coupled transport: Two-fluid model.
3. 4/14/07, 2:00 pm Modeling under constraints: Liquid crystals*
4. 4/14/07, 3:00 am Non-homogeneous systems: Surface effects.

*Following the development in "Beris and Edwards, 1994, Chapter 11"

The Dynamical Theory of Liquid Crystals

- Several levels of description:
  - Depending on the structural variable(s) used:
    - Director description, **n** (unit vector)
    - Director-scalar order parameter description, **n**, s
    - Tensor order parameter description, **m** (unit trace)
  - Depending on whether or not inertial components are kept in the structural evolution equations:
    - Inertial formulations (where both c and $\dot{c}$ are considered as variables, c representing any structural parameter)
    - Inertialess formulations
- Interconnectivity between various formulations:
  - Complexity increases as the number of structural variables increase (but also the capability of representing more states!)
  - Inertial formulations useful to deduce the form of dissipation in inertialess models

Hamiltonian/dissipation structure in the presence of constraints

- It is very important to take into account the constraints of the structural variables
- Director **n:** unit vector, $\mathbf{n}\cdot\mathbf{n} = 1$
  - Variations constrained to be perpendicular to the director: $\Delta\mathbf{n}\cdot\mathbf{n} = 0$
    - This affects the definition of the Volterra derivatives of a functional F with respect to **n**, $(\delta F/\delta \mathbf{n})_c$, since those also need to be in the same subspace as $\Delta\mathbf{n}$ **:** This is defined from the unconstrained functional $(\delta F/\delta \mathbf{n})_u$ by taking its projection to the normal to **n** space **:** $(\delta F/\delta \mathbf{n})_c = (\delta F/\delta \mathbf{n})_u - ((\delta F/\delta \mathbf{n})_u\cdot\mathbf{n})\mathbf{n}$
    - It also affects (potentially) the structure of the brackets. Formally, those can be constructed from the equivalent brackets obtained in the absence of constraints through the following substitution:

$$\frac{\delta F}{\delta \mathbf{p}} \rightarrow \frac{1}{\sqrt{(\mathbf{p}\cdot\mathbf{p})}}\left(\frac{\delta F}{\delta \mathbf{n}} - \left(\frac{\delta F}{\delta \mathbf{n}}\cdot\mathbf{n}\right)\mathbf{n}\right) = \frac{\delta F}{\delta \mathbf{n}}$$

This is obtained by exploring the relationship between d**n**/dt and d**p**/dt when **n** is formally obtained from the unconstrained (still considered unit) variable **p** as:

$$\mathbf{n} = \frac{\mathbf{p}}{\sqrt{(\mathbf{p}\cdot\mathbf{p})}};\Rightarrow \frac{d\mathbf{n}}{dt} = \frac{1}{\sqrt{(\mathbf{p}\cdot\mathbf{p})}}\left(\frac{d\mathbf{p}}{dt} - \left(\frac{d\mathbf{p}}{dt}\cdot\mathbf{n}\right)\mathbf{n}\right)$$

Hamiltonian/dissipation structure in the presence of constraints (2)

- Order parameter tensor **m:**
- Symmetric and of unit trace matrix, $m_{\alpha\beta} = m_{\beta\alpha}$; tr(**m**) = 1
  - Variations constrained to be symmetric and traceless: tr(**Δm**) = 0
    - This affects the definition of the Volterra derivatives of a functional F with respect to **m**, $(\delta F/\delta \mathbf{m})_c$, since those also need to be in the same subspace as **Δ m :** This is defined from the unconstrained functional $(\delta F/\delta \mathbf{m})_u$ by taking its projection to a symmetric and traceless space:

      $$(\delta F/\delta \mathbf{m})_c = ½\left((\delta F/\delta \mathbf{m})_u + (\delta F/\delta \mathbf{m})_u^T\right) - 1/3\left(\mathrm{tr}\left((\delta F/\delta \mathbf{m})_u \right)\right)\boldsymbol{\delta} .$$
    - It also affects (potentially) the structure of the brackets. Formally, those can be constructed from the equivalent brackets obtained in the absence of constraints through the following substitution:

$$\frac{\delta F}{\delta \mathbf{c}} \rightarrow \frac{1}{\mathrm{tr}(\mathbf{c})}\left(\frac{\delta F}{\delta \mathbf{c}} - \left(\frac{\delta F}{\delta \mathbf{c}} : \mathbf{m} \right) \boldsymbol{\delta} \right) = \frac{\delta F}{\delta \mathbf{c}} - \left(\frac{\delta F}{\delta \mathbf{c}} : \mathbf{m} \right) \boldsymbol{\delta}$$

This is obtained by exploring the relationship between d**m**/dt and d**c**/dt when **m** is formally obtained from the unconstrained variable **c** (still considered of unit trace) as:

$$\mathbf{m} = \frac{\mathbf{c}}{\mathrm{tr}(\mathbf{c})} ; \Rightarrow \frac{d\mathbf{m}}{dt} = \frac{1}{\mathrm{tr}(\mathbf{c})}\left(\frac{d\mathbf{c}}{dt} - \left(\frac{d\mathbf{c}}{dt} : \mathbf{m} \right) \boldsymbol{\delta} \right)$$

Inertial Director Theory: Variables

- For an incompressible, system we have
  - **v**, the velocity
  - s, the entropy density (alternatively, *T*, temperature)
  - **n**, the director (constrained to be a unit vector field)
  - **w**, the momentum of the director (**w** = σ d**n**/dt)

Inertial Director Theory: Hamiltonian

- The Hamiltonian (extended Helmholtz free energy of the system) is assumed to have the form:

$$A = \int_{\mathrm{V}} \left(\tfrac{1}{2} \rho v^{2} + \tfrac{1}{2\sigma} w^{2} + W + \psi \right) \mathrm{dV}$$

where *W* is the elastic (Oseen/Frank) distortion free energy density :

$$W = \tfrac{1}{2} \left(k_{11} (\operatorname{div} \mathbf{n})^{2} + k_{22} (\mathbf{n} \cdot \operatorname{curl} \mathbf{n})^{2} + k_{33} ((\mathbf{n} \cdot \nabla) \mathbf{n})^{2} \right)$$

and *ψ* the effects of an external field. For example, for magnetically susceptible material it is given as:

$$\psi = -\tfrac{1}{2} \left((\chi_{\parallel} - \chi_{\perp}) (\mathbf{n} \cdot \mathbf{H})^{2} + \chi_{\perp} \mathbf{H} \cdot \mathbf{H} \right)$$

where $\chi_{\perp}$ and $\chi_{\parallel}$ are the magnetic susceptibilities perpendicular and parallel to **n**

Inertial Director Theory : Reversible equations

- For an isothermal system, we get the standard reversible dynamics for a Hamiltonian system endowed with a vector structural parameter and its (material) time derivative:

$$\rho \frac{\mathrm{D}}{\mathrm{Dt}} v_\alpha = F_\alpha - p_{,\alpha} - \left(\frac{\partial W}{\partial n_{\beta,\gamma}} n_{\beta,\alpha} \right)_{,\gamma}$$

where

$$F_\alpha = \Phi_\beta \nabla_\alpha H_\beta$$

and

$$\Phi_\alpha = (\chi_{\|} - \chi_{\perp}) \mathbf{n} \cdot \mathbf{H} n_\alpha + \chi_{\perp} H_\alpha$$

$$\frac{\mathrm{D}}{\mathrm{Dt}} n_\alpha = \frac{1}{\sigma} \left(w_\alpha - w_\beta n_\beta n_\alpha \right)$$

$$\frac{\mathrm{D}}{\mathrm{Dt}} \mathbf{w} = -\frac{\delta H}{\delta \mathbf{n}}$$

Inertial Director Theory : Dissipation Bracket

$$[F,G] \equiv -\int Q_{\alpha\beta\gamma\varepsilon}\left(\nabla_\alpha \frac{\delta F}{\delta v_\beta}\right)\left(\nabla_\gamma \frac{\delta G}{\delta v_\varepsilon}\right) d\Omega$$

Upper convected →

$$+\int \alpha_2\left(\frac{\delta F}{\delta w_\alpha} - n_\beta \nabla_\beta \frac{\delta F}{\delta v_\alpha}\right)\left(\frac{\delta G}{\delta w_\alpha} - n_\gamma \nabla_\gamma \frac{\delta G}{\delta v_\alpha}\right) d\Omega$$

Lower convected →

$$-\int \alpha_3\left(\frac{\delta F}{\delta w_\alpha} + n_\beta \nabla_\alpha \frac{\delta F}{\delta v_\beta}\right)\left(\frac{\delta G}{\delta w_\alpha} + n_\gamma \nabla_\alpha \frac{\delta G}{\delta v_\gamma}\right) d\Omega$$

where

$$\begin{aligned} Q_{\alpha\beta\gamma\varepsilon} &= \alpha_1 n_\alpha n_\beta n_\gamma n_\varepsilon + \tfrac{1}{2}\alpha_4\left(\delta_{\alpha\gamma}\delta_{\beta\varepsilon} + \delta_{\beta\gamma}\delta_{\alpha\varepsilon}\right) \\ &+ \tfrac{1}{2}\left(\alpha_2 + \alpha_5\right)\left(\delta_{\beta\varepsilon} n_\alpha n_\gamma + \delta_{\beta\gamma} n_\alpha n_\varepsilon\right) \\ &+ \tfrac{1}{2}\left(\alpha_6 - \alpha_3\right)\left(\delta_{\alpha\varepsilon} n_\beta n_\gamma + \delta_{\alpha\gamma} n_\beta n_\varepsilon\right) \end{aligned}$$

Inertial Director Theory : Final equations

$$\rho \frac{\mathrm{D}}{\mathrm{Dt}} v_{\alpha} = F_{\alpha} - p_{,\alpha} - \left(\frac{\partial W}{\partial n_{\beta,\gamma}} n_{\beta,\alpha} \right)_{,\gamma} + t_{\alpha\gamma,\gamma}$$

where $t_{\alpha\gamma}$ is exactly the Leslie/Ericksen stress

$$\frac{\mathrm{D}}{\mathrm{Dt}} n_{\alpha} = \frac{1}{\sigma} \left(w_{\alpha} - w_{\beta} n_{\beta} n_{\alpha} \right)$$

$$\frac{\mathrm{D}}{\mathrm{Dt}} w_{\alpha} = -\frac{\delta H}{\delta n_{\alpha}} + \alpha_2 \left({}^{1}\!/_{\sigma}\, w_{\alpha} - n_{\gamma} \nabla_{\gamma} v_{\alpha} \right) - \alpha_3 \left({}^{1}\!/_{\sigma}\, w_{\alpha} + n_{\gamma} \nabla_{\alpha} v_{\gamma} \right)$$

Inertialess Director Theory: Variables

- For an incompressible, system we have
  - **v**, the velocity
  - s, the entropy density (alternatively, *T*, temperature)
  - **n**, the director (constrained to be a unit vector field)

Inertialess Director Theory: Hamiltonian

- The Hamiltonian (extended Helmholtz free energy of the system) is assumed to have the form:

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where *W* is the elastic (Oseen/Frank) distortion free energy density :

$$W = \tfrac{1}{2} \left(k_{11} (\mathrm{div}\, \mathbf{n})^2 + k_{22} (\mathbf{n} \cdot \mathrm{curl}\, \mathbf{n})^2 + k_{33} ((\mathbf{n} \cdot \nabla) \mathbf{n})^2 \right)$$

and *ψ* the effects of an external field. For example, for magnetically susceptible material it is given as:

$$\psi = -\tfrac{1}{2} \left((\chi_{\parallel} - \chi_{\perp}) \mathbf{n} \cdot \mathbf{H} + \chi_{\perp} \mathbf{H} \cdot \mathbf{H} \right)$$

where $\chi_{\perp}$ and $\chi_{\parallel}$ are the magnetic susceptibilities perpendicular and parallel to **n**

Inertialess Director Theory : Reversible equations

- For an isothermal system, we get the standard reversible dynamics for a Hamiltonian system endowed with a vector structural parameter:

$$\rho \frac{\mathrm{D}}{\mathrm{Dt}} v_\alpha = F_\alpha - p_{,\alpha} - \left(\frac{\partial W}{\partial n_{\beta,\gamma}} n_{\beta,\alpha} \right)_{,\gamma} + t_{\alpha\gamma,\gamma}$$

where

$$F_\alpha = \Phi_\beta \nabla_\alpha H_\beta$$ and $$\Phi_\alpha = (\chi_{\parallel} - \chi_\perp)\mathbf{n}\cdot\mathbf{H} n_\alpha + \chi_\perp H_\alpha$$

$$t_{\alpha\gamma} = \frac{\delta H}{\delta n_\alpha} n_\gamma$$

$$\frac{\mathrm{D}}{\mathrm{Dt}} n_\alpha - n_\beta \nabla_\beta v_\alpha + n_\alpha n_\gamma n_\beta \nabla_\beta v_\gamma = 0$$

Inertialess Director Theory : Dissipation Bracket

$$
\begin{aligned}
[F,G] \equiv & -\int Q_{\alpha\beta\gamma\varepsilon}\left(\nabla_{\alpha}\frac{\delta F}{\delta v_{\beta}}\right)\left(\nabla_{\gamma}\frac{\delta G}{\delta v_{\varepsilon}}\right)d\Omega \\
& -\int P_{\alpha\beta\gamma\varepsilon}\left(\frac{\delta F}{\delta n_{\alpha}}n_{\beta}\right)\left(\frac{\delta G}{\delta n_{\gamma}}n_{\varepsilon}\right)d\Omega \\
& -\int L_{\alpha\beta\gamma\varepsilon}\left(\nabla_{\alpha}\frac{\delta F}{\delta v_{\beta}}n_{\gamma}\frac{\delta G}{\delta n_{\varepsilon}}-\nabla_{\alpha}\frac{\delta G}{\delta v_{\beta}}n_{\gamma}\frac{\delta F}{\delta n_{\varepsilon}}\right)d\Omega
\end{aligned}
$$

where

$$
\begin{aligned}
Q_{\alpha\beta\gamma\varepsilon} = & \beta_1 n_{\alpha}n_{\beta}n_{\gamma}n_{\varepsilon} + \tfrac{1}{2}\beta_2\left(\delta_{\alpha\gamma}\delta_{\beta\varepsilon}+\delta_{\beta\gamma}\delta_{\alpha\varepsilon}\right) \\
& + \tfrac{1}{2}\beta_3\left(\delta_{\beta\varepsilon}n_{\alpha}n_{\gamma}+\delta_{\beta\gamma}n_{\alpha}n_{\varepsilon}+\delta_{\alpha\varepsilon}n_{\beta}n_{\gamma}+\delta_{\alpha\gamma}n_{\beta}n_{\varepsilon}\right)
\end{aligned}
$$

$$
P_{\alpha\beta\gamma\varepsilon} = \beta_4\left(\delta_{\alpha\gamma}\delta_{\beta\varepsilon}+\delta_{\beta\gamma}\delta_{\alpha\varepsilon}\right)
$$

$$
L_{\alpha\beta\gamma\varepsilon} = \beta_5\left(\delta_{\alpha\gamma}\delta_{\beta\varepsilon}+\delta_{\beta\gamma}\delta_{\alpha\varepsilon}\right)
$$

Inertialess Director Theory : Final equations

$$\rho \frac{\mathrm{D}}{\mathrm{Dt}} v_{\alpha} = F_{\alpha} - p_{,\alpha} - \left(\frac{\partial W}{\partial n_{\beta,\gamma}} \right)_{,\gamma} n_{\beta,\alpha} + t_{\alpha\gamma,\gamma}$$

where $t_{\alpha\gamma}$ is exactly the Leslie/Ericksen stress for suitably selected parameters

$$\frac{\mathrm{D}}{\mathrm{Dt}} n_{\alpha} - (1+\beta_5)\left(n_{\beta} \nabla_{\beta} v_{\alpha} - n_{\alpha} n_{\gamma} n_{\beta} \nabla_{\beta} v_{\gamma} \right) - \beta_5 \left(n_{\beta} \nabla_{\alpha} v_{\beta} - n_{\alpha} n_{\gamma} n_{\beta} \nabla_{\gamma} v_{\beta} \right) = -\beta_4 \frac{\delta H}{\delta n_{\alpha}}$$

Inertial Tensor Theory: Variables

- For an incompressible, system we have
  - **v**, the velocity
  - s, the entropy density (alternatively, *T*, temperature)
  - **m**, the tensor order parameter (constrained to be of unit trace), **m** = <**nn**>
  - **w**, the momentum of the tensor order parameter (**w** = σ d**m**/dt)

Inertial Tensor Theory: Hamiltonian

- The Hamiltonian (extended Helmholtz free energy of the system) is assumed to have the form:

$$A = \int_{\mathrm{V}} \left(\tfrac{1}{2}\rho v^2 + \tfrac{1}{2\sigma} w^2 + W + \psi + a_b \right) \mathrm{dV}$$

where *W,* the elastic (Oseen/Frank) distortion free energy density, is written in terms of gradients of **m**, for example:

$$W = \tfrac{1}{2}\left(b_1(\nabla \mathbf{m})^2 + b_2(\nabla \cdot \mathbf{m})^2\right)$$

ψ represents an external field. For example, for magnetically susceptible material it is given as:

$$\psi = -\tfrac{1}{2}\left((\chi_{\parallel} - \chi_{\perp})\mathbf{HH} : \mathbf{m} + \chi_{\perp}\mathbf{H} \cdot \mathbf{H}\right)$$

where $\chi_{\perp}$ and $\chi_{\parallel}$ are the magnetic susceptibilities perpendicular and parallel to **n**

Finally, a_b represents the bulk free energy that can be represented through a phenomenological Landau/de Gennes expansion of **S** = **m** – 1/3 (tr**m**)**δ**

Inertial Tensor Theory : Reversible equations

- For an isothermal system, we get the standard reversible dynamics for a Hamiltonian system endowed with a tensor structural parameter and its (material) time derivative:

$$\rho \frac{\mathrm{D}}{\mathrm{Dt}} v_{\alpha} = F_{\alpha} - p_{,\alpha} - \left(\frac{\partial W}{\partial m_{\beta\varepsilon,\gamma}} m_{\beta\varepsilon,\alpha} \right)_{,\gamma}$$

where

$$F_{\alpha} = \Phi_{\beta} \nabla_{\alpha} H_{\beta}$$

and

$$\Phi_{\alpha} = (\chi_{\|} - \chi_{\perp}) m_{\beta\alpha} H_{\beta} + \chi_{\perp} H_{\alpha}$$

$$\frac{\mathrm{D}}{\mathrm{Dt}} m_{\alpha\beta} = \frac{1}{\sigma}\left(w_{\alpha\beta} - w_{\gamma\beta} m_{\alpha\beta} \right)$$

$$\frac{\mathrm{D}}{\mathrm{Dt}} \mathbf{w} = -\frac{\delta H}{\delta \mathbf{m}} + \left(\mathbf{m} : \frac{\delta H}{\delta \mathbf{m}} \right) \boldsymbol{\delta}$$

Inertial Tensor Theory : Dissipation Bracket

$$[F,G] \equiv -\int R_{\alpha\beta\gamma\varepsilon}\left(\nabla_\alpha \frac{\delta F}{\delta v_\beta}\right)\left(\nabla_\gamma \frac{\delta G}{\delta v_\varepsilon}\right) d\Omega$$

Upper convected →

$$+\int \alpha_2^m \left(\frac{\delta F}{\delta w_{\alpha\beta}} - m_{\alpha\gamma}\nabla_\gamma \frac{\delta F}{\delta v_\beta} - m_{\beta\gamma}\nabla_\gamma \frac{\delta F}{\delta v_\alpha}\right)\left(\frac{\delta G}{\delta w_{\alpha\beta}} - m_{\alpha\gamma}\nabla_\gamma \frac{\delta G}{\delta v_\beta} - m_{\beta\gamma}\nabla_\gamma \frac{\delta G}{\delta v_\alpha}\right) d\Omega$$

Lower convected →

$$-\int \alpha_3^m \left(\frac{\delta F}{\delta w_{\alpha\beta}} + m_{\alpha\gamma}\nabla_\beta \frac{\delta F}{\delta v_\gamma} + m_{\beta\gamma}\nabla_\alpha \frac{\delta F}{\delta v_\gamma}\right)\left(\frac{\delta G}{\delta w_{\alpha\beta}} + m_{\alpha\gamma}\nabla_\beta \frac{\delta G}{\delta v_\gamma} + m_{\beta\gamma}\nabla_\alpha \frac{\delta G}{\delta v_\gamma}\right) d\Omega$$

where

$$\begin{aligned}
R_{\alpha\beta\gamma\varepsilon} = {} & \tfrac{1}{2}\alpha_1^m\left(m_{\alpha\gamma}m_{\beta\varepsilon} + m_{\alpha\varepsilon}n_{\beta\gamma}\right) + \tfrac{1}{2}\alpha_4^m\left(\delta_{\alpha\gamma}\delta_{\beta\varepsilon} + \delta_{\beta\gamma}\delta_{\alpha\varepsilon}\right) \\
& + \tfrac{1}{2}\left(\alpha_5^m\right)\left(m_{\alpha\gamma}\delta_{\beta\varepsilon} + m_{\alpha\varepsilon}\delta_{\beta\gamma} + m_{\beta\varepsilon}\delta_{\alpha\gamma} + m_{\beta\gamma}\delta_{\alpha\varepsilon}\right) \\
& + \tfrac{1}{2}\left(\alpha_6^m\right)\left(m_{\alpha\zeta}m_{\zeta\gamma}\delta_{\beta\varepsilon} + m_{\alpha\zeta}m_{\zeta\varepsilon}\delta_{\beta\gamma} + m_{\beta\zeta}m_{\zeta\varepsilon}\delta_{\alpha\gamma} + m_{\beta\zeta}m_{\zeta\gamma}\delta_{\alpha\varepsilon}\right) \\
& + \tfrac{1}{2}\left(\alpha_7^m\right)\left(m_{\alpha\zeta}m_{\zeta\gamma}m_{\beta\varepsilon} + m_{\alpha\zeta}m_{\zeta\varepsilon}m_{\beta\gamma} + m_{\beta\zeta}m_{\zeta\varepsilon}m_{\alpha\gamma} + m_{\beta\zeta}m_{\zeta\gamma}m_{\alpha\varepsilon}\right) \\
& + \tfrac{1}{2}\left(\alpha_8^m\right)\left(m_{\alpha\zeta}m_{\zeta\gamma}m_{\beta\eta}m_{\eta\varepsilon} + m_{\alpha\zeta}m_{\zeta\varepsilon}m_{\beta\eta}m_{\eta\gamma}\right)
\end{aligned}$$

Inertial Tensor Theory : Final equations

$$\rho\frac{\mathrm{D}}{\mathrm{Dt}}v_{\alpha}=F_{\alpha}-p_{,\alpha}-\left(\frac{\partial W}{\partial m_{\beta\varepsilon,\gamma}}m_{\beta\varepsilon,\alpha}\right)_{,\gamma}+T_{\beta\alpha,\beta}$$

where

$$T_{\alpha\beta}=R_{\alpha\beta\gamma\varepsilon}\left(v_{\gamma,\varepsilon}+v_{\varepsilon,\gamma}\right)+2a_{2}^{m}m_{\beta\gamma}\left(\frac{1}{\sigma}w_{\alpha\gamma}-m_{\alpha\varepsilon}v_{\gamma,\varepsilon}-m_{\varepsilon\gamma}v_{\alpha,\varepsilon}\right)+2a_{3}^{m}m_{\alpha\gamma}\left(\frac{1}{\sigma}w_{\beta\gamma}+m_{\gamma\varepsilon}v_{\varepsilon,\beta}+m_{\beta\varepsilon}v_{\varepsilon,\gamma}\right)$$

$$\frac{\mathrm{D}}{\mathrm{Dt}}m_{\alpha\beta}=\frac{1}{\sigma}\left(w_{\alpha\beta}-w_{\gamma\beta}m_{\alpha\beta}\right)$$

$$\frac{\mathrm{D}}{\mathrm{Dt}}w_{\alpha\beta}=-\frac{\delta H}{\delta m_{\alpha\beta}}+\left(\mathbf{m}:\frac{\delta H}{\delta\mathbf{m}}\right)\delta_{\alpha\beta}+a_{2}^{m}\left(\frac{1}{\sigma}w_{\alpha\beta}-m_{\alpha\gamma}v_{\beta,\gamma}-m_{\beta\gamma}v_{\alpha,\gamma}\right)$$
$$+a_{3}^{m}\left(\frac{1}{\sigma}w_{\alpha\beta}+m_{\alpha\gamma}v_{\gamma,\beta}+m_{\beta\gamma}v_{\gamma,\alpha}\right)$$

Inertialess Tensor Theory: Variables

- For an incompressible, system we have
  - **v**, the velocity
  - s, the entropy density (alternatively, *T*, temperature)
  - **m**, the tensor order parameter (constrained to be of unit trace), **m** = <**nn**>

Inertialess Tensor Theory: Hamiltonian

- The Hamiltonian (extended Helmholtz free energy of the system) is assumed to have the form:

$$A = \int_{\mathrm{V}} \left({}^{1}\!/\!_{2}\,\rho v^2 + W + \psi + a_b \right) \mathrm{dV}$$

where *W,* the elastic (Oseen/Frank) distortion free energy density, is written in terms of gradients of **m**, for example:

$$W = {}^{1}\!/\!_{2}\left(b_1(\nabla \mathbf{m})^2 + b_2(\nabla \cdot \mathbf{m})^2\right)$$

ψ represents an external field. For example, for magnetically susceptible material it is given as:

$$\psi = -{}^{1}\!/\!_{2}\left((\chi_{\|} - \chi_{\perp})\mathbf{HH} : \mathbf{m} + \chi_{\perp}\mathbf{H} \cdot \mathbf{H} \right)$$

where $\chi_{\perp}$ and $\chi_{\|}$ are the magnetic susceptibilities perpendicular and parallel to **n**

Finally, a_b represents the bulk free energy that can be represented through a phenomenological Landau/de Gennes expansion of **S** = **m** – 1/3 (tr**m**)**δ**

Inertialess Tensor Theory : Reversible equations

- For an isothermal system, we get the standard reversible dynamics for a Hamiltonian system endowed with a tensor, constrained, structural parameter:

$$\rho \frac{\mathrm{D}}{\mathrm{Dt}} v_{\alpha} = F_{\alpha} - p_{,\alpha} - \left(\frac{\partial W}{\partial m_{\beta\varepsilon,\gamma}} m_{\beta\varepsilon,\alpha} \right)_{,\gamma} + T_{\beta\alpha,\beta}$$

where

$$T_{\alpha\beta} = 2 m_{\beta\gamma} \frac{\delta H}{\delta m_{\gamma\alpha}} - 2 m_{\alpha\beta} m_{\gamma\varepsilon} \frac{\delta H}{\delta m_{\gamma\varepsilon}}$$

$$\frac{\mathrm{D}}{\mathrm{Dt}} m_{\alpha\beta} - \left(m_{\alpha\gamma} v_{\beta,\gamma} + m_{\beta\gamma} v_{\alpha,\gamma} \right) + 2 m_{\alpha\beta} m_{\gamma\varepsilon} v_{\gamma,\varepsilon} = 0$$

Inertialess Tensor Theory : Dissipation Bracket

$$[F,G] \equiv -\int R^m_{\alpha\beta\gamma\varepsilon}\left(\nabla_\alpha \frac{\delta F}{\delta v_\beta}\right)\left(\nabla_\gamma \frac{\delta G}{\delta v_\varepsilon}\right)d\Omega - \int P^m_{\alpha\beta\gamma\varepsilon}\left(\frac{\delta F}{\delta m_{\alpha\beta}}\right)\left(\frac{\delta G}{\delta m_{\gamma\varepsilon}}\right)d\Omega$$

$$-\int L^m_{\alpha\beta\gamma\varepsilon}\left(\nabla_\alpha \frac{\delta F}{\delta v_\beta}\frac{\delta G}{\delta m_{\gamma\varepsilon}} - \nabla_\alpha \frac{\delta G}{\delta v_\beta}\frac{\delta F}{\delta m_{\gamma\varepsilon}}\right)d\Omega$$

$$-\int L^m_{\eta\zeta\gamma\gamma} m_{\alpha\beta}\left(\nabla_\eta \frac{\delta F}{\delta v_\zeta}\frac{\delta G}{\delta m_{\alpha\beta}} - \nabla_\eta \frac{\delta G}{\delta v_\zeta}\frac{\delta F}{\delta m_{\alpha\beta}}\right)d\Omega$$

where

$$R^m_{\alpha\beta\gamma\varepsilon} = \tfrac{1}{2}\beta^m_1\left(m_{\alpha\gamma}m_{\beta\varepsilon} + m_{\alpha\varepsilon}n_{\beta\gamma}\right) + \tfrac{1}{2}\beta^m_4\left(\delta_{\alpha\gamma}\delta_{\beta\varepsilon} + \delta_{\beta\gamma}\delta_{\alpha\varepsilon}\right) + \tfrac{1}{2}\left(\beta^m_2\right)\left(m_{\alpha\gamma}\delta_{\beta\varepsilon} + m_{\alpha\varepsilon}\delta_{\beta\gamma} + m_{\beta\varepsilon}\delta_{\alpha\gamma} + m_{\beta\gamma}\delta_{\alpha\varepsilon}\right)$$
$$+\tfrac{1}{2}\left(\beta^m_3\right)\left(m_{\alpha\zeta}m_{\zeta\gamma}\delta_{\beta\varepsilon} + m_{\alpha\zeta}m_{\zeta\varepsilon}\delta_{\beta\gamma} + m_{\beta\zeta}m_{\zeta\varepsilon}\delta_{\alpha\gamma} + m_{\beta\zeta}m_{\zeta\gamma}\delta_{\alpha\varepsilon}\right) + \tfrac{1}{2}\left(\beta^m_6\right)\left(m_{\alpha\zeta}m_{\zeta\gamma}m_{\beta\eta}m_{\eta\varepsilon} + m_{\alpha\zeta}m_{\zeta\varepsilon}m_{\beta\eta}m_{\eta\gamma}\right)$$
$$+\tfrac{1}{2}\left(\beta^m_5\right)\left(m_{\alpha\zeta}m_{\zeta\gamma}m_{\beta\varepsilon} + m_{\alpha\zeta}m_{\zeta\varepsilon}m_{\beta\gamma} + m_{\beta\zeta}m_{\zeta\varepsilon}m_{\alpha\gamma} + m_{\beta\zeta}m_{\zeta\gamma}m_{\alpha\varepsilon}\right)$$

$$P^m_{\alpha\beta\gamma\varepsilon} = \tfrac{1}{2}\frac{1}{\beta^m_7}\left(\delta_{\alpha\gamma}\delta_{\beta\varepsilon} + \delta_{\beta\gamma}\delta_{\alpha\varepsilon} + 6m_{\alpha\beta}m_{\gamma\varepsilon}\right)$$

$$L^m_{\alpha\beta\gamma\varepsilon} = \tfrac{1}{2}\beta^m_8\left(m_{\alpha\gamma}\delta_{\beta\varepsilon} + m_{\alpha\varepsilon}\delta_{\beta\gamma} + m_{\beta\varepsilon}\delta_{\alpha\gamma} + m_{\beta\gamma}\delta_{\alpha\varepsilon}\right)$$

Inertialess Tensor Theory : Final equations

$$\rho \frac{\mathrm{D}}{\mathrm{Dt}} v_{\alpha} = F_{\alpha} - p_{,\alpha} - \left(\frac{\partial W}{\partial m_{\beta\varepsilon,\gamma}} m_{\beta\varepsilon,\alpha} \right)_{,\gamma} + T_{\beta\alpha,\beta}$$

where

$$T_{\alpha\beta} = R^{m}_{\alpha\beta\gamma\varepsilon}\left(v_{\gamma,\varepsilon} + v_{\varepsilon,\gamma}\right) + \left(2 + \beta^{m}_{8}\right) m_{\beta\gamma} \frac{\delta H}{\delta m_{\gamma\alpha}} + \left(\beta^{m}_{8}\right) m_{\alpha\gamma} \frac{\delta H}{\delta m_{\gamma\beta}} - \left(2 + \beta^{m}_{8}\right) m_{\alpha\beta} m_{\gamma\varepsilon} \frac{\delta H}{\delta m_{\gamma\varepsilon}}$$

$$\frac{\mathrm{D}}{\mathrm{Dt}} m_{\alpha\beta} - \frac{\left(2 + \beta^{m}_{8}\right)}{2}\left(m_{\alpha\gamma} v_{\beta,\gamma} + m_{\beta\gamma} v_{\alpha,\gamma}\right) - \frac{\beta^{m}_{8}}{2}\left(m_{\alpha\gamma} v_{\beta,\gamma} + m_{\beta\gamma} v_{\alpha,\gamma}\right) + 2\left(1 + \beta^{m}_{8}\right) m_{\alpha\beta} m_{\gamma\varepsilon} v_{\gamma\varepsilon} =$$

$$-\frac{1}{\beta^{m}_{7}}\left(\frac{\delta H}{\delta m_{\alpha\beta}} + 3 m_{\gamma\varepsilon} \frac{\delta H}{\delta m_{\gamma\varepsilon}} (m_{\alpha\beta} - \tfrac{1}{3} \delta_{\alpha\beta}) \right)$$

Conclusions

- The most important benefit: To be able to draw comparisons between different levels of descriptions and in this way “fill up the blanks” .
- Most important example: The demonstration of the possibility of a generalized convected derivative for **m**
  - Direct comparison between the inertialess and the inertial formalisms gives:

$$\beta_8^m = \frac{\left(2\alpha_3^m\right)}{\left(\alpha_2^m - \alpha_3^m\right)}$$

  - Even in the dissipationless limit, this parameter (being undetermined) can still be non-zero!
  - This is a crucial parameter as it regulates tumbling